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Semiclassical spectral analysis of discrete Witten Laplacians

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Abstract

A discrete analogue of the Witten Laplacian on the n-dimensional integer lattice is considered. After rescaling of the operator and the lattice size we analyze the tunnel effect between different wells, providing sharp asymptotics of the low-lying spectrum. Our proof, inspired by work of B. Helffer, M. Klein and F. Nier in continuous setting, is based on the construction of a discrete Witten complex and a semiclassical analysis of the corresponding discrete Witten Laplacian on 1-forms. The result can be reformulated in terms of metastable Markov processes on the lattice.

Contents

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Introduction

This thesis originates from problems arising in the mathematical analysis of metastable stochastic processes. The latter is an (old) topic, which - especially in very recent years - has been receiving growing attention, and a substantial literature is nowadays available on the subject (see for example the monograph [85] or the lecture notes [10] and [53] for recent overviews).

Generally speaking, a system evolving in time is said to be metastable, if there exist distinct critical time scales, each one related to a so-called metastable state: the latter appears stable as long as the system is observed on shorter time scales than the critical one, but it becomes unstable if the time scale is sufficiently large. In particular, the qualitative behaviour of the system changes abruptly depending on the time scale of observation.

Metastability phenomena show up in the dynamical behaviour of a large variety of complex real world systems. From a mathematical point of view the dynamic of such systems may be modelled by means of stochastic processes; the underlying mechanism leading to metastability effects is then explained in terms of suitable scaling limits, phase transitions and universality features, which are central concepts of modern probability theory and statistical mechanics.

The basic stochastic process exhibiting metastable behaviour is the small noise diffusion in a multiwell potential in n-dimensional Euclidean space, where each local minimum of the potential corresponds to a metastable state (see equation (0.1) below). Manifold tools have successfully be applied to its analysis and complement each other to shape a rather satisfactory mathematical understanding of this fundamental model. These include mainly large deviation techniques (see for example [33],[17]), capacity estimates in a potential theoretic framework ([13], [14], [96]), but also more analytic approaches, based for example on spectral asymptotics, WKB expansions, etc. ([24],[77],[54], [42], see also the overview [22] and the very recent preprint [78], based on the two-scale approach for logarithmic Sobolev inequalities and optimal mass transport techniques).

In this diffusive setting a particularly sharp result, concerning the so-called Eyring-Kramers formula (sometimes also called Arrhenius' Law), which quantifies the average critical time scales at which metastable transitions occur, was obtained in the paper [42] by B. Helffer, M. Klein and F. Nier.

Their method is dubbed Witten complex (or supersymmetric) approach to metastability.[1]

The main result in [42] is formulated in terms of asymptotic expansions of the exponentially small eigenvalues of the generator, which very precisely encode part of the metastable behaviour of the process (see equation (0.12) below). Indeed the authors consider tunneling through non resonant wells of a particular Schrödinger operator, also known as Witten Laplacian, this point of view being an equivalent reformulation of the stochastic metastability problem in the (reversible) diffusive case.

Their proof efficiently exploits the particular Laplacian-type structure of the mentioned Schrödinger operator (or, equivalently, of the generator of the process). In particular it turns out that, from a spectral point of view, it is more convenient to work with the "square root" of the Witten Laplacian, given by the so-called Witten differential. Its extension to the algebra of differential forms gives rise to a complex in the sense of cohomology theory, and involving the Hodge-type extension of the Witten Laplacian to 1-forms becomes an important ingredient of this approach.

These algebraic/geometric constructions, which merge the problem in the larger framework of the exterior algebra of differential forms, are then used in combination with sophisticated analytical results previously developed in a series of papers (starting with [45]) by B. Helffer and J. Sjöstrand, devoted to the semiclassical analysis of tunnel effects. In particular rather explicit WKB-type expansions and Agmon-type estimates on the decay of eigenfunctions contained in [48] are instrumental in the Helffer-Klein-Nier proof.

While the more probabilistic approaches based on large deviations theory and/or potential theory turned out to be to great extent model independent and adaptable to various (physically more relevant) situations other than the diffusive model considered so far, the analytical methods suffer generally from being rather limited in scope. In particular, the Witten complex approach mentioned above restricts so far to the setting of diffusions on manifolds [2] and it would be an important goal to push further the frontiers of its applicability to metastability problems, by extracting as much as possible its general features based on algebraic structural properties.

[1] For a similar point of view see also [99] by J. Kurchan and S. Tanase-Nicola.

[2] We mention here that after [42] the Witten complex approach was extended by allowing various boundary conditions, see [44] and [72].

Besides the classical small noise diffusion model in Euclidean space discussed so far, another fundamental, and relatively simple class of stochastic processes on which to experiment new techniques and test their scope and flexibility, is its discrete counterpart, obtained from the continuous space model by restricting the motion to discrete subsets of Euclidean space (see (0.7) below for an instance of this). It is worth mentioning that such metastable discrete diffusions naturally arise also in the context of (disordered) mean field models in Statistical mechanics as the Random field Curie-Weiss model, after reduction in terms of suitable order parameters ([11]).

In the discrete space setting, much has been studied with the forementioned probabilistic techniques (see for example [11] and [12] for results obtained with a potential theoretic approach). On the other hand, when switching from the continuous case to the discrete one, analytic spectral-theoretic and semiclassical methods are less developed. Indeed, already in the simplest case of lattices (i.e. discrete subgroups of $\mathbb{R}^n$) as state space, a rigorous analytic treatment becomes more problematic and challenging: generally the combinatorial advantages are here less relevant, and besides the reduction of space symmetries, the failure of the Leibniz rule is beyond other drawbacks maybe the most unpleasant fact of the discrete calculus. Very recently M. Klein and E. Rosenberger started a series of papers, developing a systematic analysis of the semiclassical tunneling effect for discrete Schrödinger operators on the rescaled integer lattice (see [64, 65, 66], but also [49] for previous investigations). Their work is mainly based on microlocalization techniques and partly provides some of the tools needed for a purely analytic approach to metastability in discrete setting, which could possibly lead to results comparable in strength to the one obtained with the aid of the Witten complex in [42].

This program of an analytic approach to metastability for discrete diffusions is accomplished in the present thesis, by carefully working out all the missing elements that permit to carry over to the discrete case the analysis à la Helffer-Klein-Nier.

In particular, a Schrödinger operator on the n-dimensional integer lattice is considered, which is naturally linked to the discrete diffusions under examination and which can be seen as a discrete equivalent of the Witten Laplacian on the level of functions. A substantial part of the thesis is devoted to the definition of a suitable algebraic and geometric framework, which makes it possible to extend this discrete Witten Laplacian (at first only defined on functions on the lattice) on a larger space of discrete differential forms, keeping all the relevant supersymmetric properties. The definitions we propose appear to be new. Indeed, even if in the literature one can find several attempts of formalizing a discrete differential calculus[3], none of them seems to be well-suited to the problem we consider nor of direct applicability.

After suitable rescaling of the discrete Witten Laplacians and the lattice size, crucial semiclassical properties (e.g. harmonic approximation, WKB expansions) are derived on the full algebra of discrete forms. These are analogous to the Helffer-Sjöstrand results mentioned above. On the basis of these preparations, complete asymptotic expansions for the low-lying spectrum of the discrete Witten Laplace are finally obtained, following essentially the strategy of [42].

Besides improving existing results with a new method, this thesis can also be seen as a first step in upgrading the Witten-complex strategy from an ad-hoc tool to a more systematic approach to metastability problems. On the other hand, although the contents of this work were worked out with the express purpose of applying it to metastability questions, they are in fact independent of that, and, we believe, also interesting from a purely algebraic and analytic point of view.

The rest of this introduction is structured in four subsections as follows. Even if the bulk of the thesis is not written directly in terms of metastable stochastic processes - it is indeed mainly analytic and partly algebraic/geometric in flavour (as the Witten complex approach is)-, we shall start with an informal discussion of the formentioned metastable diffusions both in continuous and discrete setting, and clarify their relationship. Indeed, most of the heuristic arguments and choices of abstract definitions are better understood with this probabilistic metaphor on the background.

In the second subsection the relation between metastability and spectral properties is explained in this context. Moreover we recall the Helffer-Klein-Nier result contained in [42] and state the analogous result for the discrete case, which is the main theorem of the thesis.

In the third subsection we informally sketch the main ideas of the Witten complex approach as developed in [42]. In doing this, we point to the main

[3]The topic of a discrete discrete differential calculus became quite popular in recent years. Just to mention a few works: [15], [79], [39], [26], [98]. Robin Forman considers in the context of his discrete Morse theory also discrete Witten Laplacians associated with cell complexes ([32]).

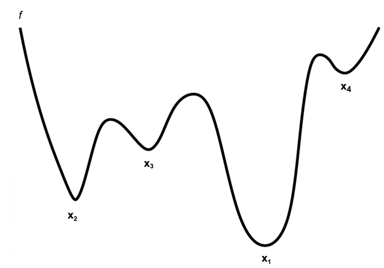

FIGURE 1. An energy function with four wells in dimension 1.

difficulties arising in the discrete case and briefly describe, how these have been resolved in the present work.

Finally, in the last subsection, a detailed description of the contents of the thesis is given.

Continuous and discrete metastable diffusions.

Let be given a multiwell energy landscape in n-dimensional Euclidean space, i.e. a function $f : \mathbb{R}^n \to \mathbb{R}$, having several local minima. For simplicity we assume f to be smooth, even if the following considerations hold under much weaker regularity assumptions.

We shall consider a deterministic motion along the (negative) gradient flow, stochastically perturbed by a small Brownian noise. The intensity of the stochastic input is given by a parameter $0 < \varepsilon \ll 1$. To be specific, we consider the stochastic equation of motion

$$dX_t \;=\; -2\nabla f(X_t)\;dt \;+\; \sqrt{2\varepsilon}\;dW_t \quad , \tag{0.1}$$

where $X_t \in \mathbb{R}^n$ denotes the ε-dependent state at time t of the system, $\nabla := (\frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_n})$ is the standard gradient and $(W_t)_{t\geq 0}$ is a standard Brownian motion in $\mathbb{R}^n$. In particular we have for the mean and variance of the stochastic perturbation we are considering,

$$E(\sqrt{2\varepsilon}W_t) \;=\; 0 \quad \text{and} \quad \mathrm{Var}\,(\sqrt{2\varepsilon}W_t) \;=\; 2\varepsilon t$$

for every $t \geq 0$.

It follows from the standard theory of stochastic differential equations (see for example [34]) that for each fixed $\varepsilon > 0$ and initial condition $x \in \mathbb{R}^n$ equation (0.1) admits a unique (possibly exploding) solution $X^{x,\varepsilon} :=$

$(X_t^{x,\varepsilon})_{t\geq 0}$, characterized by having almost surely continuous sample paths and by satisfying almost surely

$$X_t^{x,\varepsilon} \;=\; x \;+\; \int_0^t 2\nabla f(X_s^{x,\varepsilon})ds \;+\; \sqrt{2\varepsilon}W_t$$

for every $t \geq 0$ (up to explosion).

The focus here is on the family of probability measures $(\mathbb{P}_{x,\varepsilon})_{x\in\mathbb{R}^n,\varepsilon>0}$ on the path space $C(\mathbb{R}_+;\mathbb{R}^n)$ induced by the $X^{x,\varepsilon}$'s, rather than on the particular pathwise realization given by the latter.[4] As is well known, for each $\varepsilon > 0$ the family $(\mathbb{P}_{x,\varepsilon})_{x\in\mathbb{R}^n}$ is Markovian, and can be directly constructed starting from the (formal) generator

$$G_{f,\varepsilon} \;=\; -\varepsilon\Delta \;+\; 2\nabla f\cdot\nabla \tag{0.2}$$

by means e.g. of the martingale approach (see [58], [94]). Here $\Delta := \sum_{j=1}^n \frac{\partial^2}{\partial x_j^2}$ denotes the Laplacian in $\mathbb{R}^n$. The martingale method is based on the characterization of $(\mathbb{P}_{x,\varepsilon})_{x\in\mathbb{R}^n}$ as the unique strongly Markovian family on continuous path space satisfying for every $\alpha \in C_c^2(\mathbb{R}^n;\mathbb{R})$ (i.e. twice continuously differentiable and with compact support), every $x \in \mathbb{R}^n$ and $\varepsilon > 0$

$$\mathbb{P}_{x,\varepsilon}(\varphi_0 = x) \;=\; 1$$

and

$$\alpha(\varphi_t) \;-\alpha(\varphi_0) \;-\; \int_0^t G_{\varepsilon,f}\alpha\;(\varphi_s)\;ds \quad \text{is a martingale under} \quad \mathbb{P}_{x,\varepsilon} \quad .$$

This formalizes the idea of $\mathbb{P}_{x,\varepsilon}$ giving the distribution of the "integral lines" of $G_{\varepsilon,f}$. Indeed, if instead of $G_{f,\varepsilon}$ only the first order term $\mathcal{T}_f = 2\nabla f\cdot\nabla$ is taken, the solution of the martingale problem would be given by the Dirac measure on the solution of the characteristic equations

$$\begin{cases} \dot{\varphi}_t \;=\; -2\nabla f(\varphi_t) \\ \varphi_0 = x \end{cases} \qquad .$$

Another way to construct $\mathbb{P}_{x,\varepsilon}$ from $G_{f,\varepsilon}$ relies on the important relation

$$\mathbb{E}_{x,\varepsilon}\big(\alpha(\varphi_t)\big) \;=\; e^{-tG_{f,\varepsilon}}\;\alpha\;(x) \quad , \tag{0.3}$$

where $\mathbb{E}_{x,\varepsilon}$ denotes expectation with respect to $\mathbb{P}_{x,\varepsilon}$ and $\alpha : \mathbb{R}^n \to \mathbb{R}$ is bounded and measurable. Note that the right hand side of (0.3) is formal, since we did not specify the domain of $G_{f,\varepsilon}$, nor the space in which the exponential is taken. A far reaching method to deal rigorously with this kind of approach considers suitable L^2 spaces and is linked to the theory of Dirichlet forms ([35], [75]). In the present setting of a deterministic drift given by a

[4] In the explosive case the state space $\mathbb{R}^n$ is augmented by adding a fictitious point at infinity, the "cemetery" for the process.

gradient vector field it is particularly convenient to work in the weighted space $L^2(\mathbb{R}^n; e^{-2f/\varepsilon}dx)$. This is due to the fact that in this weighted space the generator $G_{f,\varepsilon}$ is symmetric and therefore powerful functional-analytic tools for selfadjoint operators become available. Indeed, a simple computation gives with $\mathrm{div} := \sum_{i=1}^n \frac{\partial}{\partial x_i}$

$$G_{f,\varepsilon}\ \alpha \ = \ \varepsilon\ e^{2f/\varepsilon}\ \ \mathrm{div}\ e^{-2f/\varepsilon}\ \nabla\ \alpha \tag{0.4}$$

and symmetry follows via integration by parts.

Now let $\langle \cdot, \cdot \rangle$ be the canonical inner product in $\mathbb{R}^n$, $|\cdot|$ the associated euclidean norm and assume to fix ideas that

$$\lim_{|x|\to\infty} \frac{\langle \nabla f(x), x\rangle}{|x|} \ = \ +\infty \quad , \tag{0.5}$$

which implies a superlinear growth of f at infinity, and in particular that $Z_\varepsilon := \int e^{-2f(x)/\varepsilon}dx$ is finite.

The symmetry of $G_{f,\varepsilon}$ reflects the fact that the corresponding Markov process with initial distribution $Z_\varepsilon^{-1}\ e^{-2f/\varepsilon}dx$ is reversible: its distribution is stationary in time and forward and backward evolutions are indistinguishable. To be precise, let $\rho_\varepsilon(x) := Z_\varepsilon^{-1}e^{-2f/\varepsilon}$ and

$$\mathbb{P}_{\rho_\varepsilon,\varepsilon} \ := \ \int \mathbb{P}_{x,\varepsilon}\ \rho_\varepsilon(x)\ dx \quad .$$

Then $\mathbb{P}_{\rho_\varepsilon,\varepsilon}$ is invariant under time shift, and can be canonically extended to a distribution on $C(\mathbb{R};\mathbb{R}^n)$ which is invariant under inversion of time. The measure $\rho_\varepsilon dx$ is also called the Gibbs measure of the model.

The main issue we are interested in concerns the long time behaviour of trajectories under $\mathbb{P}_{x,\varepsilon}$ when ε is small. Note that for fixed $\varepsilon > 0$ this problem is settled by suitable ergodicity results, implying that for "nice" measurable sets $A \subset \mathbb{R}^n$ and $x \in \mathbb{R}^n$

$$\lim_{t\to\infty} \mathbb{P}_{x,\varepsilon}(\varphi(t) \in A) \ = \ \int_A \rho_\varepsilon(x)\ dx$$

(see [61] for precise statements).

In the joint limit $t \to \infty$ and $\varepsilon \to 0$ it is not hard to see that the result depends on the order in which the limits are taken. Indeed, letting first $\varepsilon \to 0$, the deterministic gradient flow will dominate and for $t \to \infty$ push the process to the local minimum corresponding to the well of the initial position x.

On the other hand, letting first $t \to \infty$, the process beeing ergodic will distribute according to the Gibbs measure $\rho_\varepsilon dx$. The latter concentrates for $\varepsilon \to 0$ on the deepest possible state of the energy, as a simple Laplace

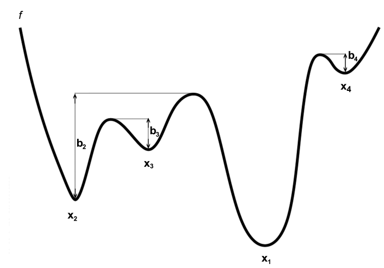

FIGURE 2. The energy barriers associated with local minima in the example of Figure 1. From the global minimum of course no transition to deeper wells is possible.

asymptotics shows. As a result, in this reversed order the global minimum of f is reached regardless of the initial condition x.

In between these two extreme situations, intermediate scalings, with say $t = t(\varepsilon)$ as a diverging function for $\varepsilon \to 0$, will lead to a whole range of possible outcomes: for short time scales (i.e. t growing slowly when ε approaches 0) the process remains trapped in the local basin of attraction; for sufficiently large time scales (i.e. t growing fast) the process wil feel the influence of the Gibbs measure, favouring deepest possible states, and perform a so-called metastable transition (or tunneling) to some deeper well.

This separation of time scales is usually referred to as metastable behaviour, and represents an instance of a dynamical phase transition. The small noise diffusion determined by (0.1) is considered a paradigmatic model for this phenomenon.

The previous heuristic picture is made precise by getting quantitative estimates on the critical times scales at which metastable transitions occur, i.e on the mean times necessary to go from a local minimum to a (small neighbourhood) of a deeper one. As already mentioned, this is a well-known and well-studied problem to which several different techniques have been applied. The rule of thumb, also called Arrhenius' Law, is that the critical transition times are exponentially large when $\varepsilon \to 0$: denoting by x_j a generic local minimum of f and by τ_j the hitting time of a small neighbourhood of the set of minima of f which lie deeper than x_j, we have roughly

$$\mathbb{E}_{x_j,\varepsilon}\, \tau_j \quad \approx \quad e^{b_j/\varepsilon} \qquad \text{when } \varepsilon \to 0 \quad , \tag{0.6}$$

with $b_j > 0$ the minimal "height of the energy barrier" which separates x_j from a deeper well (see Figure 2). The $\approx$ qualifies here in asymptotic equivalence on logarithmic scale, which does not see the prefactor in front of the exponential.

Arrhenius' Law admits sharper asymptotics (its versions taking account also of the prefactor are sometimes called Eyring-Kramers formulas), generalisations and variants, depending on various assumptions made on the geometry of the energy landscape (see [5] for an overview). A particular sharp result obtained by means of spectral methods will be discussed more rigorously in the next subsection. Before that, we shall introduce a modification of the small noise diffusion model, by passing to its discrete counterpart.

While being paradigmatic in many aspects, the process determined by (0.1) has features which appear to be not relevant at all for the metastability phenomenon to happen. One of them regards the continuity of paths [5]: if we insist on the long time behaviour of the process being given by the Gibbs measure $e^{-2f(x)/\varepsilon}dx$, one expects the same qualitative behaviour as before also in the presence of jumps, provided these are not too big[6].

We shall not consider general jump processes in $\mathbb{R}^n$ but stick for simplicity to the case in which the motion is restricted to the n-dimensional integer lattice $\mathbb{Z}^n$, rescaled with another small parameter $\delta > 0$, giving the mesh of the discretization. To keep suitable ergodicity properties, we shall work now with the Gibbs measure being absolutley continuous with respect to the counting measure dx_δ on $\delta\mathbb{Z}^n$, i.e. with

$$\rho_\varepsilon \; dx_\delta \; := \; Z_{\delta,\varepsilon}^{-1} \; e^{-2f(x)/\varepsilon} \; dx_\delta \quad ,$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is a smooth multiwell energy landscape, satisfying (0.5) exactly as before, and

$$Z_{\delta,\varepsilon} \; := \; \sum_{x \in \delta\mathbb{Z}^n} e^{-2f(x)/\varepsilon} \quad .$$

As before, we introduce the process we have in mind by describing first its sample paths: in the present discrete space setting, it is more customary (and simple) to do this by fixing the jump rates of the process ([84]), rather than the stochastic differential equation, which would be driven by a Poisson process ([58]). To fix the ideas, among the (plenty of) continuous time

[5]Another aspect which a priori is not relevant for metastability concerns the reversibility of the process. Irreversible stochastic process - or equivalently - non selfadjoint generators are not treated here. We mention that large deviation approaches hardly rely on reversibility assumptions, and are therefore particularly well-suited in this more general context. See also [30]. Spectral-theoretic approaches are less developed.

[6]The metastability picture is destroyed for example if one allows jumps from one local minimum to the other in times of order 1.

processes reversible with respect to the Gibbs measure, we take a nearest neighbour walk with jump rate from $x \in \delta\mathbb{Z}^n$ to a nearest neighbour[7] $y \in \delta\mathbb{Z}^n$ given by

$$r_{\delta,\varepsilon}(x,y) \ := \ \frac{\varepsilon}{\delta^2}\exp\{-\frac{2}{\varepsilon}[f(\frac{x+y}{2}) - f(x)]\} \ . \qquad (0.7)$$

The continuous time Markov process $X^{x,\delta,\varepsilon} := (X_t^{x,\delta,\varepsilon})_{t\geq 0}$ with state space $\delta\mathbb{Z}^n$ constructed from the jump rates (0.7) can be thought of as follows[8]: let

$$r_{\delta,\varepsilon}(x) \ := \sum_{y\in\delta\mathbb{Z}^n:|x-y|=\delta} r_{\delta,\varepsilon}(x,y)$$

and let

$$p_{\delta,\varepsilon}(x,y) \ := \begin{cases} \frac{r_{\delta,\varepsilon}(x,y)}{r_{\delta,\varepsilon}(x)} & \text{if } x-y\in\delta\mathbb{Z}^n \ \text{ and } \ |x-y| = \delta \\ 0 & \text{otherwise} \end{cases} \ .$$

The process $X^{x,\delta,\varepsilon}$ starts in $x \in \delta\mathbb{Z}^n$, waits an exponentially distributed time of parameter $r_{\delta,\varepsilon}(x)$ and jumps with probability $p_{\delta,\varepsilon}(x,y)$ to y, where it stays for a further exponentially distributed time with parameter $r_{\delta,\varepsilon}(y)$ and then jumps to a third state z with probability $p_{\delta,\varepsilon}(y,z)$ etc.

Note the validity of the detailed balance condition expressing reversibility of the process with respect to the Gibbs measure: for every $x, y \in \mathbb{R}^n$

$$e^{-2f(x)/\varepsilon} \ r_{\delta,\varepsilon}(x,y) \ = \ e^{-2f(y)/\varepsilon} \ r_{\delta,\varepsilon}(y,x) \ .$$

In this discrete model the generator is formally given by

$$G_{f,\delta,\varepsilon} \ \alpha \ (x) \ := \sum_{y\in\delta\mathbb{Z}^n:|x-y|=\delta} r_{\delta,\varepsilon}(x,y) \ [\ \alpha(x) \ - \ \alpha(x+y)\ ] \ , \qquad (0.8)$$

with $\alpha : \delta\mathbb{Z}^n \to \mathbb{R}$. This can also be rewritten as

$$G_{f,\delta,\varepsilon} \, \alpha \, (x) \ := \ \sum_{j=1}^n \ \{\ r^+_{\delta,\varepsilon,j}(x)\,[\,\alpha(x) - \alpha(x{+}\delta e_j)\,] + r^-_{\delta,\varepsilon,j}(x)\,[\,\alpha(x) - \alpha(x{-}\delta e_j)\,]\ \} \ ,$$

where $(e_1, \dots, e_n)$ denotes the canonical basis of $\mathbb{R}^n$ and

$$r^+_{\delta,\varepsilon,j}(x) \ := \ r_{\delta,\varepsilon}(x, x+\delta e_j) \quad \text{ and } \quad r^-_{\delta,\varepsilon,j}(x) \ := \ r_{\delta,\varepsilon}(x, x-\delta e_j) \ .$$

As before, the main issue we are concerned with is about the long time behaviour of the distribution of $X_t^{x,\delta,\varepsilon}$. Besides t and ε, a third (small) parameter δ is now entering the game, and manifold situations can be considered.

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[7]By definition, $y \in \delta\mathbb{Z}^n$ is nearest neighbour of $x \in \delta\mathbb{Z}^n$ if $|x-y| = \delta$.

[8]This is true at least if f behaves sufficiently well at infinity.

Heuristically, if the mesh δ of the lattice goes to zero much faster than the parameter ε, one will see essentially the continuous space small noise diffusion given by (0.1). This is an appearance of the Donsker-Varadhan invariance principle. Indeed, a simple Taylor expansion gives for $\alpha \in C_c^\infty(\mathbb{R}^n;\mathbb{R})$ and every $\varepsilon > 0$

$$G_{f,\delta,\varepsilon}\ \alpha \quad \to \quad G_{f,\varepsilon}\ \alpha \qquad \text{for} \quad \delta \to 0$$

uniformly on compact sets.

In this work we shall restrict to the particular case in which $\delta = \varepsilon$. This is the scaling which appears for example in the classical large deviation theory for sample paths of random walks (see Mogulskii's theorem in [25]). Moreover it has some interesting applications in the study of certain mean field models in statistical mechanics, as the random field Curie Weiss model. In fact, after a suitable coarse graining, obtained by introducing macroscopic variables (or order parameters), the dynamic induced on the latter will essentially be described by generators of the type (0.8). The limit $\delta = \varepsilon \to 0$ corresponds with this interpretation to the thermodynamic limit of infinite volume (see [11], [7] and the recent thesis [91]). From this point of view, the discrete model with $\delta = \varepsilon$ is the more "physical" with respect to its continuous counterpart.

Clearly not all features of the discrete process $X^{x,\delta,\varepsilon}$ are well approximated by the continuous process $X^{x,\varepsilon}$ when $\delta = \varepsilon \to 0$. Indeed, this slower scaling is critical, in that it changes the law of large numbers of the process: in the limit $\delta = \varepsilon \to 0$ the generator of the discrete diffusion converges again to a deterministic transport, but this time along a different vector field, where the hyperbolic sine of the derivatives of f appear. More precisely, we have with $\sinh \nabla f(x) := (\sinh \frac{\partial}{\partial x_1} f(x), \ldots, \sinh \frac{\partial}{\partial x_n} f(x))$ that for $\alpha \in C_c^\infty(\mathbb{R}^n;\mathbb{R})$

$$G_{f,\varepsilon,\varepsilon}\ \alpha\ (x) \quad \to \quad 2 \sinh \nabla f(x) \cdot \nabla \alpha\ (x) \qquad \text{for} \quad \varepsilon \to 0 \tag{0.9}$$

uniformly on compact sets, to be compared with

$$G_{f,\varepsilon}\ \alpha\ (x) \quad \to \quad 2 \nabla f(x) \cdot \nabla \alpha\ (x) \qquad \text{for} \quad \varepsilon \to 0\ \ . \tag{0.10}$$

The continuous approximation seems therefore not well-suited if e.g. metastable transition paths are considered. More generally it is not completely clear which properties of the diffusion are universal also in the slow lattice scaling $\delta = \varepsilon \to 0$ and some caution is needed when transferring insights from one model to the other.

The focus here is again on the mean critical time scales at which metastable transitions happen. More specifically, we are interested in sharp versions (i.e.

considering also the prefactor) of Arrhenius' Law

$$\tilde{\mathbb{E}}_{x_j,\varepsilon}\ \tau_j \quad \approx \quad e^{b_j/\varepsilon} \qquad \text{when } \varepsilon \to 0 \tag{0.11}$$

in the lattice model determined by (0.8) when $\delta = \varepsilon$. Here $\tilde{\mathbb{E}}_{x,\varepsilon}$ denotes the expectation with respect to the path measure[9] induced by the discrete process $\tilde{X}^{x,\varepsilon} := X^{x,\varepsilon,\varepsilon}$, and the x_j's, b_j's and τ_j's are as in (0.6).

In the next subsection we shall reformulate this problem in a spectral-theoretic framework and present the main result of this thesis, which provides an answer to it, by establishing explicitly the prefactor. It will follow from this result, that for the sake of computing mean critical time scales, the continuous diffusion still gives the right answer, at least in leading order in ε. We mention that sharp versions of Arrhenius'law in this discrete setting were already considered in [11] using potential theory (see also [7]).

Remark 0.1. *Large parts of the thesis do not restrict to the nearest neighbour case: more generally we consider also the case in which the support of the jumps is just symmetric, finite and generates the integer lattice. To be specific, let $E \subset \mathbb{Z}^n$ be finite and symmetric (i.e. $v \in E$ implies $-v \in E$), assume that every $x \in \mathbb{Z}^n$ can be written as linear combination with integer coefficients of elements in E, and consider instead of* (0.8) *the generator*

$$G_{f,E,\delta,\varepsilon}\ \alpha\ (x) \ := \sum_{y \in \delta E} r_{\delta,\varepsilon}(x,y)\ [\ \alpha(x)\ -\ \alpha(x+y)\ ]\quad ,$$

which reduces to (0.8) *in the case*

$$E \ = \ \{e_1, \dots, e_n, -e_1, \dots, -e_n\}\quad .$$

In the limit $\delta = \varepsilon \to 0$ the relevant geometry is now not the one given by the standard euclidean scalar product on $\mathbb{R}^n$, but by the scalar product g_E induced by E, given by

$$g_E(x,y) \ := \ \sum_{i,j=1}^{n} G_{i,j}\ x_i x_j \quad ,$$

where $G := (G_{i,j})$ is the inverse of the matrix $(\sum_{x\in E} x_i x_j)_{i,j}$. Note that g_E equals the standard scalar product when $E = \{e_1, \dots, e_n, -e_1, \dots, -e_n\}$. Accordingly, the corresponding continuous diffusion is now determined by the equation

$$dX_t \ = \ -2G^{-1}\nabla f(X_t)\ dt \ + \ \sqrt{2hG^{-1}}dW_t \quad .$$

[9] Note that the path space consists now of piecewise constant functions.

The more general case of discrete processes related to reversible diffusions with inhomogeneous diffusion matrix, that is of the type

$$dX_t \;=\; -2G^{-1}(X_t)\nabla f(X_t)\;dt \;+\; h\;\nabla\cdot G^{-1}(X_t)dt \;+\; \sqrt{2hG^{-1}}dW_t \;\;,$$

is not explicitly considered here, but is in principle treatable along the same lines.

Spectral picture of metastability and main result.

It is another rule of thumb that in presence of metastability effects some asymptotic degeneracy of eigenvalues is lurking beneath the surface. We refer in particular to [60] for early ideas advocating eigenvalue degeneracy as ultimate characteristic of first order phase transitions. See also [37] for a more recent attempt to formalize this principle in a rather general setting.

In the particular case of the two models we are considering (i.e. the continuous diffusion determined by (0.2) and the discrete diffusion determined by (0.8), with $\delta = \varepsilon$) the papers [14] and [12] provide rigorous results which accurately specify the way the metastable behaviour is encoded into the spectrum of the respective generators $G_{f,\varepsilon}$ and $\tilde{G}_{f,\varepsilon} := G_{f,\varepsilon,\varepsilon}$. [10]

Here is the punch line: consider $G_{f,\varepsilon}$ as an operator in $L^2(\mathbb{R}^n, e^{-2f/\varepsilon}dx)$, where it is selfadjoint and nonnegative, and assume that f has a finite number $x_1, \ldots, x_{m_0}$ of local minima at which for simplicity it takes distinct values. In particular there exists by (0.5) a unique global minimum which we shall label with x_1. Note also that 0 is an eigenvalue of $G_{f,\varepsilon}$, which we shall label with $\nu_{1,\varepsilon}$, corresponding to the eigenfunction identically equal to 1. The point is that the next m_0 eigenvalues $\nu_{2,\varepsilon}, \ldots, \nu_{m_0,\varepsilon}$ following $\nu_{1,\varepsilon}$ are exponentially small in ε. Then there is a big gap, the rest of the spectrum being bounded from below by a constant (see Figure 3).

Moreover each of the $m_0 - 1$ nearly vanishing eigenvalues has a precise probabilistic meaning: if the local minima $x_2, \ldots, x_{m_0}$ of f and the eigenvalues $\nu_{2,\varepsilon}, \ldots, \nu_{m_0,\varepsilon}$ of $G_{f,\varepsilon}$ are ordered in a suitable way [11], one gets for

[10]To be fair in [12] the discrete diffusion is considered only on bounded domains, but the results should be extendable to the non-compact setting by assuming suitable conditions on f at infinity.

[11]Note that the global minimum x_1 is excluded: it plays of course a special role, since no metastable transition to a deeper minimum is possible)

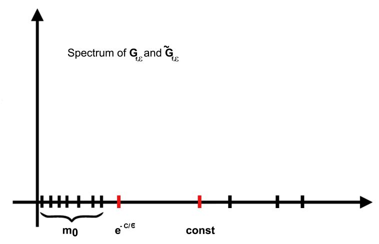

FIGURE 3. The spectrum of the generators. There are exactly m_0 exponentially small eigenvalues, where m_0 is the number of wells in the energy landscape described by f.

every $i = 2, \dots, m_0$

$$\frac{1}{\nu_{i,\varepsilon}} \;=\; \mathbb{E}_{x_i,\varepsilon}\, \tau_i \;\; (1 \;+\; o(1)) \quad , \tag{0.12}$$

where τ_i (as in (0.6)) denotes the hitting time of a small neighbourhood of the set of minima of f which lie deeper than x_i.

Exactly the same spectral feature emerges when analyzing $\tilde{G}_{f,\varepsilon}$ as an operator in $L^2(\mathbb{R}^n, e^{-2f/\varepsilon}dx_\varepsilon) \simeq \ell^2(\varepsilon\mathbb{Z}^n, e^{-2f/\varepsilon})$: also in this discrete case, there are besides $\tilde{\nu}_{1,\varepsilon} = 0$ further $m_0 - 1$ exponentially small eigenvalues, denoted by $\tilde{\nu}_{2,\varepsilon}, \dots, \tilde{\nu}_{m_0,\varepsilon}$ and satisfying

$$\frac{1}{\tilde{\nu}_{i,\varepsilon}} \;=\; \tilde{\mathbb{E}}_{x_i,\varepsilon}\, \tau_i \;\; (1 \;+\; o(1)) \quad . \tag{0.13}$$

The problem of determining the asymptotic behaviour of the mean metastable transition times $\mathbb{E}_{x_j,\varepsilon}\tau_j$ (see (0.6)) and $\tilde{\mathbb{E}}_{x_j,\varepsilon}\tau_j$ (see (0.11)) can therefore be phrased as a problem of spectral asymptotics of the respective generators $G_{f,\varepsilon}$ and $\tilde{G}_{f,\varepsilon}$.

The spectral-theoretic point of view towards metastability opens the door to the use of a variety of methods wich are non-probabilistic in nature. The following Theorem 0.2, based on the Witten complex approach mentioned before, gives complete asymptotic expansions on the m_0 exponentially small eigenvalues of the generators $G_{f,\varepsilon}$ and $\tilde{G}_{f,\varepsilon}$. In the light of (0.12) and (0.13) it can be seen as a particularly sharp version of Arrhenius' Law. The statement concerning $G_{f,\varepsilon}$ derives from the already mentioned result of [42]; the statement concerning $\tilde{G}_{f,\varepsilon}$ constitutes the main result of this thesis.

In order to be able to formulate the theorem, one has to attach to each minimum x_i of f (except the global minimum) a corresponding so-called

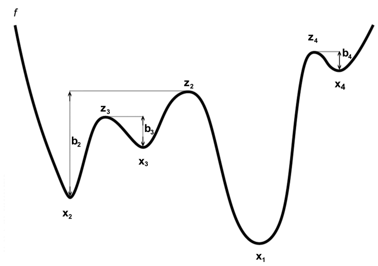

FIGURE 4. To each local minimum x_i (except the global one) corresponds a relevant saddle point z_i.

relevant saddle point z_i, which can be informally characterized as follows: first attach to each trajectory of the process, leading from the minimum in question to one of the deeper minima, a cost given by the maximum value of f along the trajectory; then consider the optimal trajectories, i.e. the ones which minimize the cost. A relevant saddle point z_i corresponding to x_i is a point which maximizes f along an optimal trajectory (see Figure 4, for exact definitions we refer to Section 13).

We call the difference $f(z_i) - f(x_i)$ the energy barrier corresponding to x_i and assume now that the minima are ordered by decreasing energy barrier, with x_1, the global minimum, having infinite energy barrier by definition. The first m_0 eigenvalues $(\nu_{i,\varepsilon})_{i=1,\ldots,m_0}$ of $G_{f,\varepsilon}$ and the first m_0 eigenvalues $(\tilde{\nu}_{i,\varepsilon})_{i=1,\ldots,m_0}$ of $\tilde{G}_{f,\varepsilon} = G_{f,\varepsilon,\varepsilon}$ are assumed to be in ascending order. The precise assumptions (implying in particular that the relevant saddle point z_i is well-defined and unique) are given after the theorem.

Theorem 0.2.

For every $i = 2, \ldots, m_0$ there exist (uniquely determined) sequences $(P_{i,k})_{k\in\mathbb{N}_0}$ and $(\tilde{P}_{i,k})_{k\in\mathbb{N}_0}$ in $\mathbb{R}$ such that

$$\nu_{i,\varepsilon} \sim \Big(\sum_{k=0}^{\infty} \varepsilon^k \quad P_{i,k} \Big) \; e^{-\frac{2[f(z_i)-f(x_i)]}{\varepsilon}} \tag{0.14}$$

and

$$\tilde{\nu}_{i,\varepsilon} \sim \Big(\sum_{k=0}^{\infty} \varepsilon^k \quad \tilde{P}_{i,k} \Big) \; e^{-\frac{2[f(z_i)-f(x_i)]}{\varepsilon}} \quad . \tag{0.15}$$

Moreover

$$P_{i,0} = \tilde{P}_{i,0} = \frac{|\kappa_{f,i}|}{\pi} \, \frac{\big[\det \operatorname{Hess} f(x_i)\big]^{\frac{1}{2}}}{|\det \operatorname{Hess} f(z_i)|^{\frac{1}{2}}} \quad , \tag{0.16}$$

where $\kappa_{f,i}$ denotes the unique negative eigenvalue of Hess $f(z_i)$.

Formula (0.14) has to be understood as follows: for every integer N we have

$$\nu_{i,\varepsilon}\, e^{\frac{2[f(z_i)-f(x_i)]}{\varepsilon}} \;-\; \sum_{k=0}^{N} \varepsilon^k \;\; P_{i,k} \;=\; \mathcal{O}(\varepsilon^{N+1}) \;\; .$$

Similarly for formula (0.15).

Note that $\nu_{1,\varepsilon}$ and $\tilde{\nu}_{1,\varepsilon}$ do not appear in the theorem because we shall work for simplicity in the case that $\nu_{1,\varepsilon} = \tilde{\nu}_{1,\varepsilon} = 0$, which is the typical situation from a probabilistic point of view. But more general situations are possible, in which there is no global minimum for f, $e^{-2f/\varepsilon}$ is not integrable/summable, and $\nu_{1,\varepsilon}$, $\tilde{\nu}_{1,\varepsilon}$ are different from zero and exponentially small. This cases are encompassed in [42] for the continuous diffusion.

In general there are three types of assumptions underlying theorems as Theorem 0.2:

- one sort of assumption concerns the regularity of f: to obtain complete expansions as the ones displayed in (0.14) and (0.15) one needs $f \in C^\infty(\mathbb{R}^n)$. With weaker regularity requirements the expansions will break down after some power in ε, depending on the smoothness of f. We restrict here as in [42] for simplicity to the case $f \in C^\infty(\mathbb{R}^n)$ and avoid to keep track of how much smoothness is needed to carry over each step in the proof.

- one needs suitable conditions on f at infinity, to assure the existence of discrete spectrum in the neighbourhood of 0. These can be skipped of course when working on a compact state space. In [42] rather weak (but not optimal) assumptions are made in terms of the first and second derivatives of f: they require that there exist constants $C', C'' > 0$ such that for every x outside a compact set $K \subset \mathbb{R}^n$

  $$|\nabla f(x)| \;\geq\; C' \quad \text{and} \quad |\,\mathrm{Hess}\, f(x)| \;\leq\; C''|\nabla f(x)|^2 \;\; .$$

  As we already mentioned this does not imply that $\nu_{1,\varepsilon} = 0$. In this thesis, to obtain Theorem 0.2 for the discrete generator, we work under the simplifying assumption that f is a positive definite quadratic function outside a compact set, implying in particular that $\nu_{1,\varepsilon} = \tilde{\nu}_{1,\varepsilon} = 0$. This is a purely technical assumption chosen to facilitate proofs at several places, but surely more general cases could be considered, where Theorem 0.2 still holds also in the discrete setting. (for further discussion on how this assumption can be relaxed see Section 9).

- there is another bunch of assumptions, whose role is mainly to pick up a typical situation, thus simplifying the statement of the theorem by avoiding situations which need taxonomic information: to be specific, we shall assume in this work that
  (i) f is a Morse function

  Moreover, denoting by $\mathcal{C}$ the set of critical points of f, and by $\mathcal{C}^{(0)}, \mathcal{C}^{(1)} \subset \mathcal{C}$ its subsets containing respectively the critical points of index 0 and 1,
  (ii) the critical values $\{f(x) : x \in \mathcal{C}\}$ are distinct
  (iii) the quantities $\{f(\zeta^{(1)}) - f(\zeta^{(0)}) : \zeta^{(1)} \in \mathcal{C}^{(1)}, \zeta^{(0)} \in \mathcal{C}^{(0)}\}$ are distinct.

  Note that assumptions (i)-(iii) are generic in the category of smooth functions. If one of these generic assumptions is dropped, one has to distinguish case by case and if necessary modify both the proof and the statement of the theorem regarding the prefactor: if e.g. some minimum is degenerate, the first term in the expansion may vanish; if (ii) is dropped, the uniqueness of the relevant saddle point attached to a minimum is potentially violated and different scenari can appear: in particular it becomes necessary to understand if the multiple saddle points have to be climbed up "in series" (i.e. if there is a metastable transition path issuing from a minimum and crossing several relevant saddle point) or 'in parallel" (the process can choose among different metastable transition paths, related to different relevant saddle points); if (iii) is dropped, one has to be careful since degeneracy of the eigenvalues of the generator is possible.

  The details for these extensions are not contained in the thesis, and in fact not available in the literature as far as we know, at least for the discrete case. For further information around that topic in the continuous setting see [5],[96].

We end this subsection with a few more comments around Theorem 0.2:

As already anticipated in (0.6) (in combination with (0.12)) and (0.11) (in combination with (0.13)), the rate of the exponential decay of the small eigenvalues is given by the energy barrier $2[f(x_i) - f(z_i)]$ (the factor 2 appears in accordance with the fact that we have chosen the Gibbs measure to be proportional to $e^{-2f/\varepsilon}$ instead of $e^{-f/\varepsilon}$). The strength of Theorem 0.2

rests on the statements regarding the asymptotics of the "prefactors".[12] Rigorous results on the prefactor in such a general setting can be already found in [96], [14],[13], [29],[78] for the continuous diffusion and in [11],[12], where the leading term of the prefactor is found to be of order 1 in ε. That the subleading term in the prefactor is of order ε (and more generally, that complete expansions of the type indicated in Theorem 0.2 exist) appears to be new in the discrete setting, while in continuous setting it is due, as mentioned before, to [42].

The explicit expression (0.16) for the leading term, where the quadratic part of f around the involved critical points appears, also seems to be not available so far in the literature, as far as the discrete setting is concerned (but see also [7] for similar situations). Note that according to (0.16) there is no distinction in the leading terms between the continuous and the discrete model. One can see (0.16) therefore also as a statement of validity of the diffusive approximation, at least for the sake of computing leading terms of metastable transition times, even in the scaling $\delta = \varepsilon$. The geometric constraint imposed on the process by forcing it to move on the lattice becomes appreciable only starting from the second term in the expansion.

The Witten complex approach to metastability.

As already stressed at the beginning of the introduction, the main motivation for this thesis arises from the so-called Witten complex or supersymmetric method in the context of metastability problems introduced in [42] (see also [43] and [83] for more pedagogic expositions).

To illustrate the main points of this approach it is convenient to rewrite the generator $G_{f,\varepsilon}$ as introduced in (0.2) in terms of the (de Rham) exterior differential

$$d \;:\; C_c^\infty(\mathbb{R}^n;\Lambda^0\mathbb{R}^n) \;\to\; C_c^\infty(\mathbb{R}^n;\Lambda^1\mathbb{R}^n) \;\; .$$

Here $C_c^\infty(\mathbb{R}^n;\Lambda^0\mathbb{R}^n) \simeq C_c^\infty(\mathbb{R}^n;\mathbb{R})$ is the space of smooth compactly supported 0-forms and $C_c^\infty(\mathbb{R}^n;\Lambda^1\mathbb{R}^n) \simeq C_c^\infty(\mathbb{R}^n;\mathbb{R}^n)$ is the space of smooth compactly supported 1-forms, and the generator can be rewritten as (see

[12] As mentioned in [12] a good understanding of the prefactor becomes important in applications to disordered models to control additional fluctuations on the long-time behaviour due to the disorder.

also (0.4))

$$G_{f,\varepsilon} \;=\; \varepsilon\, d_\varepsilon^{*f}\, d \quad \text{with} \quad d_\varepsilon^{*f} \;:=\; e^{2f/\varepsilon}\, d^*\, e^{-2f/\varepsilon} \quad .$$

Here $d^* : C_c^\infty(\mathbb{R}^n;\Lambda^1\mathbb{R}^n) \;\to\; C_c^\infty(\mathbb{R}^n;\Lambda^0\mathbb{R}^n)$ denotes the formal adjoint of d with respect to the scalar products in the "flat" spaces $L^2(\mathbb{R}^n, dx;\Lambda^0\mathbb{R}^n)$ and $L^2(\mathbb{R}^n, dx;\Lambda^1\mathbb{R}^n)$. Observe that, on the other hand, d_ε^{*f} is the formal adjoint of d when considering the scalar products of the weighted spaces $L^2(\mathbb{R}^n, e^{-2f/\varepsilon}dx;\Lambda^0\mathbb{R}^n)$ and $L^2(\mathbb{R}^n, e^{-2f/\varepsilon}dx;\Lambda^1\mathbb{R}^n)$. Thus the generator $G_{f,\varepsilon}$ can be seen as nothing but the Laplacian in the weighted space $L^2(\mathbb{R}^n, e^{-2f/\varepsilon}dx;\mathbb{R})$. [13]

The spirit of the supersymmetric approach (see also [99] besides [42]) is to obtain new insights on the problem by broadening the view and considering the Hodge-type extension of the "Laplacian" $G_{f,\varepsilon}$ on the full algebra of differential forms. To be specific, denoting for $p = 0,\dots,n-1$ by

$$d^{(p)} \;:\; C_c^\infty(\mathbb{R}^n;\Lambda^p\mathbb{R}^n) \;\to\; C_c^\infty(\mathbb{R}^n;\Lambda^{p+1}\mathbb{R}^n)$$

the de Rham exterior differential acting on the space of p-forms and by

$$d^{*,(p)} \;:\; C_c^\infty(\mathbb{R}^n;\Lambda^{p+1}\mathbb{R}^n) \;\to\; C_c^\infty(\mathbb{R}^n;\Lambda^p\mathbb{R}^n)$$

its adjoint with respect to the scalar products of the flat spaces $L^2(\mathbb{R}^n, dx;\Lambda^p\mathbb{R}^n)$, one defines for every $p = 0,\dots,n$

$$G_{\varepsilon,f}^{(p)} \;:\; C_c^\infty(\mathbb{R}^n;\Lambda^p\mathbb{R}^n) \;\to\; C_c^\infty(\mathbb{R}^n;\Lambda^p\mathbb{R}^n) \quad ,$$

by setting[14]

$$G_{\varepsilon,f}^{(p)} \;:=\; \varepsilon\, d_\varepsilon^{*f,(p)}\, d^{(p)} \;+\; \varepsilon\, d^{(p-1)}\, d_\varepsilon^{*f,(p-1)} \quad ,$$
$$\text{with} \quad d_\varepsilon^{*f,(p)} \;:=\; e^{2f/\varepsilon}\, d^{*,(p)}\, e^{-2f/\varepsilon} \quad .$$

We shall henceforth drop in general the superscript (p) on the operators if the direct sum acting on the full algebra of forms is intended. The main feature of the Hodge Laplacian $G_{f,\varepsilon}$ is that it commutes with d as expressed by the so-called intertwining relation:

$$G_{f,\varepsilon}\, d \;=\; d\, G_{f,\varepsilon} \quad . \tag{0.17}$$

Observe that this has the following implication: if u_ε is an eigenfunction corresponding to the eigenvalue $\nu_\varepsilon \neq 0$ for $G_{f,\varepsilon}^{(0)}$, then $\alpha_\varepsilon := du_\varepsilon$ is an eigenform for $G_{f,\varepsilon}^{(1)}$, still corresponding to the eigenvalue ν_ε. The identity (0.17) is

[13]Note that this is a general structural property of reversible Markov processes.

[14]Here and in analogous situations below we have by convention $d^{(-1)} \equiv d_\varepsilon^{*f,(-1)} \equiv d^{(n)} \equiv d_\varepsilon^{*f,(n)} \equiv 0$

a simple consequence of the complex property $d^2 \equiv 0$, the term "complex" referring to the fact that this property qualifies the sequence

$$C_c^\infty(\mathbb{R}^n;\Lambda^0\mathbb{R}^n) \xrightarrow{d^{(0)}} C_c^\infty(\mathbb{R}^n;\Lambda^1\mathbb{R}^n) \xrightarrow{d^{(1)}} C_c^\infty(\mathbb{R}^n;\Lambda^2\mathbb{R}^n) \xrightarrow{d^{(2)}} \dots \xrightarrow{d^{(n-1)}} C_c^\infty(\mathbb{R}^n;\Lambda^n\mathbb{R}^n)$$

as a chain complex in the sense of cohomology theory. Analogous considerations hold for d_ε^{*f}.

To better understand the origin of the idea of extending the generator to higher forms, it may be useful to provide some background related to Witten's ideas on Morse inequalities contained in his famous paper [103]. We shall first slightly change point of view and pass from the weighted spaces $L^2(\mathbb{R}^n, e^{-2f/\varepsilon}dx;\Lambda^p\mathbb{R}^n)$ to the flat spaces $L^2(\mathbb{R}^n, dx;\Lambda^p\mathbb{R}^n)$ by conjugating the operators with the unitary transformation given by multiplication with $e^{-f/\varepsilon}$. To be precise consider for every $p = 0, \dots, n$

$$\Delta_{f,\varepsilon}^{(p)} \;:=\; \varepsilon\, e^{-f/\varepsilon}\, G_{f,\varepsilon}^{(p)}\, e^{f/\varepsilon}$$

and for every $p = 0, \dots, n-1$

$$d_{f,\varepsilon}^{(p)} \;:=\; \varepsilon\, e^{-f/\varepsilon}\, d^{(p)}\, e^{f/\varepsilon}$$

$$\text{and} \quad d_{f,\varepsilon}^{*,(p)} \;:=\; \varepsilon\, e^{-f/\varepsilon}\, d_\varepsilon^{*f,(p)}\, e^{f/\varepsilon} \;=\; \varepsilon\, e^{f/\varepsilon}\, d^{*,(p)}\, e^{-f/\varepsilon} \quad .$$

Note that $d_{f,\varepsilon}^{(p)}$ and $d_{f,\varepsilon}^{*,(p)}$ are formally adjoint in the flat L^2 spaces and that the complex property $d_{f,\varepsilon}^2 \equiv 0$ still holds. Note also that

$$\Delta_{f,\varepsilon}^{(p)} \;=\; d_{f,\varepsilon}^{*,(p)}\, d_{f,\varepsilon}^{*,(p)} \;+\; d_{f,\varepsilon}^{(p-1)}\, d_{f,\varepsilon}^{*,(p-1)}$$

and, up to the factor ε which we introduced to conform with common conventions, $\Delta_{f,\varepsilon}^{(p)}$ has the same spectrum of $G_{f,\varepsilon}^{(p)}$. The two point of views are indeed formally equivalent[15] and we shall stick to the flat space setting to conform with [42] and [103]. A simple computation gives

$$\Delta_{f,\varepsilon}^{(0)} \;=\; -\varepsilon^2\Delta \;+\; |\nabla f|^2 \;-\varepsilon\,\Delta f$$

and more generally

$$\Delta_{f,\varepsilon}^{(p)} \;=\; \Delta_{f,\varepsilon}^{(0)} \otimes \mathrm{Id} \;+\; \varepsilon\; 2\,\mathrm{Hess}^{(p)} f \quad , \tag{0.18}$$

with $\mathrm{Hess}^{(p)} f$ denoting the natural action of a symmetric matrix on a p-form, so that in particular $\mathrm{Hess}^{(1)} f = \mathrm{Hess}\, f$. This can be seen as a Schrödinger

[15] The difference between the two settings is psychological: the operators in the weighted L^2 space are linked to the intuition coming from the diffusion process, and the considered scaling is a small noise asymptotic; the operators in the flat L^2 space turn out to be Schrödinger-type operators and the small parameter is here "Planck's constant". Standard methods of semiclassical analysis are here more natural and readily available.

operator with the potential given as a sum of the leading term $|\nabla f|^2$ and the subleading term $-\Delta f + 2\,\mathrm{Hess}^{(p)} f$.

The "deformed" Hodge Laplacian $\Delta_{f,\varepsilon}$ and the "deformed" de Rham differential $d_{f,\varepsilon}$ are known as Witten Laplacian and Witten differential respectively, with the latter giving rise to the Witten complex

$$C_c^\infty(\mathbb{R}^n;\Lambda^0\mathbb{R}^n) \overset{d_{f,\varepsilon}^{(0)}}{\to} C_c^\infty(\mathbb{R}^n;\Lambda^1\mathbb{R}^n) \overset{d_{f,\varepsilon}^{(1)}}{\to} C_c^\infty(\mathbb{R}^n;\Lambda^2\mathbb{R}^n) \overset{d_{f,\varepsilon}^{(2)}}{\to} \dots \overset{d_{f,\varepsilon}^{(n-1)}}{\to} C_c^\infty(\mathbb{R}^n;\Lambda^n\mathbb{R}^n) \ .$$

These operators were used by Edward Witten in [103] to give an analytical proof of the Morse inequalities on compact manifolds. An account on this can be found in the survey paper [9] by R. Bott (see also [48] for a more rigorous version of Witten's ideas and [67], where in the introduction a very brief review of the impact of Witten's complex in topology and analysis can be found).

Note that the intertwining relation (0.17) becomes now

$$\Delta_{f,\varepsilon}\, d_{f,\varepsilon} \ = \ d_{f,\varepsilon}\, \Delta_{f,\varepsilon} \ . \tag{0.19}$$

The key feature of the Witten Laplacian on the algebra of forms is to complete very nicely the spectral picture given in Figure 3 by involving in its low-lying spectrum not only the minima of f but *all* its critical points. Indeed, with m_p denoting the number of critical points of index p of f, one has that $\Delta_{f,\varepsilon}^{(p)}$ has exactly m_p exponentially small eigenvalues with the rest of its spectrum being bounded from below by a positive constant times ε (recall that the spectrum of $\Delta_{f,\varepsilon}^{(p)}$ differs by a factor ε from the one of $G_{f,\varepsilon}$). In particular

$$\dim \mathrm{Ran}\, 1_{[0,\varepsilon^{6/5})}(\Delta_{f,\varepsilon}^{(p)}) \ = \ m_p \ . \tag{0.20}$$

This is seen by suitably "decoupling" the wells of the leading potential $|\nabla f|^2$, each of which corresponds to a critical point of f. It turns then out that only the m_p wells corresponding to the critical points of index p contribute to the low-lying spectrum $\mathrm{Spec}(\Delta_{f,\varepsilon}^{(p)}) \cap [0,\varepsilon^{6/5})$. In other terms, in the case of $\Delta_{f,\varepsilon}^{(p)}$ the m_p wells corresponding to the critical points of index p are resonant in $[0,\varepsilon^{6/5})$, all the others are non-resonant.

Note en passant that once the very rough estimate (0.20) is established it is not a long way to prove the Morse inequalitites, at least in their simplest form, stating that for every $p = 0, \ldots, n$

$$b_p \ \leq \ m_p \ \ , \tag{0.21}$$

where b_p is the p-th Betti number, which by Hodge theory equals the kernel of the classical Hodge Laplacian $\Delta_H^{(p)}$ on p-forms. Indeed it is sufficient to note that $\Delta_{f,\varepsilon}^{(p)}$ has the same kernel as $\Delta_H^{(p)}$ for every ε and (0.21) follows immediatley from (0.20).

We shall now return to the much harder problem of finding sharp spectral asymptotics for the small eigenvalues of $G_{f,\varepsilon}^{(0)}$, or equivalently of $\Delta_{f,\varepsilon}$, the Witten Laplacian on functions. [16] Now a simple decoupling is not sufficient and the interaction between the resonant wells has to be analyzed. In the semiclassical spectral theory of Schrödinger operators the typical strategy ([45],[18]) to understand the splitting of nearly degenerate eigenvalues, due to tunneling between different resonant wells, can be very roughly summarized as follows:

Step 1 Construct locally for each resonant well of the potential a quasimode[17] (typically through a WKB Ansatz). To have some chance to catch the splitting effect the quasimodes must have as large as possible support so that at least some overlap among them occurs.

Step 2 Reduce to a finite dimensional linear algebra problem by studying the operator restricted to the eigenspace corresponding to the considered spectral interval. This restricted operator is represented as a matrix by chosing as basis the quasimodes projected on the eigenspace. If the quasimodes are sufficiently well chosen one can hope to be able to compute approximately the spectrum of this matrix.

To implement this general strategy in the case of $\Delta_{f,\varepsilon}^{(0)}$ in order to obtain (0.14) is a rather daunting task, mainly for the following three reasons: the tunneling between two minima of f occurs by passing through a non-resonant well, namely the well associated to the corresponding relevant

[16] We may add at this point that sharp asymptotics of the low-lying spectrum for $p > 0$ are obtained in the preprint [73]. This case is even more difficult since for $p = 0$ one has the advantage of knowing that $\Delta_{f,\varepsilon}^{(0)} e^{-f/\varepsilon} = 0$

[17] A quasimode is a function which satisfies the eigenvalue equation only approximately. According to [18] the term quasimode appeared first in [2].

saddle point. This is a particularly difficult situation since WKB expansions starting from a minimum break down at the saddle point, and it is therefore hard to get overlapping quasimodes. Moreover, as we know from the probabilistic model (see in particular (0.12)), the tunneling between two minima which is responsible for the appearance of a given non-zero small eigenvalue may also occur through a well associated to a third minimum, which is weakly resonant in the terminology of [46], [47] and further complicates the situation. Apart from this, one has to face another complication in Step 2, related to the fact that the small eigenvalues have distinct exponential decay. Indeed, when diagonalizing the matrix of the operator, error terms propagate additively (see [48]) and therefore quantities of order of the larger exponentially small eigenvalues destroy the possibility to accurately estimate the smaller ones.

All these obstructions are elegantly avoided in [42] by exploiting the particular Witten complex structure. The guiding ideas are:

1) Use of the fact that $\Delta_{f,\varepsilon}^{(0)} e^{-f/\varepsilon} = 0$ and of the intuition coming from the behaviour of the stochastic process to construct quasimodes for each minimum, whose support is sufficiently large to intersect a small neigbourhood of the corresponding relevant saddle point.

   More precisely consider for each minimum x_i the "metastable basin of attraction" $\mathcal{B}_i$ given by the connected component of $\{f < f(z_i)\}$ containing x_i and take as quasimode roughly $e^{-f/\varepsilon} 1_{\mathcal{B}_i}$ suitably normalized to one.

   Note that these quasimodes may go far beyond the corresponding well by including possible weakly resonant wells encountered on the way to the relevant saddle point. But they loose there efficiency around the relevant saddle point.

2) The lack of good information in the small region around the relevant saddle points is patched up by using a local WKB expansion for the eigenvalue problem of the Witten Laplacian $\Delta_{f,\varepsilon}^{(1)}$, which is acting on 1-forms. These WKB expansions had already been constructed in [48] by Helffer and Sjöstrand.

3) Instead of analyzing directly the small eigenvalues of $\Delta_{f,\varepsilon}$ one considers their square roots, characterized as singular values of $d_{f,\varepsilon}$. Note that if $\nu_\varepsilon \neq 0$ is a small eigenvalue of $\Delta_{f,\varepsilon}^{(0)}$ with normalized

eigenfunction u_ε, then

$$\nu_\varepsilon = \langle \Delta^{(0)}_{f,\varepsilon} u_\varepsilon, u_\varepsilon\rangle \;=\; \langle d_{f,\varepsilon} u_\varepsilon, d_{f,\varepsilon} u_\varepsilon\rangle \;=\; \langle d_{f,\varepsilon} u_\varepsilon, \frac{d_{f,\varepsilon} u_\varepsilon}{\|d_{f,\varepsilon} u_\varepsilon\|}\rangle \;\; \sqrt{\nu_\varepsilon}$$

$$\text{i.e.} \quad \sqrt{\nu}_\varepsilon \;=\; \langle d_{f,\varepsilon} u_\varepsilon, \alpha_\varepsilon\rangle \;\;, \tag{0.22}$$

where $\alpha_\varepsilon := \frac{d_{f,\varepsilon} u_\varepsilon}{\|d_{f,\varepsilon} u_\varepsilon\|}$ is a normalized eigenform of $\Delta^{(1)}_{f,\varepsilon}$ thanks to the intertwining relation (0.19). More generally, it is not hard to show starting from (0.19) that the image of $d_{f,\varepsilon}$ restricted to the eigenspace $\mathrm{Ran}\, 1_{[0,\varepsilon^{6/5})}(\Delta^{(0)}_{f,\varepsilon})$ is contained in the eigenspace $\mathrm{Ran}\, 1_{[0,\varepsilon^{6/5})}(\Delta^{(1)}_{f,\varepsilon})$, which by (0.20) has dimension m_1.

Considering singular values instead of eigenvalues turns out to be a twofold advantage: on one hand, as can be seen from (0.22), it naturally drags in the WKB expansions of the point 2) (which are approximations for the α_ε above) and no cumbersome matching of the WKB expansions with the quasimodes of point 1) is needed. On the other hand, it greatly facilitates the final linear algebra problem. This last point has to do with the following simple fact regarding stability of singular values: if B_ε is an arbitrary matrix, then multiplication with a quasi-orthogonal matrix S_ε (i.e. $S_\varepsilon = S + \mathcal{O}(\varepsilon^\infty)$ with S orthogonal), does not change the i-th singular value $\mu_{i,\varepsilon}$ up to an error which appears *multiplicatively* and not additively, i.e. (in case of left multiplication just to give an example)

$$\mu_{i,\varepsilon}(S_\varepsilon B_\varepsilon) \;=\; \mu_{i,\varepsilon}(B_\varepsilon)\;(1 + \mathcal{O}(\varepsilon^\infty)) \;\;.$$

We stress that the proof in [42] takes advantage of the formalism of differential forms[18] and of several important results, which were previously established in [48]: in particular (0.20) in the cases $p = 0, 1$ and the construction of WKB expansions on the level of 1-forms. Besides local existence of the latter, [42] takes from [48] a very detailed analysis along the instanton of the leading WKB amplitude and the WKB phase function and a priori estimates on the semiclassical decay of the eigenforms, also called semiclassical Agmon estimates.

In this thesis the strategy underlying [42] is adapted to the discrete model defined by (0.8) (for $\delta = \varepsilon$), without loss of strength in the conclusions (see Theorem 0.2).

Several hindrances appeared along the way, first of all due to the fact that the discrete setting was lacking the necessary foundations to build on.

[18]Note that even if only the Witten Laplacians for $p = 0, 1$ are considered, also the space of 2-forms appears implicitly in the definition of $\Delta^{(1)}_{f,\varepsilon}$.

Therefore we had to start from scratch: an important step was to define a suitable algebra of differential forms, well-suited to the discrete geometry determined by the process. This generalized algebra consists of forms which are "nonlinear" in the tangent space and which are well-suited for describing not only infinitesimal displacements, but also jumps.[19]

In this framework of generalized forms we introduce an invariantly defined discrete differential complex, its Witten-type deformation and finally a discrete Witten Laplacian having the following key properties: on one hand, it is unitary equivalent to the generator (0.8) when restricted to the level of functions (i.e. 0-forms). On the other hand it shares all the relevant analytic and algebraic properties of its continuous analogue, in particular the intertwining property (0.19). Pursuing this route the formulas rapidly become quite annoying when compared to their continuous analogues, due to the failure of the Leibniz rule in discrete setting. In order to be able to efficiently handle these expressions in later sections and gain in transparency it became almost mandatory to spend some time in developing an ad hoc compact notation.

On this basis one can proceed with a first, rough asymptotic spectral analysis, yielding the discrete analogue of (0.20) for $p = 0, 1$, and by exhibiting local WKB expansions for the discrete Witten Laplacian on 1-forms around critical points of f having index 1. The rough spectral analysis of the low-lying spectrum is achieved as in the continuous case with a harmonic approximation (see [89], [21]). But here additional problems appear, due to the nonlocality of the discrete operators. These are solved following [65], where microlocalization techniques are exploited.

The WKB expansions are constructed using standard techniques ([45],[27], [66]): a proof of existence amounts to show local solvability of singular eikonal equations and singular linear transport equations. The associated approximate eigenvalues are shown to be $\mathcal{O}(\varepsilon^\infty)$ mimicking an argument contained in [40] which exploits the intertwining relations. A refined analysis along the instanton, as the one contained in [48] for the continuous case, is more complicated and indeed still missing. The complications arise from the fact that the transport occurs now around non-gradient vector fields (compare (0.9) and (0.10)) and that the solution of the eikonal equation (the so-called Agmon distance) is a distance which is not arising from a

[19] We point to the fact that with these generalizations the cotangent space at a point has now the same dimension of the state space only in the special case in which nearest neighbour jumps are considered, as in (0.8). In general it will be larger.

scalar product. Indeed, it turns out to be just a Finslerian distance (see [64] for more information on this).

Only after this rather long spadework (accomplished in Part I and Part II of the thesis) one reaches the point where [42] starts. One of the main tasks one has to face when trying to carry over their strategy without losing accuracy in the remainder estimates is to efficiently deal with Laplace-type asymptotics of sums. Indeed, when computing the scalar products appearing in the interaction matrix or normalization constants, quantities like the following appear all over the time:

$$\sum_{x \in \varepsilon\mathbb{Z}^n} a(x) e^{-\varphi(x)/\varepsilon} \quad .$$

This problem is solved here by consistently using the Poisson summation formula, which permits to reduce to classical Laplace integrals.

The fact that the constant functions are in the kernel of the discrete generator (0.8) implies, as in the continuous case, that $e^{-f/\varepsilon}$ is in the kernel of the discrete Witten Laplacian on functions. We can therefore again work very efficiently on the level of functions with quasimodes roughly given by $e^{-f/\varepsilon} 1_{\mathcal{B}_i}$, where $\mathcal{B}_i$ is a metastable basin of attraction as before. However, with respect to [42] we slightly change the precise definition of each of these quasimodes, by pushing the border of its support closer to the relevant saddle point as ε goes to zero (see Section 14). With this trick, we avoid at once both the use of Agmon estimates (which were developed in [64] on the level of functions but not on the level of discrete 1-forms) and the need of a refined analysis of the WKB expansions along the instanton. Indeed, that our 1-form quasimodes are slightly worse, is balanced by the fact that our 0-form quasimodes are slightly better than in [42]: no harm in the final result occurs.

We like to mention that, while the avoidance of Agmon estimates somehow streamlines the presentation, a refined analysis on the instanton of the discrete WKB expansions would be still desirable even when the forementioned trick is applied: without this information the proof of the complete expansions of the eigenvalues given in (0.15) becomes computationally much more involved (see Section 15).

For the final linear algebra problem we follow essentially the induction process proposed in [71], which is a streamlined version of the one contained in [42].

Outline of the thesis.

The thesis is divided into four parts. Part I ("Discrete geometries on affine spaces") has a foundational character: it is mainly concerned with definitions and basic properties of de Rham-type complexes, Hodge-type and Witten-type Laplacians in affine space. The point is that the geometry we consider on the latter is *not* the classical geometry induceed by a scalar product on the tangent space, but the geometry determined by a reversible Markov jump process. For simplicity we limit ourselves to discrete processes, i.e. those which are constrained to move on a lattice, but the formalism is presented in a way which lends itself to straightforward generalizations. We have chosen to consequently give a coordinate-free representation, enlightnening the geometric content of the considered objects, which would be hidden in a more concrete development in the coordinate space $\mathbb{R}^n$.

In Part II ("Semiclassical Witten Laplacians") we introduce a small scaling parameter ε and derive basic asymptotic properties of the correspnding rescaled discrete Witten Laplacians concerning the low-lying spectrum.

In Part III ("Asymptotics of small eigenvalues of $\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$") we use the precedently developed framework and tools to derive sharp asymptotics for the low-lying spectrum of the discrete Witten Laplacian on 0-forms.

Finally, in Part IV ("Appendix"), we present some general abstract results, which are used at crucial points in the main text and which, to our knowledge, are not available in the literature in the precise form we need. Moreover we confine to the last section some straightforward computations, needed in Part II.

Below we give a short description of the content of each section.

Part I

Section 1.

We fix some basic notation concerning the space we are working on, namely an n-dimensional affine space M, with underlying vector space V. Then we introduce spaces of symmetric and alternating p-functions, denoted by $F_s(M \times V^p)$ and $F_a(M \times V^p)$, which generalize the classical spaces of (covariant) symmetric and alternating p-tensors by dropping the linearity condition. Motivation and geometric interpretation concerning the definition of p-functions is provided with a brief excursus on p-cells.

Section 2.

We introduce various formal operators acting on the spaces of p-functions. In particular an exterior difference operator δ is defined on the antisymmetric algebra $\mathcal{F}_a(M \times V) := \oplus_{p=0}^{\infty} F_a(M \times V^p)$. The operator δ is the analogue of the De Rham exterior differential on classical forms and satisfies the basic complex property $\delta^2 = 0$.

Section 3.

A discrete geometry on M is defined in terms of a finite, symmetric and lattice generating jump distribution μ on the vector space V. If also one of the corresponding ergodic components in M is chosen, one gets a lattice graph Λ_μ, which determines scalar products on spaces of p-functions for every p. The choice of μ permits to define a formal operator δ^{*_μ} on the alternating algebra $\mathcal{F}_a(M \times V)$, which is dual to δ.

Section 4.

We introduce a formal Hodge Laplacian $\mathcal{L}_\mu$ acting on $\mathcal{F}_a(M \times V)$ and compute representation formulas.

Section 5.

The discussion of Section 3 is generalized to cover the case in which a weight function ρ is given on M, describing inhomogeneities in space and thus possibly breaking the translation invariance. A couple (μ, ρ) is called an inhomogeneous discrete geometry. If a corresponding weighted lattice graph $\Lambda_{\rho\mu}$ is chosen, one gets weighted scalar products on the spaces of p functions. The dual $\delta^{*\rho\mu}$ of δ is introduced in this setting.

Section 6.

Representation formulas for the formal Hodge Laplacian $\mathcal{L}_{\rho\mu}$ associated with an inhomogeneous discrete geometry are derived. Suitable realizations $\mathcal{L}_{\Lambda_{\rho\mu}}$ in the L^2 spaces determined by lattice graphs $\Lambda_{\rho\mu}$ are introduced by Friedrichs extensions.

Section 7.

Here we focus our attention on $\mathcal{L}_{\rho\mu}^{(0)}$, the restriction of the Hodge Laplacian to the level of functions and discuss its probabilistic interpretation, recalling some standard facts about generators of semigroups, Dirichlet forms and construction of Markov processes.

Section 8.

We slightly change our point of view: the function ρ is treated as a deformation parameter of the operators δ, $\delta^{*\mu}$, rather than an inhomogeneity perturbing the discrete geometry μ. This point of view is unitarily equivalent to the one developed in Section 5 and 6 and leads to the discrete Witten Laplacian $\mathcal{H}_{\rho,\mu}$, and its L^2 realizations $\mathcal{H}_{\rho,\Lambda_\mu}$ with respect to lattice graphs.

Part II

Section 9.
We rescale both ρ and μ with a small parameter $\varepsilon > 0$ by setting $\rho_\varepsilon := e^{-2f/\varepsilon}$ and $\mu_\varepsilon(\cdot) := \mu(\varepsilon^{-1}\cdot)$, with f a smooth real function. We derive useful representation formulas for the leading symbols of the corresponding rescaled Witten Laplacians. Moreover the basic assumptions made throughout Part II are declared.

Section 10.
The aim of this section is to provide a rough spectral analysis of the low-lying spectrum of $\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$ and $\mathcal{H}^{(1)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$ via harmonic approximation. The dimensions of the low eigenspaces are related to the number of critical points of f of index 0 and 1.

Section 11.
We construct through a WKB Ansatz quasimodes corresponding to the small eigenvalues of the semiclassical Witten Laplacian for $p = 1$. The main result is stated in Theorem 11.1. It says that in a sufficiently small neighbourhood Ω around a a critical point of index 1 of f one can find a smooth phase function φ and a smooth amplitude a_ε such that

$$e^{\frac{\varphi}{\varepsilon}} \ \mathcal{H}^{(1)}_{\rho_\varepsilon,\mu_\varepsilon} \ a_\varepsilon e^{-\frac{\varphi}{\varepsilon}} \Big|_{\Omega} \sim 0 \ .$$

Part III

Section 12.
In this short section we fix the setup and the precise assumptions underlying Part III.

Section 13.
The aim of this section is to introduce a convenient labelling of the local minima of f, to attach to each of them a so-called relevant saddle point at

which exit from the metastable basin of attraction of the considered minimum occurs. The metastable basins of attraction are smoothed in proximity of the relevant saddle point, where a corner occurs. These "modified" basins of attraction will be useful in the definition of the quasimodes on the level of function in the following Section 14. The discussion in this section concerns only the geometry of f: the Witten Laplacian, in particular the discrete nature of the one we are considering in this work, plays no role here.

Section 14.

Following [42] we attach to every minimum of f a quasimode for $\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$ and to every critical point of index 1 of f a quasimode for $\mathcal{H}^{(1)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$. The former is obtained by cutting the ground state $e^{-\frac{f}{\varepsilon}}$ outside the basin of attraction of the considered minimum; the latter by using a WKB-expansion, cut around a small neigbourhood of the considered saddle point, as constructed in Section 11. The cut-off function $\chi^{(0)}_{i,s,\varepsilon}$ attached to the i-th minimum is supported in a small neigbourhood of the modified basin of attraction and will depend both on ε and a second parameter $s > 0$. Every choice of $s \in [\frac{1}{2}, 1)$ will be fine to obtain asymptotic expressions for the low-lying eigenvalues of $\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$, with $s = \frac{1}{2}$ giving the best (but not optimal) error estimate. The convenience of developing the theory also for different values of s will show up only in Section 17, where comparing two possible choices of s (say $s = \frac{1}{2}$ and $s = \frac{\sqrt{2}}{2}$) one can easily get rid of the fictitious dependence on s of the results and thus obtain optimal error estimates.

Section 15.

In this section we analyze the asymptotic behaviour as $\varepsilon \to 0$ of the (square root of the) approximate eigenvalues $\nu^{\text{app}}_{i,s,\varepsilon}$ determined by the quasimodes of the previous section. The key instrument here is the Poisson summation formula which permits to reduce sums over the scaled lattice to integrals. Once the passage to integrals is achieved one can comfortably change from coordinates adapted to the lattice to coordinates adapted to the local structure of f.

Section 16.

In this section we establish a sharp asymptotic relation between the approximate eigenvalues computed in Section 15 and the actual small eigenvalues of $\mathcal{H}^{(0)}_{\Lambda_{\rho_\varepsilon,\mu_\varepsilon}}$. This is obtained by projecting the quasimodes on the eigenspaces $\dim \operatorname{Ran} 1_{[0,\varepsilon^{6/5})}(\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}})$ and $\dim \operatorname{Ran} 1_{[0,\varepsilon^{6/5})}(\mathcal{H}^{(1)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}})$ and studying the singular values of the distorted differential d_{ρ_ε}, considered as a map from $\dim \operatorname{Ran} 1_{[0,\varepsilon^{6/5})}(\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}})$ to $\dim \operatorname{Ran} 1_{[0,\varepsilon^{6/5})}(\mathcal{H}^{(1)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}})$. The good properties of the quasimodes established in Section 14 permit to conclude with a straightforward Gaussian elimination, following [71].

Section 17.

The results of Section 15 and Section 16 are combined to get the main theorem of this thesis (Theorem 17.1), giving complete expansions of the first m_0 eigenvalues of $\mathcal{H}^{(0)}_{\Lambda_{\rho_\varepsilon,\mu_\varepsilon}}$ with explicit leading prefactor. Equation (0.15) in Theorem 0.2 of this introduction is a direct consequence, noting that the eigenvalues of the discrete Witten Laplacian differ by a factor ε from the eigenvalues of $\tilde{G}_{f,\varepsilon}$.

Part IV

Appendix A.

We state a theorem on local existence of solutions for a class of matrix-valued singular linear transport equations under suitable compatibility conditions. This result is instrumental for the construction of WKB expansions as done in Section 11. The scalar case is a classical result which is proved for example in [27] or [40]. The higher-dimensional result requires only minor modifications to the proof and is used for example in [48]. For completeness, we give a detailed proof adapting the one of [27].

Appendix B.

We consider a class of matrix valued discrete Schrödinger operators on the scaled lattice $\varepsilon\mathbb{Z}^n$. Criteria for essential selfadjointness and localization of the essential spectrum are given. Moreover we state a result which quantifies the error commited when approximating the discrete spectrum with the one of suitable harmonic oscillators sitting at the bottom of the wells of the potential (harmonic approximation). The proof is omitted since it amounts in slightly modifying the arguments in [65], where only the scalar case is treated.

Appendix C.

We consider sums of the type

$$\sum_{x\in\varepsilon\mathbb{Z}^n} a(x)e^{-\varphi(x)/\varepsilon} \quad ,$$

with compactly supported and smooth amplitude a and smooth phase φ, having a unique non degenerate global minimum. Complete asymptotics are obtained by rescaling properly and using the Poisson summation formula to reduce to the case of a classical Laplace integral.

Appendix D.

We consider an $m_1 \times m_0$ matrix B_ε (which in the application of Section 16.1 corresponds to the discrete Witten differential $\delta_{\rho_\varepsilon}^{(0)}$ restricted on the m_0-dimensional eigenspace $\operatorname{Ran} 1_{[0,\varepsilon^{6/5})}(\mathcal{H}^{(1)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}})$). It is shown, following essentially [71], that if approximately orthogonal bases $e_{1,\varepsilon},\dots,e_{m_0,\varepsilon}$ and $f_{1,\varepsilon},\dots,f_{m_1,\varepsilon}$ are found, such that the matrix $(\langle f_{i,\varepsilon}, B_\varepsilon e_{j,\varepsilon}\rangle)$ is approximately diagonal, then the diagonal of the latter matrix well approximates the singular values of B_ε.

Appendix E.

This last section contains some definitions and complementary computations used throughout Part II.

Part I. Discrete geometries on affine spaces

This first part has a foundational character: it is mainly concerned with definitions and basic properties of de Rham-type complexes, Hodge-type and Witten-type Laplacians in affine space. The point is that the geometry we consider on the latter is *not* the classical geometry induced by a scalar product on the tangent space, but the geometry determined by a reversible Markov jump process. For simplicity we limit ourselves to discrete processes, i.e. those which are constrained to move on a lattice, but the formalism is presented in a way which lends itself to straightforward generalizations. We have chosen to consequently give a coordinate-free representation, enlightnening the geometric content of the considered objects, which would be hidden in a more concrete development in the coordinate space $\mathbb{R}^n$. In this part no scaling limits appear.

1. A generalized tensor algebra

We list in this section some basic terminology and notation that will be used throughout this work.

The set of natural numbers is denoted by $\mathbb{N}_*$ if 0 is excluded and by $\mathbb{N}_0$ otherwise.

Let V be a real vector space of dimension $n \in \mathbb{N}_*$. Its generic elements are denoted by v, w. For the elements of the p-th Cartesian product V^p we use the notation $\mathbf{v} := (v_1, \dots, v_p)$.

Given $\pi \in \mathcal{P}_p$, the set of permutations of $\{1, \dots, p\}$, and $\mathbf{v} \in V^p$ we write $\pi\mathbf{v} := (v_{\pi_1}, \dots, v_{\pi_p})$, where π_j is the image of j under π. Similarly, for $\mathbf{s} := (s_1, \dots, s_p) \in \{-1, 1\}^p$ and $\wp := (\pi, \mathbf{s}) \in \mathcal{P}_p^{\mathrm{sign}} := \mathcal{P}_p \times \{-1, 1\}^p$ (the set of signed permutations of p elements), we let $\mathbf{sv} := (s_1 v_1, \dots, s_p v_p)$ resp. $\wp\mathbf{v} := (s_1 v_{\pi_1}, \dots, s_p v_{\pi_p})$. Moreover $\mathrm{sign}(\mathbf{s}) := s_1 \cdots s_p$ and $\mathrm{sign}(\wp) := \mathrm{sign}(\pi)\,\mathrm{sign}(\mathbf{s})$.

The basic space considered throughout this work is an affine space M with underlying real vector space V of fixed dimension $n \in \mathbb{N}_*$. The action of $v \in V$ on a point $\zeta \in M$ is a point in M denoted as usual by $\zeta + v$. For $\mathbf{v} \in V^p$ and $\zeta \in M$ we define

$$\zeta + \mathbf{v} := \zeta + v_1 + \cdots + v_p \quad .$$

We shall refer later to this situation and notation shortly with the phrase "M is an n-dimensional affine space".

On M the canonical smooth structure inherited from V is considered. The classical "tangential" or infinitesimal point of view on smooth manifolds leads to the notion of tensor fields over the tangent bundle

$$TM \ := \ \bigsqcup_{\zeta \in M} T_\zeta M \quad ,$$

with $T_\zeta M$ denoting the tangent space of M at ζ.

Since M is affine, there are of course canonical identifications: $T_\zeta M \simeq V$ for every $\zeta \in M$ and $TM \simeq M \times V$. Despite of this it is convenient in the present context to clearly distinguish between $T_\zeta M$ and V, reflecting their distinct physical interpretation: the former describes possible infinitesimal displacements of a particle, the latter possible jumps (or finite displacements).

The following definitions of this section attach to the trivial bundle $M \times V$ a tensor algebra tailored to the forementioned physical interpretation of V. The new tensor algebra is a Fock-type algebra. With the identification $T_\zeta M \simeq V$ it can be seen as an extension of the usual tensor algebra obtained by dropping the linearity assumption.

The idea behind the proposed algebraic formalism stems from some simple considerations on cubical cells. This underlying geometric picture is sketched briefly in the next subsection. We shall refer to it occasionally for various geometric interpretations, but it is not strictly necessary for the following development.

Excursus on p-cells.

Let M be an n-dimensional affine space and let $p \in \mathbb{N}_0$. A **p-cell** in M is a set of 2^p not necessarily distinct points $\zeta_1, \ldots, \zeta_{2^p} \in M$, called the vertices of the cell, satisfying the following property: there exist $\mathbf{v} \in V^p$ and an enumeration $\mathbf{s}^{(1)}, \ldots, \mathbf{s}^{(2^p)}$ of the elements of $\{-1, 1\}^p$ such that

$$\zeta_j \ = \ \zeta_1 \ + \ \frac{1}{2} \sum_{k=1}^{p} \left(v_k + s_k^{(j)} v_k\right) \quad . \tag{1.1}$$

We call a p-cell **nondegenerate** if all its vertices are distinct[20] and **degenerate** otherwise. Observe that a p-cell is nondegenerate if and only if all the v_k's can be taken different from zero and such that for $k \neq l$ both $v_k \neq v_l$ and $v_k \neq -v_l$ hold.

All the possible orderings of the points of a nondegenerate p-cell, $p \geq 1$, are divided into two equivalence classes by the equivalence relation given by the sign of a permutation. An orientation on a nondegenerate p-cell is a choice of one of this equivalence classes and an **oriented p-cell** is a nondegenerate p-cell together with an orientation. Observe that for a 0-cell, i.e. a point, there is just one possible orientation. Thus every 0-cell is canonically oriented, no change of orientation is possible, and there is no distinction between oriented and non-oriented 0-cells. By convention degenerate p-cells are included among the oriented p-cells assigning to them both possible orientations. This means that a change of orientation leaves degenerate p-cells invariant.

Clearly the representation of p-cells given in (1.1) is not unique. Therefore it is not very handy to describe with it elementary operations one would like to perform on (oriented) cells. To facilitate algebraic manipulations it is convenient to change parametrization. To this purpose observe that a couple $(\zeta, \mathbf{v}) \in M \times V^p$ describes a p-cell $\{\zeta_1, \ldots, \zeta_{2^p}\}$ by taking an arbitrary enumeration $\mathbf{s}^{(1)}, \ldots, \mathbf{s}^{(2^p)}$ of the elements of $\{-1, 1\}^p$ and letting for $j = 1, \ldots, 2^p$

$$\zeta_j \;:=\; \zeta \;+\; \frac{1}{2} \sum_{k=1}^{p} s_k^{(j)} v_k$$

(i.e. ζ is the "center" of the cell). Plainly this cell does not depend on the chosen enumeration $\mathbf{s}^{(1)}, \ldots, \mathbf{s}^{(2^p)}$ nor on the ordering of the v_k's. Moreover every p-cell can be described in this way. It follows that the set of cells is in bijection with the set $M \times V^p / \sim_{\mathcal{N}}$, where the equivalence relation $\sim_{\mathcal{N}}$ in V^p is given by

$$\mathbf{v} \;\sim_{\mathcal{N}}\; \mathbf{w} \quad \text{if} \quad \exists \wp \in \mathcal{P}_p^{\text{sign}} \quad \text{s.t. } \mathbf{v} \;=\; \wp \mathbf{w} \;. \tag{1.2}$$

The cell corresponding to $(\zeta, [\mathbf{v}]) \in M \times V^p / \sim_{\mathcal{N}}$ is denoted by $\mathrm{Cell}(\zeta, [\mathbf{v}])$. Observe that $\mathrm{Cell}(\zeta, [\mathbf{v}])$ is nondegenerate if and only if for the representative $\mathbf{v}$ (and therefore for every other representative) all the v_k's are different from zero and such that for $k \neq l$ both $v_k \neq v_l$ and $v_k \neq -v_l$ hold.

[20]Observe that in general even a nondegenerate p-cell is not p-dimensional, where the dimension of a cell is defined as the dimension of its convex hull. This happens only under the stronger condition that the v_k's above can be chosen linearly independent.

Similarly there is a canonical bijection between the set of oriented cells and $M \times V^p / \sim_{\mathcal{O}}$, with $\sim_{\mathcal{O}}$ defined via

$$\mathbf{v} \;\sim_{\mathcal{O}}\; \mathbf{w} \quad \text{if} \quad \exists \wp \in \mathcal{P}_p^{\text{sign}} \quad \text{with} \quad \text{sign}(\wp) = 1 \quad \text{s.t. } \mathbf{v} \;=\; \wp \mathbf{w} \;\; . \tag{1.3}$$

Given $(\zeta, [\mathbf{v}]) \in M \times V^p / \sim_{\mathcal{O}}$ we denote by $\text{Cell}_{\text{sign}}(\zeta, [\mathbf{v}])$ the oriented cell given by the points

$$\zeta_j \;:=\; \zeta \;+\; \frac{1}{2} \sum_{k=1}^{p} s_k^{(j)} v_k \qquad \text{for} \quad j = 0, \ldots, 2^p \quad ,$$

with $\mathbf{s}^{(1)}, \ldots, \mathbf{s}^{(2^p)}$ following the lexicographic order in $\{-1, 1\}^p$ and orientation determined by the ordering $(\zeta_1, \ldots, \zeta_{2^p})$ if the cell is nondegenerate.

Note that with the canonical identification $T_\zeta M \simeq V$, where $T_\zeta M$ denotes the tangent space of M at $\zeta \in M$, one can think of a $\text{Cell}(\zeta, [\mathbf{v}])$ as an infinitesimal cell for every $(\zeta, \mathbf{v}) \in M \times V^p$.

Recall that a classical (covariant) p-tensor on M is just a smooth function $\alpha : M \times V^p \to \mathbb{R}$, which is p-multilinear in V. A particular important subspace of the space of p-tensors is the one of antisymmetric p-tensors, the so-called forms. They satisfy for every $\pi \in \mathcal{P}_p$, $\zeta \in M$ and $\mathbf{v} \in V^p$

$$\alpha(\zeta, \pi \mathbf{v}) \;=\; \text{sign}(\pi)\; \alpha(\zeta, \mathbf{v}) \;\; .$$

By linearity it follows that also for $\wp \in \mathcal{P}_p^{\text{sign}}$

$$\alpha(\zeta, \wp \mathbf{v}) \;=\; \text{sign}(\wp)\; \alpha(\zeta, \mathbf{v}) \;\; .$$

A p-form α can therefore be thought of as a function on oriented *infinitesimal* p-cells, which changes sign by changing orientation of the cell.[21]

The choice of an Euclidean scalar product - or, equivalently, the choice of a Brownian motion - gives a geometry on M which is completely described by means of infinitesimal displacements. In this case the usual tensors are the natural objects to consider. On the other hand, in presence of a richer geometry arising from displacements (jumps) that can happen at every finite length, the linearity condition on the tensors may be too restrictive.[22] In the next subsection we introduce a notation to describe the algebra of tensors obtained by dropping the linearity condition.

[21] An analogous interpretation holds for a symmetric tensor: it is essentially a function on infinitesimal (nonoriented) cells.

[22] A fortiori tensors are not suitable if the underlying space is discrete. In this case there is no notion of tangent vector space available since *only* finite displacements are allowed.

The algebra of p-functions on M.

Recall that M is an affine space with underlying real vector space V of dimension $n \in \mathbb{N}_0$. For $p \in \mathbb{N}_0$ let

$$F(M \times V^p) := \mathbb{R}^{M \times V^p} \quad ,$$

the set of real functions on $M \times V^p$. We shall refer to it as the **space of p-functions** on M. Observe that $F(M \times V^p)$ is a (infinite dimensional) vector space.

The direct sum $\mathcal{F}(M \times V) := \oplus_{p=0}^{\infty} F(M \times V^p)$ is a graded algebra with respect to the (pointwise) tensor product

$$\otimes : F(M \times V^p) \times F(M \times V^{p'}) \to F(M \times V^{p+p'})$$

defined via

$$\alpha \otimes \beta(\zeta, (\mathbf{v}, \mathbf{w})) \;:=\; \alpha(\zeta, \mathbf{v})\; \beta(\zeta, \mathbf{w}) \quad .$$

Observe that $\otimes$ is not commutative. In the language of graded algebras a p-function is a homogeneous element of degree p in $\mathcal{F}(M \times V)$.

We are interested mainly in the two subspaces of $\mathcal{F}(M \times V)$ given by the alternating resp. symmetric functions over V. Here an $\alpha \in F(M \times V^p)$ is called **alternating** (or antisymmetric) if for every $\wp \in \mathcal{P}_p^{\mathrm{sign}}$

$$\alpha(\zeta, \wp\mathbf{v}) \;=\; \mathrm{sign}(\wp)\; \alpha(\zeta, \mathbf{v}) \quad . \tag{1.4}$$

On the other hand we call an $\alpha \in F(M \times V^p)$ **symmetric** if for every $\wp \in \mathcal{P}_p^{\mathrm{sign}}$

$$\alpha(\zeta, \wp\mathbf{v}) \;=\; \alpha(\zeta, \mathbf{v}) \quad . \tag{1.5}$$

Observe that if α is alternating, then automatically for every $\zeta \in M$ and every $\mathbf{v} \in V^p$ with the property that $v_i = v_j$ or $v_i = -v_j$ for some $i \neq j$ or $v_i = 0$ for some i

$$\alpha(\zeta, \mathbf{v}) = 0 \quad . \tag{1.6}$$

We denote by $F_a(M \times V^p) \subset F(M \times V^p)$ the vector subspace of alternating p-functions and define $\mathcal{F}_a(M \times V) := \oplus_{p=0}^{\infty} F_a(M \times V^p)$. The latter is not a subalgebra of $\mathcal{F}(M \times V)$, but it is again a graded algebra itself with the (pointwise) wedge product $\wedge$ defined for $\alpha \in F_a(M \times V^p)$, $\beta \in F_a(M \times V^{p'})$ via

$$\alpha \wedge \beta \;:=\; \mathrm{Alt}^{(p+p')}\; \alpha \otimes \beta \quad .$$

Here for $p \in \mathbb{N}_0$, $\mathrm{Alt}^{(p)} : F(M \times V^p) \to F_a(M \times V^p)$ denotes the **alternating operator** defined as

$$\mathrm{Alt}^{(p)}\, \alpha(\zeta, \mathbf{v}) \ := \ \frac{1}{p!2^p} \sum_{\wp \in \mathcal{P}_p^{\mathrm{sign}}} \mathrm{sign}(\wp)\ \alpha(\zeta, \wp\mathbf{v}) \quad .$$

Analogous considerations hold mutatis mutandis for the space of symmetric p-functions $F_s(M \times V^p) \subset F(M \times V^p)$. We repeat them to fix the notation. $\mathcal{F}_s(M \times V) := \oplus_{p=0}^{\infty} F_s(M \times V^p)$ is a graded algebra with the symmetrized tensor product $\odot$ defined for $\alpha \in F_s(M \times V^p)$, $\beta \in F_s(M \times V^{p'})$ via

$$\alpha \odot \beta \ := \ \mathrm{Sym}^{(p+p')}\, \alpha \otimes \beta \quad .$$

Here for $p \in \mathbb{N}_0$, $\mathrm{Sym}^{(p)} : F(M \times V^p) \to F_s(M \times V^p)$ denotes the **symmetrizing operator** defined as

$$\mathrm{Sym}^{(p)}\, \alpha(\zeta, \mathbf{v}) \ := \ \frac{1}{p!2^p} \sum_{\wp \in \mathcal{P}_p} \alpha(\zeta, \wp\mathbf{v}) \quad .$$

Observe that $\wedge$ is anticommutative , while $\odot$ is commutative.

We intentionally avoid at this point to introduce topologies on $\mathcal{F}(M \times V)$ or even on $F(M \times V^p)$. This will be the main topic of Section 3. Nevertheless we point out that by introducing a measure on $M \times V$, the corresponding L^2 space would yield a construction reminiscent of the Fock algebra appearing in Quantum Field Theory. Then $F_a(M \times V^p)$ (resp. $F_s(M \times V^p)$) corresponds to the space of fermionic (resp. bosonic) states with p-particles.

Sometimes it is convenient to view the space of p-functions not as the space of real functions on $M \times V^p$ but as the space of functions from M to $\mathbb{R}^{V^p}$. The latter can be seen as the space of p-functions obtained by fixing a base point $\zeta \in M$. In this context we shall use the notation $\mathbb{R}_a^{V^p}$ to denote the space of antisymmetric real functions on V^p. More precisely $\omega \in \mathbb{R}^{V^p}$ is by definition in $\mathbb{R}_a^{V^p}$ if for every $\wp \in \mathcal{P}_p^{\mathrm{sign}}$

$$\omega(\wp\mathbf{v}) \ = \ \mathrm{sign}(\wp)\ \omega(\mathbf{v}) \quad . \tag{1.7}$$

In the symmetric case the symbol $\mathbb{R}_s^{V^p}$ is used. Moreover we shall write for an $\alpha \in F(M \times V^p)$,

$$\alpha_{\mathbf{v}}(\zeta) \ := \ \alpha(\zeta, \mathbf{v})$$

and denote for every fixed $\mathbf{v} \in V^p$ by $\alpha_{\mathbf{v}}$ the function $\zeta \mapsto \alpha(\zeta, \mathbf{v})$.

Remark 1.1.

The discussion on cells of the previous subsection gives the following geometric intepretation of $F_a(M \times V^p)$ resp. $F_s(M \times V^p)$ for $p \in \mathbb{N}_*$: an alternating p-function is a function on oriented p-cells which changes sign by changing orientation; in particular it is 0 *on degenerate p-cells which by convention are invariant under change of orientation. A symmetric p-function is a function on cells. For $p = 0$, p-functions are just functions on M and there is no distinction between antisymmetric and symmetric functions.*

Linear and smooth p-functions.

Let $p \in \mathbb{N}_0$. We shall consider in particular the subspace $F_{\text{lin}}(M \times V^p)$ of $F(M \times V^p)$, consisting of functions which are multilinear with respect to V^p. More precisely, an $\alpha \in F(M \times V^p)$ is by definition an element of $F_{\text{lin}}(M \times V^p)$ if for every $\zeta \in M$, $\mathbf{v} \in V^{p-1}$ and every $j = 1, \ldots, p$ the function

$$w \mapsto \alpha(\zeta, v_1, \ldots, v_{j-1}, w, v_j, \ldots, v_p)$$

is linear over V.

If we restrict to antisymmetric (resp. symmetric) multilinear p-functions we shall use the symbols $F_{a,\text{lin}}(M \times V^p)$ (resp. $F_{s,\text{lin}}(M \times V^p)$).

For the (finite dimensional) subspace of multilinear elements of $\mathbb{R}^{V^p}$ we use the standard notation T^pV^*, whose antisymmetric and symmetric versions are denoted by $T^p_aV^*$ and $T^p_sV^*$.

Another subspace of $F(M \times V^p)$ which will be considered throughout is the space of smooth p-functions. More precisely, we shall denote by $C^\infty(M; \mathbb{R}^{V^p})$ the set of functions $\alpha \in F(M \times V^p)$ s.t. $\zeta \mapsto \alpha(\zeta, \mathbf{v})$ is infinitely many times differentiable for every $\mathbf{v} \in V^p$. Here, restricting to antisymmetric (resp. symmetric) smooth p-functions we shall use the symbols $C^\infty(M; \mathbb{R}^{V^p}_a)$ (resp. $C^\infty(M; \mathbb{R}^{V^p}_s)$). Similarly we write $C^\infty(M; T^pV^*)$, $C^\infty(M; T^p_aV^*)$ and $C^\infty(M; T^p_sV^*)$ in the multilinear cases.

Observe that via the canonical identification $T_\zeta M \simeq V$ an $\alpha \in C^\infty(M; T^pV^*)$ can be identified with a classical covariant linear p-tensor on the tangent bundle of M.

2. The exterior difference operator δ

Let M be an affine space with underlying real vector space V of dimension n. In this section we shall introduce some basic (formal) operators acting on the algebra $\mathcal{F}(M \times V)$. In particular an exterior difference operator is defined on the antisymmetric algebra $\mathcal{F}_a(M \times V)$ (see Definition 2.5 below), which is the analogue of the De Rham exterior differential on classical forms.

We use here the following notation to describe the operations of removing, adding and exchanging vectors given an element $\mathbf{v}$ of the Cartesian product V^p, $p \in \mathbb{N}_0$.

- For every $w \in V$ and every $j \in \{0, \cdots, p\}$ define $\mathbf{v}_{+(w,j)} \in V^{p+1}$ by
$$\mathbf{v}_{+(w,j)} = (v_1, \ldots, v_{j-1}, w, v_{j+1}, \ldots, v_p) \quad .$$
- For $j = \{1, \cdots, p\}$ define $\mathbf{v}_{-(j)} \in V^{p-1}$ by
$$\mathbf{v}_{-(j)} = (v_1, \cdots, v_{j-1}, v_{j+1}, \cdots, v_p) \quad .$$
- For every $w \in V$, every $j \in \{0, \cdots, p\}$ and $l \in \{1, \cdots, p+1\}$ define $\mathbf{v}_{\substack{+(w,j)\\-(l)}} \in V^p$ by
$$\mathbf{v}_{\substack{+(w,j)\\-(l)}} := \hat{\mathbf{v}}_{-(l)} \quad ,$$
with $\hat{\mathbf{v}} := \mathbf{v}_{+(w,j)}$. Similarly, for every $w \in V$, every $j \in \{0, \cdots, p+1\}$ and $l \in \{1, \cdots, p\}$ define $\mathbf{v}_{\substack{-(l)\\+(w,j)}} \in V^p$ by
$$\mathbf{v}_{\substack{-(l)\\+(w,j)}} := \hat{\mathbf{v}}_{+(w,j)} \quad ,$$
with $\hat{\mathbf{v}} := \mathbf{v}_{-(l)}$

Definition 2.1 (Translation, difference and sum operators).
Let M be an n-dimensional affine space. For every $p \in \mathbb{N}_0$ define the formal operators $\mathcal{T}^{(p)}, \mathcal{T}^{\star,(p)}, \mathcal{D}^{(p)}, \mathcal{D}^{\star,(p)}, \mathcal{S}^{(p)} : F(M \times V^p) \to F(M \times V^{p+1})$ respectively by

$$\mathcal{T}^{(p)}\alpha\ (\zeta, \mathbf{v}) \ := \ \alpha(\zeta + v_1/2, \mathbf{v}_{-(1)}) \quad , \quad \mathcal{T}^{\star,(p)}\alpha\ (\zeta, \mathbf{v}) \ := \ \alpha(\zeta - v_1/2, \mathbf{v}_{-(1)}) \quad ,$$
$$\mathcal{D}^{(p)} \ := \ \mathcal{T}^{(p)} - \mathcal{T}^{\star,(p)} \quad , \quad \mathcal{D}^{\star,(p)} \ := \ \mathcal{T}^{\star,(p)} - \mathcal{T}^{(p)} \quad ,$$
$$\mathcal{S}^{(p)} \ := \ \frac{1}{2}[\ \mathcal{T}^{(p)} + \mathcal{T}^{\star,(p)}\ ] \quad .$$

Observe that

$$\mathcal{D}^{(p)}\alpha\ (\zeta,\mathbf{v})\ =\ \alpha(\zeta+v_1/2,\mathbf{v}_{-(1)})\ -\ \alpha(\zeta-v_1/2,\mathbf{v}_{-(1)})\ \ ,$$

$$\mathcal{S}^{(p)}\alpha\ (\zeta,\mathbf{v})\ =\ \frac{1}{2}\alpha(\zeta+v_1/2,\mathbf{v}_{-(1)})\ +\ \frac{1}{2}\alpha(\zeta-v_1/2,\mathbf{v}_{-(1)})$$

and that

$$\mathcal{D}^{\star,(p)} = -\mathcal{D}^{(p)}\ \ .$$

The choice of the first entry as acting variable in the above definition is just a convention to fix the notation. Of course any other choice could have been made for developing the following concepts. We shall also consider for every $w \in V$ the operators $T_w^{(p)}, T_w^{\star,(p)} : F(M \times V^p) \to F(M \times V^p)$ given for $\alpha \in F(M \times V^p)$, $(\zeta,\mathbf{v}) \in M \times V^p$ by

$$\mathcal{T}_w^{(p)}\alpha\ (\zeta,\mathbf{v})\ :=\ \mathcal{T}^{(p)}\alpha\ (\zeta,w,\mathbf{v})\ \ ,\ \ \mathcal{T}_w^{\star,(p)}\alpha\ (\zeta,\mathbf{v})\ :=\ \mathcal{T}^{\star,(p)}\alpha\ (\zeta,w,\mathbf{v})\ \ . \tag{2.1}$$

The operators $\mathcal{D}_w^{(p)}, \mathcal{D}_w^{\star,(p)}, \mathcal{S}_w^{(p)} : F(M \times V^p) \to F(M \times V^p)$ are defined analogously.

The factor $\frac{1}{2}$ in the definition of $\mathcal{S}^{(p)}$ is chosen in order to normalize the following rule for the discrete differentiation of a pointwise product of p-functions.

Proposition 2.2 (Product rules for $\mathcal{D}^{(p)}$ and $\mathcal{S}^{(p)}$).
For every $p \in \mathbb{N}_0$ and $\alpha,\beta \in F(M \times V^p)$

$$\mathcal{D}^{(p)}(\alpha\beta)\ =\ \mathcal{D}^{(p)}\alpha\ \ \mathcal{S}^{(p)}\beta\ +\ \mathcal{S}^{(p)}\alpha\ \ \mathcal{D}^{(p)}\beta$$

and

$$\mathcal{S}^{(p)}(\alpha\beta)\ =\ \mathcal{S}^{(p)}\alpha\ \ \mathcal{S}^{(p)}\beta\ -\ \frac{1}{4}\mathcal{D}^{(p)}\alpha\ \ \mathcal{D}^{(p)}\beta\ \ .$$

Proof. Dropping for simplicity the superscript (p) we have

$$\begin{aligned}\mathcal{D}(\alpha\beta)\ &=\ \mathcal{T}(\alpha\beta)\ -\ \mathcal{T}^\star(\alpha\beta)\ =\ \mathcal{T}\alpha\ \ \mathcal{T}\beta\ -\ \mathcal{T}^\star\alpha\ \ \mathcal{T}^\star\beta\ = \\ &=\ \frac{1}{2}\mathcal{T}\alpha\ \ \mathcal{T}\beta\ +\ \frac{1}{2}\mathcal{T}\alpha\ \ \mathcal{T}\beta\ -\ \frac{1}{2}\mathcal{T}\alpha\ \ \mathcal{T}^\star\beta\ +\ \frac{1}{2}\mathcal{T}\alpha\ \ \mathcal{T}^\star\beta\ + \\ &\quad -\frac{1}{2}\mathcal{T}^\star\alpha\ \ \mathcal{T}^\star\beta\ -\ \frac{1}{2}\mathcal{T}^\star\alpha\ \ \mathcal{T}^\star\beta\ +\ \frac{1}{2}\mathcal{T}^\star\alpha\ \ \mathcal{T}\beta - \frac{1}{2}\mathcal{T}^\star\alpha\ \ \mathcal{T}\beta\ = \\ &=\ \mathcal{D}\alpha\ \ \mathcal{S}\beta\ +\ \mathcal{S}\alpha\ \ \mathcal{D}\beta\ \ .\end{aligned}$$

An analogous computation yields the statement for $\mathcal{S}^{(p)}$. □

Let $k \in \mathbb{N}_*$. The k**-th translation, difference and sum operators**

$$\mathcal{T}^{k,(p)}, \mathcal{T}^{\star,k,(p)}, \mathcal{D}^{k,(p)}, \mathcal{D}^{\star,k,(p)}, \mathcal{S}^{k,(p)} : F(M \times V^p) \to F(M \times V^{p+k})$$

are obtained by k-times application of the respective operators. So for example

$$\mathcal{T}^{k,(p)} \ := \ \mathcal{T}^{(p+k-1)} \dots \mathcal{T}^{(p)} \quad .$$

We shall also use for every $\mathbf{w} \in V^k$ the symbols $\mathcal{T}_{\mathbf{w}}^{k,(p)}, \mathcal{T}_{\mathbf{w}}^{\star,k,(p)}, \mathcal{D}_{\mathbf{w}}^{k,(p)}, S_{\mathbf{w}}^{k,(p)}$ defined in the obvious way starting from (2.1). So for example

$$\mathcal{D}_{\mathbf{w}}^{k,(p)} \ := \ \mathcal{D}_{w_1}^{(p)} \dots \mathcal{D}_{w_k}^{(p)} \quad .$$

If $w_1 = w_2 = \cdots = w_k = w$ we shall also write $\mathcal{T}_w^{k,(p)}$, etc.

Observe that for each $\mathbf{w} \in V^k$

$$\mathcal{D}_{\mathbf{w}}^{k,(p)} \ = \sum_{\mathbf{s} \in \{-1,1\}^k} \operatorname{sign}(\mathbf{s}) \ \mathcal{T}_{\mathbf{sw}}^{k,(p)} \tag{2.2}$$

and

$$S_{\mathbf{w}}^{k,(p)} \ = \ \frac{1}{2} \sum_{\mathbf{s} \in \{-1,1\}^k} \mathcal{T}_{\mathbf{sw}}^{k,(p)} \quad . \tag{2.3}$$

In particular

$$\mathcal{D}_{w_1,w_2}^{2,(p)} \ = \ \mathcal{T}_{w_1}^{(p)} \mathcal{T}_{w_2}^{(p)} - \mathcal{T}_{w_1}^{(p)} \mathcal{T}_{w_2}^{\star,(p)} - \mathcal{T}_{w_1}^{\star,(p)} \mathcal{T}_{w_2}^{(p)} + \mathcal{T}_{w_1}^{\star,(p)} \mathcal{T}_{w_2}^{\star,(p)} \tag{2.4}$$

and, taking second differences on the diagonal gives:

$$\mathcal{D}_{w,w}^{2,(p)} \alpha \ (\zeta, \mathbf{v}) \ = \ \alpha(\zeta + w, \mathbf{v}) + \alpha(\zeta - w, \mathbf{v}) - 2\alpha(\zeta, \mathbf{v}) \quad . \tag{2.5}$$

Remark 2.3. *It follows from (2.2) and (2.3) that for each $k \in \mathbb{N}_*$, $p \in \mathbb{N}_0$, $\alpha \in F(M \times V^p)$, $\wp = (\pi, \mathbf{s}) \in \mathcal{P}_k^{\mathrm{sign}}$ and $\mathbf{w} \in V^k$, we have*

$$\mathcal{D}_{\wp \mathbf{w}}^{k,(p)} \ = \ \operatorname{sign}(\mathbf{s}) \ \mathcal{D}_{\mathbf{w}}^{k,(p)}$$

and similarly

$$\mathcal{S}_{\wp \mathbf{w}}^{k,(p)} \ = \ \mathcal{S}_{\mathbf{w}}^{k,(p)} \quad .$$

In particular, for $\pi \in \mathcal{P}_k$,

$$\mathcal{D}^{k,(p)} \alpha(\zeta, \pi \mathbf{w}, \mathbf{v}) \ = \ \mathcal{D}^{k,(p)} \alpha(\zeta, \mathbf{w}, \mathbf{v}) \quad , \tag{2.6}$$

which expresses the symmetry of the difference operator in the acting variables.

For every $k \in \mathbb{N}_*$ the direct sums $\oplus_{p=0}^{\infty}\mathcal{T}^{k,(p)}$, $\oplus_{p=0}^{\infty}\mathcal{T}^{\star,k,(p)}$, $\oplus_{p=0}^{\infty}\mathcal{D}^{k,(p)}$, $\oplus_{p=0}^{\infty}\mathcal{D}^{\star,k,(p)}$ and $\oplus_{p=0}^{\infty}\mathcal{S}^{k,(p)}$ are denoted respectively by $\mathcal{T}^k$, $\mathcal{T}^{\star,k}$, $\mathcal{D}^k$, $\mathcal{D}^{\star,k}$ and $\mathcal{S}^k$. The superscript k is dropped in the case $k = 1$.

Remark 2.4. *Let for $k, p \in \mathbb{N}_0$, $\alpha \in C^\infty(M; \mathbb{R}^{V^p})$ and $\bar{\zeta}, \mathbf{v} \in M \times V^p$ the function $V \ni w \mapsto \nabla_w^{k,(p)}\alpha_{\mathbf{v}}\ (\bar{\zeta}) := \nabla^{k,(p)}\alpha\ (\bar{\zeta}, w, \mathbf{v})$ be the k-th differential of $\alpha_{\mathbf{v}}$ at the point $\bar{\zeta}$. Observe that $\nabla^{(p)} := \nabla^{1,(p)}$, restricted on the space $C^\infty(M; \mathbb{R}^{V^p})$ of smooth linear tensors, is the usual covariant derivative on an affine space. A formal Taylor series expansion gives*

$$\mathcal{D}_w^{(p)}\alpha\ (\zeta, \mathbf{v}) \sim \sum_{\substack{k=1 \\ k\ odd}}^{\infty} \frac{\nabla_w^{k,(p)}\alpha(\zeta, \mathbf{v})}{k!2^{k-1}} \quad .$$

Since the first term in the expansion equals $\nabla^{(p)}$, the difference operator can be seen as a discrete version of the covariant derivative acting on tensors. For the sum operator we have

$$\mathcal{S}_w^{(p)}\alpha(\zeta, \mathbf{v}) \sim \sum_{\substack{k=0 \\ k\ even}}^{\infty} \frac{\nabla_w^{k,(p)}\alpha(\zeta, \mathbf{v})}{k!2^{k}} \quad .$$

Here the first term is the identity operator. In other terms the sum operator becomes trivial in linear approximation.

Next we define an analogue of the de Rham exterior differential which will play a major role in the sequel.

Definition 2.5 (Exterior difference operator and symmetric sum operator).

Let M be an n-dimensional affine space. For $p \in \mathbb{N}_0$ we define

- *the formal exterior difference operators $\delta^{(p)} : F_a(M \times V^p) \to F_a(M \times V^{p+1})$ by*

$$\delta^{(p)} \ := \ (p+1)\,\mathrm{Alt}^{(p+1)}\ \mathcal{D}^{(p)}$$

  and set $\delta := \oplus_{p=0}^{\infty}\delta^{(p)}$.
- *the formal symmetric sum operators $\sigma^{(p)} : F_s(M \times V^p) \to F_s(M \times V^{p+1})$ by*

$$\sigma^{(p)} \ := \ (p+1)\,\mathrm{Sym}^{(p+1)}\,\mathcal{S}^{(p)}$$

  and set $\sigma := \oplus_{p=0}^{\infty}\sigma^{(p)}$

From the definition it follows that $\delta^{(p)}$ has the representation

$$\delta^{(p)}\alpha\ (\zeta, \mathbf{v}) = \sum_{l=1}^{p+1} (-1)^{l+1}\ \mathcal{D}^{(p)}\alpha(\zeta, v_l, \mathbf{v}_{-(l)})\quad . \tag{2.7}$$

Proposition 2.6 (**Complex property for** δ**).**
For every $p \in \mathbb{N}_0$

$$\delta^{(p+1)}\delta^{(p)} \equiv 0\quad .$$

Proof. As in the infinitesimal case, this is a consequence of the "Schwarz Lemma",

$$\mathcal{D}^{2,(p)}_{w_1,w_2} = \mathcal{D}^{2,(p)}_{w_2,w_1}\quad ,$$

valid for every $(w_1, w_2) \in V^2$ as remarked in (2.6). In fact for $\zeta \in M$, $\mathbf{v} \in V^{p+2}$, observing that the j-th vector appearing in $\mathbf{v}_{-(l)}$ is v_j if $j < l$ and is v_{j+1} if $j \geq l$ and using the notation $\mathbf{v}_{-(l,j)} := \left(\ \mathbf{v}_{-(l)}\ \right)_{-(j)}$ we have

$$\delta^{(p+1)}\delta^{(p)}\ \alpha(\zeta, \mathbf{v}) =$$

$$= \sum_{l=2}^{p+2}\sum_{j=1}^{l-1} (-1)^{l+j}\ \mathcal{D}^{2,(p)}_{v_l,v_j}\alpha\ (\zeta, \mathbf{v}_{-(l,j)}) + \sum_{l=1}^{p+1}\sum_{j=l}^{p+1} (-1)^{l+j}\ \mathcal{D}^{2,(p)}_{v_l,v_{j+1}}\alpha\ (\zeta, \mathbf{v}_{-(j+1,l)}) =$$

$$= \sum_{l=2}^{p+2}\sum_{j=1}^{l-1} (-1)^{l+j}\ \mathcal{D}^{2,(p)}_{v_l,v_j}\alpha\ (\zeta, \mathbf{v}_{-(l,j)}) + \sum_{l=1}^{p+1}\sum_{j=l+1}^{p+2} (-1)^{l+j-1}\ \mathcal{D}^{2,(p)}_{v_l,v_j}\alpha\ (\zeta, \mathbf{v}_{-(j,l)}) =$$

$$= \sum_{l=2}^{p+2}\sum_{j=1}^{l-1} (-1)^{l+j}\ \left[\ \mathcal{D}^{2,(p)}_{v_l,v_j}\alpha\ (\zeta, \mathbf{v}_{-(l,j)}) - \mathcal{D}^{2,(p)}_{v_j,v_l}\alpha\ (\zeta, \mathbf{v}_{-(l,j)})\ \right] =$$

$$= 0\quad .$$

$\square$

Remark 2.7. *The operator* δ *can be given a simple geometric interpretation in terms of oriented cells: recall (1.3) and let* $(\zeta, [\mathbf{v}]) \in M \times V^{p+1}/\sim_{\mathcal{O}}$*. For simplicity we assume that* $\mathrm{Cell}_{\mathrm{sign}}(\zeta, [\mathbf{v}])$ *is nondegenerate. In the degenerate case similar considerations as the following can be made, and the same conclusions will remain valid. The boundary of the convex hull of* $\mathrm{Cell}_{\mathrm{sign}}(\zeta, [\mathbf{v}])$*, denoted by* $\partial\,\mathrm{Cell}_{\mathrm{sign}}(\zeta, [\mathbf{v}])$*, is composed of convex hulls of* p*-cells,* $2(p+1)$

in number and oriented in the standard way using the outer normal. More precisely, we have

$$\partial\,\mathrm{Cell}_{\mathrm{sign}}(\zeta,[\mathbf{v}]) =$$

$$= \bigcup_{j=1}^{p+1} \left[\ (-1)^{j+1}\,\mathrm{Cell}_{\mathrm{sign}}(\zeta + v_j/2, [\mathbf{v}_{-(j)}])\ \cup\ (-1)^{j}\,\mathrm{Cell}_{\mathrm{sign}}(\zeta - v_j/2, [\mathbf{v}_{-(j)}])\ \right] \quad ,$$

where multiplying an oriented cell with -1 *amounts to a change of orientation*[23]*. Interpreting an* $\alpha \in F_a(M \times V^p)$ *as a function on oriented p-cells (see Remark 1.1), it follows that, for* $(\zeta, \mathbf{v}) \in M \times V^{p+1}$, $\delta^{(p)}\alpha(\zeta, \mathbf{v})$ *equals the sum of the values of* α *on* $\partial\,\mathrm{Cell}_{\mathrm{sign}}(\zeta, [\mathbf{v}])$*. Requiring that functions on cells are additive w.r.t. to the union, this fact can be written compactly as*

$$\delta\alpha = \alpha\partial \quad ,$$

which can be recognized as a version of the Stokes formula. Observe that for $p = 0$ *this recovers the usual meaning of the discrete differential of a function* $f : M \to \mathbb{R}$ *evaluated on an oriented* 1*-cell* $\{\zeta_1, \zeta_2\}$ *(an "edge") as the difference* $f(\zeta_2) - f(\zeta_1)$*.*

With the geometric interpretation just given the complex property translates to the obvious statement that the boundary of a boundary of a cell vanishes.

[23] Here, to cover also the case $p = 0$, we adopt the convention that a 0-cell has two possible orientations given by ± 1.

3. Discrete geometries and lattice graphs

A (euclidean) geometric structure can be introduced in the affine space M by fixing a scalar product on the underlying vector space V or - equivalently - on V^*, the dual of V. This scalar product is then extended in a canonical way: first, for every $p \in \mathbb{N}_0$, to a scalar product on T^pV^*, the p-th tensor product of V^*, and then to square integrable sections of $F_{\text{lin}}(M \times V^p)$ by means of the induced (Riemannian) volume form. More precisely, given a scalar product $g : V^* \times V^* \to \mathbb{R}$, one defines for every $p \in \mathbb{N}_0$

$$\langle \alpha, \beta \rangle_g^{(p)} := \int_M g^p\Big(\alpha(\zeta, \cdot), \beta(\zeta, \cdot)\Big) \ \text{Vol}(d\zeta) \quad , \tag{3.1}$$

where $d\,\text{Vol}$ is the unique Haar measure (depending on g) assigning unitary measure to a parallelepide spanned by an orthonormal basis of V, g^p is the p-th tensor product of the given scalar product[24] g, and $\alpha, \beta \in L^2(M \times V^p, g) := \{\alpha \in F_{\text{lin}}(M \times V^p) : \zeta \mapsto \alpha(\zeta, \mathbf{v})$ is Borel measurable $\forall \mathbf{v} \in V^p$ and $\langle \alpha, \alpha \rangle_g^{(p)} < \infty\}$.

Such a geometry is homogeneous, in the sense that the metric tensor g is independent of the base point $\zeta \in M$. Moreover it is infinitesimal, in the sense that it is defined only on the linear tensor algebra.

The aim of this section is to introduce homogeneous geometric structures in M which take into account finite displacements, by assigning suitable scalar products on the full space $F(M \times V)$, containing also *nonlinear* 1-functions. These are extended in a canonical way to $F(M \times V^p)$ for every $p \in \mathbb{N}_0$. The set of this kind of geometries is much broader, since every finite geometry contains in particular an infinitesimal geometry. In this work the attention is restricted to discrete geometries corresponding to a finite number of admissible jumps, as introduced below. Inhomogeneous perturbations of discrete geometries wil be considered starting from Section 5.

We assume given as data an n-dimensional affine space M together with a symmetric measure μ on the underlying vector space V, endowed with

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[24] Recall that for $p \in \mathbb{N}_*$ g^p is a scalar product on $T^p(V^*)$, defined by setting for pure tensors

$$g^p(\alpha_1 \otimes \cdots \otimes \alpha_p, \beta_1 \otimes \cdots \otimes \beta_p) = g(\alpha_1, \beta_1) \dots g(\alpha_p, \beta_p) \tag{3.2}$$

and then extending by linearity. For $p = 0$ we define in formula (3.1) above $g^0\big(\alpha(\zeta), \beta(\zeta)\big) := \alpha(\zeta)\beta(\zeta)$. Observe that from (3.2) it follows that in particular

$$g^p(\alpha_1 \wedge \cdots \wedge \alpha_p, \beta_1 \wedge \cdots \wedge \beta_p) = \frac{1}{p!} \det\big(g(\alpha_i, \beta_j)\big)_{i,j} \quad .$$

the canonical Borel sigma-algebra. The symmetry condition means that $\mu(S) = \mu(-S)$ for every Borel set S of M. We assume furthermore that μ has finite support, i.e. that μ is a finite linear combination of Dirac measures. The set

$$E = \operatorname{supp} \mu \setminus \{0\}$$

will be called the **set of admissible jumps** in M and μ can be thought of as a weight attached to each admissible jump.[25] By the symmetry of μ it follows that also E is symmetric, i.e. $v \in E$ implies $-v \in E$. In particular the cardinality of E is even.

For simplicity we assume from the outset that E generates a **lattice** Γ in V although at least some parts of the following discussion could be treated in a more general setting.

Recall that a lattice Γ in V is by definition a discrete subgroup of V with finite covolume. In our particular case of V being a vector space this is equivalent to asking that Γ is a discrete subgroup which spans the whole V.

We call a symmetric measure μ on V which has finite, lattice generating support for short a **(homogeneous) discrete geometry**. Given a discrete geometry we denote always by E the associated set of admissible jumps and by Γ the lattice generated by E. The **size** of a discrete geometry is defined as half the cardinality of E and denoted by N.

Remark 3.1. *The simplest examples of discrete geometries are those of size n, which are obtained by taking*

$$E = \{e_1, \ldots, e_n, -e_1, \ldots, -e_n\} \quad ,$$

where $e_1, \ldots, e_n$ form a basis of V, and by taking as μ the delta measure on the set E:

$$\mu(\{v\}) \;=\; 1$$

if $v \in E$, and $\mu(S) = 0$ if $S \cap E = \emptyset$. We refer to discrete geometries of size n also as **(simple) nearest neighbour geometries**. *Observe that the set E corresponding to an arbitrary discrete geometry must contain necessarily n independent vectors and their opposites. So the minimal size of a discrete geometry is n. On the other hand, as is well known, a finite symmetric subset of V with cardinality $2N > 2n$ and containing n independent vectors does not necessarily generate a lattice. A simple counterexample is $E = \{1, \sqrt{2}, -1, -\sqrt{2}\}$ for $n = 1$.*

[25] The value of μ in 0 will play no role in the sequel and is defined only for notational convenience.

Given an n-dimensional affine space M with discrete geometry μ, consider the set M/Γ consisting of the equivalence classes of the equivalence relation $\sim_\Gamma$ defined by

$$\zeta \sim_\Gamma \zeta' \ \text{ if } \ \zeta - \zeta' \in \Gamma \quad .$$

To each $\Lambda \in M/\Gamma$ can be given canonically the structure of an undirected weighted graph, denoted by Λ_μ, which is embedded in M. The vertices of Λ_μ are by definition the elements of the chosen equivalence class Λ. A pair $\{\zeta, \eta\}$ of vertices is an edge if and only if there exists an $e \in E$ such that $\zeta = \eta + e$. The weight of this edge is defined to be $\mu(\{e\})$. We call a graph Λ_μ obtained in this way briefly a **lattice graph** in M associated to the given discrete geometry μ. The letter Λ is used to denote the set of its vertices. Observe that Λ_μ is locally finite (even of bounded degree) since E is finite by assumption. A particle moving in M with the constraint E (i.e. only jumps in directions given by E are allowed) is forced to remain on a particular Λ_μ, and every vertex in Λ_μ can potentially be visited. One can think of a choice of Λ_μ as a choice of an "ergodic component".

A discrete geometry μ attaches a nonnegative weight to 1-cells. More generally, for $p \in \mathbb{N}_0$ a weight is attached to p-cells in a natural way through the product measures $\mu^p := \otimes^p \mu$. We denote in the sequel for every $\Lambda \in M/\Gamma$ the counting measure on Λ by $d\Lambda$ (or $\Lambda(d\zeta)$ if we want to stress that the integration variable is ζ).

Definition 3.2 (Scalar products).
Let M be an n-dimensional affine space with discrete geometry μ. For every $p \in \mathbb{N}_0$ and lattice graph Λ_μ define $\| \cdot \|^{(p)}_{\Lambda_\mu} : F(M \times V^p) \to [0, \infty]$ by setting

$$\|\alpha\|^{(p)}_{\Lambda_\mu} \ := \ \Big(\ \frac{1}{p!2^p} \int_{M \times V^p} \alpha^2(\zeta + \mathbf{v}/2, \mathbf{v}) \ \ \Lambda(d\zeta) \otimes \mu^p(d\mathbf{v}) \ \Big)^{\frac{1}{2}} \quad .$$

On $L^2(M \times V^p, \Lambda_\mu) := \{\alpha \in F(M \times V^p) : \|\alpha\|^{(p)}_{\Lambda_\mu} < \infty\}$ the (degenerate) scalar product $\langle \cdot, \cdot \rangle^{(p)}_{\Lambda_\mu}$ is defined via

$$\langle \alpha, \beta \rangle^{(p)}_{\Lambda_\mu} \ := \ \frac{1}{p!2^p} \int_{M \times V^p} \alpha(\zeta + \mathbf{v}/2, \mathbf{v}) \ \beta(\zeta + \mathbf{v}/2, \mathbf{v}) \ \ \Lambda(d\zeta) \otimes \mu^p(d\mathbf{v}) \quad .$$

We drop the superscript (p) and write just $\|\cdot\|_{\Lambda_\mu}$ and $\langle\cdot,\cdot\rangle_{\Lambda_\mu}$ if no confusion arises.

Remark 3.3. *In fact by $L^2(M\times V^p,\Lambda_\mu)$ we will henceforth mean with usual abuse of notation the corresponding set of equivalence classes of functions. Since $d\Lambda$ and μ are purely atomic on $M\times V$ this is equivalent to consider functions on suitable discrete subsets. More precisely, let for $p\in\mathbb{N}_0$*

$$\Lambda^{(p)} := \{(\zeta,\mathbf{v})\in M\times E^p \ s.t.\ \zeta-\mathbf{v}/2\in\Lambda\} \quad .$$

Observe that in particular $\Lambda^{(0)}=\Lambda$ and that $\Lambda^{(p)}$ is countable for every p. Moreover

$$L^2(M\times V^p,\Lambda_\mu) \ \simeq \ \{\alpha\in\mathbb{R}^{\Lambda^{(p)}} \ s.t.\ \frac{1}{p!2^p}\sum_{(\zeta,\mathbf{v})\in\Lambda^{(p)}}\alpha^2(\zeta,\mathbf{v})\ \mu^p(\{\mathbf{v}\})<\infty\} \quad .$$

Nevertheless, for the purposes we have in mind it is more convenient to work with equivalence classes of functions defined on the whole bundle $M\times V^p$. Observe that even with this convention, $d\Lambda$ and μ being counting measures, the corresponding scalar product can be rewritten as

$$\langle\alpha,\beta\rangle^{(p)}_{\Lambda_\mu} \ := \ \frac{1}{p!2^p}\sum_{(\zeta,\mathbf{v})\in M\times E^p}\alpha(\zeta+\mathbf{v}/2,\mathbf{v})\ \beta(\zeta+\mathbf{v}/2,\mathbf{v})\ \mu^p(\mathbf{v}) \quad .$$

In accordance with previous established notation we use the subscripts a and s to restrict function spaces to antisymmetric resp. symmetric functions. More precisely, we let

$$L^2_a(M\times V^p,\Lambda_\mu) \ := \ L^2(M\times V^p,\Lambda_\mu)\bigcap F_a(M\times V^p)$$

and

$$L^2_s(M\times V^p,\Lambda_\mu) \ := \ L^2(M\times V^p,\Lambda_\mu)\bigcap F_s(M\times V^p) \quad .$$

It is worth to emphasize that the scalar products $\langle\cdot,\cdot\rangle^{(p)}_{\Lambda_\mu}$ are not induced directly by the product measures $d\Lambda\otimes\mu^p$ on $M\times V^p$ since a shift appears in the definition. To describe this shift it is convenient to introduce the following notation.

Let $p\in\mathbb{N}_0$ and define the **shift operator** $\tau: M\times V^p\to M\times V^p$ as the bijection given by

$$\tau(\zeta,\mathbf{v}) \ := \ (\zeta-\frac{\mathbf{v}}{2},\mathbf{v}) \quad .$$

Its pushforward $\tau_*: F(M\times V^p)\to F(M\times V^p)$ acts as

$$\tau_*\alpha(\zeta,\mathbf{v}) \ := \ \alpha(\zeta+\frac{\mathbf{v}}{2},\mathbf{v}) \tag{3.3}$$

and gives the set ismorphism

$$F(M \times V^p) \;\simeq\; \tau_* F(M \times V^p) \quad ,$$

where $\tau_* F(M \times V^p)$ denotes the image of $F(M \times V^p)$ under τ_*. Using τ we have

$$\langle \alpha, \beta \rangle_{\Lambda_\mu}^{(p)} \;:=\; \frac{1}{p!2^p} \int_{M \times V^p} \tau_*(\alpha\beta)\; d\Lambda \otimes \mu^p \quad .$$

It will also be convenient to introduce the notation $\| \cdot \|_\mu^{(p)}$ and $\langle \cdot, \cdot \rangle_\mu^{(p)}$ to denote the norm and scalar product induced by μ on $\mathbb{R}^{V^p}$: for $\omega, \omega' \in \mathbb{R}^{V^p}$ let

$$\langle \omega, \omega' \rangle_\mu^{(p)} \;:=\; \frac{1}{p!2^p} \int_{V^p} \omega_{\mathbf{v}}\, \omega'_{\mathbf{v}}\; \mu^p(d\mathbf{v}) \quad \text{and} \quad \|\omega\|_\mu^{(p)} \;:=\; \sqrt{\langle \omega, \omega \rangle_\mu^{(p)}} \;. \tag{3.4}$$

Again we shall drop the superscript (p) in (3.4) if no confusion is possible. Moreover we shall write $\mathbb{R}^{V^p,\mu}$ to emphasize that we consider the space $\mathbb{R}^{V^p}$ as a Hilbert space with scalar product $\langle \cdot, \cdot \rangle \mu$. In accordance with the notation introduced around (1.7) we also write $\mathbb{R}_a^{V^p,\mu}$ and $\mathbb{R}_s^{V^p,\mu}$ for the corresponding restrictions to alternating resp. symmetric functions. Note that with (3.4) and (3.3) one has (recall that we use the notation $\Lambda(d\zeta)$ instead of $d\Lambda$ to stress that ζ is the integration variable)

$$\langle \alpha, \beta \rangle_{\Lambda_\mu}^{(p)} \;:=\; \int_M \langle \tau_*\alpha(\zeta), \tau_*\beta(\zeta) \rangle_\mu^{(p)}\; \Lambda(d\zeta) \quad . \tag{3.5}$$

Remark 3.4. *Let $\alpha \in F_s(M \times V^p) \cup F_a(M \times V^p)$. Then $\alpha^2 \in F_s(M \times V^p)$ and therefore (recall Remark 1.1) it is a function on nonoriented p-cells. With this interpretation the square of $\| \cdot \|_{\Lambda_\mu}^{(p)}$ amounts to a weighted sum of the values of α^2 over all nonoriented p-cells, the weight being given by μ^p.*

Remark 3.5. *Since, as observed in* (1.6)*, $\alpha(\zeta, \mathbf{v}) = 0$ if $\alpha \in F_a(M \times V^p)$ and $\mathbf{v}$ is such that $v_i = v_j$ for some $i \neq j$, one deduces that*

$$L_a^2(M \times V^p, \Lambda_\mu) \;=\; \{0\} \qquad \textit{for} \quad p > N \quad ,$$

where N is the size of μ.

It may be convenient in some situations to consider suitable coordinates adapted to the lattice, and a different description of p-cells based on the following remark.

Remark 3.6. *Recall the discussion on cells in Section 1, in particular* (1.2)*. We say that the oriented p-cell given by $(\zeta, [\mathbf{v}]) \in M \times V^p / \sim_{\mathcal{O}}$ is an* **oriented E-generated p-cell** *if $\mathbf{v} \in E^p$. A* **positive orientation** *is defined by selecting for every couple of nondegenerate, oriented E-generated p-cells with opposite orientation one of the two orientations. If such a selection is given, combining Remark 1.1 and Remark 3.3 leads to the observation that an element of $L^2_a(M \times V^p, \Lambda_\mu)$ is determined by the values of one of its representatives on the set of positively oriented* [26] *E-generated p-cells which are contained in Λ.*

Coordinates adapted to the lattice graph Λ_μ.

Given an n-dimensional affine space M with discrete geometry μ of size N and a lattice graph Λ_μ we choose

(i) N elements of E by selecting one vector for every couple of opposite vectors in E and then order this selection arbitrarily. This produces first a set denoted by $E_{\frac{1}{2}} = \{e_1, \ldots, e_N\}$ and then an array denoted by $\overrightarrow{E} = (e_1, \ldots, e_N)$.
(ii) a point O in Λ and a basis $\mathscr{B}_\Gamma = (b_1, \ldots, b_n)$ of the lattice Γ.

Observe that in general E does not contain a basis of Γ. A simple counterexample in dimension 1 is given by taking $E := \{2e, 3e, -2e, -3e\}$ for an arbitrary nonzero vector e. But if E is a nearest neighbour geometry (i.e. $N = n$) one can make the choices above with $b_j = e_j$ for every $j = 1, \ldots, n$. In the sequel we will assume $b_j = e_j$ if $N = n$, although this is not always necessary.

Remark 3.7. *We note that there is a canonical way to select $E_{\frac{1}{2}}$ and $\overrightarrow{E}$ as described in* (i) *once a basis of V is given: define $E_{\frac{1}{2}}$ as the subset of E consisting of vectors with first nonzero coordinate being positive, and $\overrightarrow{E}$ by ordering the coordinate vectors according to the lexicographic order. Thus it is in fact enough to make the choice (ii). This point of view is convenient when dealing with uncountable E, as in the case of general jump processes.*

[26] Observe that positively oriented p-cells are by definition nondegenerate.

The choice (i) defines positively oriented E-generated cells in the obvious way (Cell$(\zeta,[\mathbf{v}])$ is positively oriented if $[\mathbf{v}]$ has a representative which is a subarray of $\overrightarrow{E}$) and permits to establish a one-to-one correspondence

$$\Phi : M \times \left[E^p/\sim\mathcal{O}\right]_+ \to M \times \mathcal{M}_N^p \quad ,$$

where $M \times \left[E^p/\sim\mathcal{O}\right]_+$ denotes the set of positively oriented E-generated p-cells and $\mathcal{M}_N^p$ is the set of increasing multiindices of length $p \in \mathbb{N}_0$, i.e.

$$\mathcal{M}_N^p := \left\{\ I = (i_1, \ldots, i_p) \in \{1, \ldots, N\}^p : i_1 < \cdots < i_p \ \right\} \quad . \tag{3.6}$$

This correspondence is described by the following recipe. Given a $[\mathbf{v}] \in E^p/\sim_{\mathcal{O}}$ take a representative $\mathbf{v}$, reorder and change the signs of its components $(v_1, \ldots, v_p)$ according to $\overrightarrow{E}$. The resulting vector $\hat{\mathbf{v}} \in E^p$ is (well-defined and is) associated with the multiindex $I_{\hat{\mathbf{v}}} := \{i_1, \ldots, i_p\} \in \mathcal{M}_N^p$ having the property that

$$\hat{\mathbf{v}} = \mathbf{e}_{I_{\hat{\mathbf{v}}}} \quad ,$$

where $\mathbf{e}_{I_{\hat{\mathbf{v}}}} := (e_{i_1}, \ldots, e_{i_p})$. Finally set for every $(\zeta, [\mathbf{v}]) \in M \times \left[E^p/\sim_{\mathcal{O}}\ \right]_+$

$$\Phi(\zeta, [\mathbf{v}]) := (\Phi_1(\zeta, [\mathbf{v}]), \Phi_2([\mathbf{v}])) := (\zeta - \hat{\mathbf{v}}/2, I_{\hat{\mathbf{v}}}) \quad .$$

Observe that the set of points of the cell given by $(\zeta, [\mathbf{v}]) \in M \times \left[E^p/\sim_{\mathcal{O}}\ \right]_+$ is contained in Λ if and only if $\Phi_1(\zeta, [\mathbf{v}]) \in \Lambda$. Recall also that the cardinality of $\mathcal{M}_N^p$ is $\binom{N}{p}$.

It follows from the considerations of Remark 3.3 that for every $p \in \mathbb{N}_0$ there is a Hilbert space isomorphism

$$L^2_a(M \times V^p, \Lambda_\mu) \ \simeq \ L^2(\Lambda; \mathbb{R}^{\mathcal{M}_N^p, \mu}) \quad , \tag{3.7}$$

where

$$L^2(\Lambda; \mathbb{R}^{\mathcal{M}_N^p, \mu}) \ := \ \left\{\ (\alpha_I)_{I \in \mathcal{M}_N^p} : \Lambda \to \mathbb{R}^{\mathcal{M}_N^p} \ \text{ s.t. } \sum_{\zeta \in \Lambda} \sum_{I \in \mathcal{M}_p^N} \alpha_I^2(\zeta)\ \mu_I < \infty\ \right\}$$

$$\text{and} \qquad \mu_I := \mu^p\ (\{\mathbf{e}_I\}) \quad . \tag{3.8}$$

The isomorphism we consider in (3.7) maps an $\alpha \in L^2_a(M \times V^p, \Lambda_\mu)$ to an $(\alpha_I)_{I \in \mathcal{M}_p^N} \in L^2(\Lambda; \mathbb{R}^{\mathcal{M}_N^p, \mu})$ via

$$\alpha_I(\zeta) \ := \ \alpha(\zeta + \mathbf{e}_I/2, \mathbf{e}_I) \quad .$$

The choice (ii) introduces in M coordinates $x := (x_1, \ldots, x_n) \in \mathbb{R}^n$ with respect to $(O, \mathscr{B}_\Gamma)$. Since $\mathscr{B}_\Gamma$ is a basis of Γ it follows that a point $\zeta \in M$ is in Λ if and only if its coordinates are integers. This isomorphism $\Lambda \simeq \mathbb{Z}^n$ gives

$$L^2(\Lambda; \mathbb{R}^{\mathcal{M}_N^p, \mu}) \ \simeq \ L^2(\mathbb{Z}^n; \mathbb{R}^{\mathcal{M}_N^p, \mu}) \quad , \tag{3.9}$$

where

$$L^2(\mathbb{Z}^n;\mathbb{R}^{\mathcal{M}^p_N,\mu}) \;:=\; \{\, (\alpha_I)_{I\in\mathcal{M}^p_N} : \mathbb{Z}^n \to \mathbb{R}^{\mathcal{M}^p_N} \text{ s.t. } \sum_{x\in\mathbb{Z}^n}\sum_{I\in\mathcal{M}^N_p} \alpha_I^2(x)\,\mu_I < \infty \,\} \;.$$

Putting together (3.7) and (3.9) gives finally

$$L^2_a(M\times V^p,\Lambda_\mu) \;\simeq\; L^2(\mathbb{Z}^n;\mathbb{R}^{\mathcal{M}^p_N,\mu}) \quad . \tag{3.10}$$

The operator $\delta^{*\mu}$.

The choice of a discrete geometry permits to define a formal operator which is dual to δ in a sense that will be specified in Proposition 3.10.

Definition 3.8.

Let M be an affine space with discrete geometry μ. For $p\in\mathbb{N}_0$ define the formal operator $\delta^{*\mu,(p)} : F_a(M\times V^{p+1}) \to F_a(M\times V^p)$ by setting

$$\delta^{*\mu,(p)}\;\alpha(\zeta,\mathbf{v}) \;:=\; \frac{1}{2}\int_V \mathcal{D}^{\star,(p+1)}_w\alpha\;(\zeta,w,\mathbf{v})\;\mu(dw) \quad .$$

Moreover let $\delta^{*\mu} \;:=\; \oplus_{p=0}^{\infty}\delta^{*\mu,(p)}$.

Observe that $\delta^{*\mu}$ depends on the chosen discrete geometry μ while δ does not. Since in the above definition α is antisymmetric, and therefore $\alpha(\zeta,w,\mathbf{v}) = 0$ if $w = v_j$ or $w = -v_j$ for some $j = 1,\ldots,p$, the integral can be restricted to the set $V\setminus\{\pm v_1,\ldots,\pm v_p\}$. More precisely, using the shorthand notation $V\setminus\pm\mathbf{v}$ for the latter, the following holds:

$$\delta^{*\mu,(p)}\alpha(\zeta,\mathbf{v}) \;:=\; \frac{1}{2}\int_{V\setminus\pm\mathbf{v}} \mathcal{D}^{\star,(p+1)}_w\alpha\;(\zeta,w,\mathbf{v})\;\mu(dw) \quad . \tag{3.11}$$

Moreover it will be convenient in the sequel to have the representation

$$\delta^{*\mu,(p)}\alpha(\zeta,\mathbf{v}) \;= \tag{3.12}$$

$$= \;\frac{1}{2(p+1)}\sum_{j=1}^{p+1}(-1)^{j+1}\int_{V\setminus\pm\mathbf{v}} \mathcal{D}^{\star,(p+1)}_w\;\alpha(\zeta,\mathbf{v}_{+(w,j)})\;\mu(dw) \quad .$$

Recalling that μ is purely atomic we also get

$$\delta^{*\mu,(p)}\alpha(\zeta,\mathbf{v}) \;:=\; \frac{1}{2}\sum_{w\in E\setminus\pm\mathbf{v}} \mathcal{D}^{\star,(p+1)}_w\alpha\;(\zeta,w,\mathbf{v})\;\mu(\{w\}) \quad . \tag{3.13}$$

Remark 3.9. *Observe that for every lattice graph Λ_μ and $\alpha \in L^2_a(M \times V^p, \Lambda_\mu)$ the expressions $\delta\alpha$ and $\delta^{*_\mu}\alpha$ are well-defined (i.e. independent of the chosen representative). Moreover the translation invariance of $d\Lambda$ gives $\delta\alpha \in L^2_a(M \times V^{p+1}, \Lambda_\mu)$ and $\delta^{*_\mu}\alpha \in L^2_a(M \times V^{p-1}, \Lambda_\mu)$. More precisely*

$$\|\delta\alpha\|^{(p+1)}_{\Lambda_\mu} \;\leq\; 2(p+1)\sum_{v\in E}\mu(\{v\})\;\|\alpha\|^{(p)}_{\Lambda_\mu}$$

and

$$\|\delta^{*_\mu}\alpha\|^{(p-1)}_{\Lambda_\mu} \;\leq\; \|\alpha\|^{(p)}_{\Lambda_\mu} \quad .$$

Proposition 3.10.
For every $p \in \mathbb{N}_0$, every lattice graph Λ_μ and $\alpha \in L^2_a(M \times V^p, \Lambda_\mu)$, $\beta \in L^2_a(M \times V^{p+1}, \Lambda_\mu)$

$$\langle \delta^{(p)}\alpha, \beta\rangle^{(p+1)}_{\Lambda_\mu} \;=\; \langle \alpha, \delta^{*_\mu,(p)}\beta\rangle^{(p)}_{\Lambda_\mu} \quad .$$

Proof. First observe that if $\gamma \in L^2(M\times V^{p+1}, \Lambda_\mu)$ and $\beta \in L^2_a(M\times V^{p+1}, \Lambda_\mu)$, then

$$\int_{M\times V^{p+1}} (\mathrm{Alt}\,\gamma)\;\beta\;d\Lambda\otimes\mu^{p+1} \;=\; \int_{M\times V^{p+1}} \gamma\;\beta\;d\Lambda\otimes\mu^{p+1}$$

and also

$$\int_{M\times V^{p+1}} \tau_*\big(\,(\mathrm{Alt}\,\gamma)\;\beta\,\big)\;d\Lambda\otimes\mu^{p+1} \;=\; \int_{M\times V^{p+1}} \tau_*\big(\,\gamma\;\beta\,\big)\;d\Lambda\otimes\mu^{p+1} \quad .$$

It follows that

$$\begin{aligned}\langle \delta^{(p)}\alpha, \beta\rangle^{(p+1)}_{\Lambda_\mu} \;&=\; \frac{1}{(p+1)!2^{p+1}}\int_{M\times V^{p+1}} \tau_*\big(\,(\delta^{(p)}\alpha)\;\beta\,\big)\;\;d\Lambda\otimes\mu^{p+1} \;=\\ &=\; \frac{p+1}{(p+1)!2^{p+1}}\int_{M\times V^{p+1}} \tau_*\big(\,(\mathcal{D}^{(p)}\alpha)\;\beta\,\big)\;d\Lambda\otimes\mu^{p+1} \quad .\end{aligned}$$

So, using the invariance of $d\Lambda$ under the action of E, one gets

$$\langle \delta^{(p)}\alpha, \beta\rangle^{(p+1)}_{\Lambda_\mu} =$$

$$= \frac{1}{p!2^{p+1}} \int_{M\times V^{p+1}} \big[\ \alpha(\zeta + w_1/2 + \mathbf{w}/2, \mathbf{w}_{-(1)}) - \alpha(\zeta - w_1/2 + \mathbf{w}/2, \mathbf{w}_{-(1)})\ \big]$$

$$\beta(\zeta + \mathbf{w}/2, \mathbf{w})\ \Lambda(d\zeta) \otimes \mu^{p+1}(d\mathbf{w}) =$$

$$= \frac{1}{p!2^{p}} \int_{M\times V^{p}} \alpha(\zeta + \mathbf{u}/2, \mathbf{u})$$

$$\big[\ -\frac{1}{2}\int_V \beta(\zeta + w/2 + \mathbf{u}/2, w, \mathbf{u}) - \beta(\zeta - w/2 + \mathbf{u}/2, w, \mathbf{u})\ \mu(dw)\ \big]$$

$$\Lambda(d\zeta) \otimes \mu^{p}(d\mathbf{u})$$

$$= \langle \alpha, \delta^{*_\mu,(p)}\beta\rangle^{(p)}_{\Lambda_\mu} \quad .$$

□

Remark 3.11. *Let α, β be as above and - say - continuous and compactly supported with respect to the space variable ζ. Then the previous proposition continues to be valid also by taking instead of $d\Lambda$ a Lebesgue measure (invariant with repect to all translations) on M or more generally any Borel measure which is invariant with respect to E-translations.*

Remark 3.12. *The subscript Λ_μ attached to a formal operator on p-functions will indicate that we consider it as an operator in the L^2 space corresponding to the lattice graph Λ_μ. More precisely, for every $p \in \mathbb{N}_0$ and lattice graph Λ_μ we set*

$$\delta^{(p)}_{\Lambda_\mu} : L^2_a(M \times V^p, \Lambda_\mu) \to L^2_a(M \times V^{p+1}, \Lambda_\mu)$$

and

$$\delta^{*_\mu,(p)}_{\Lambda_\mu} : L^2_a(M \times V^{p+1}, \Lambda_\mu) \to L^2_a(M \times V^{p}, \Lambda_\mu)$$

by restricting respectively $\delta^{(p)}$ to $L^2_a(M \times V^p, \Lambda_\mu)$ and $\delta^{*_\mu,(p)}$ to $L^2_a(M \times V^{p+1}, \Lambda_\mu)$. This is well defined by Remark (3.9). Both $\delta^{(p)}_{\Lambda_\mu}$ and $\delta^{*_\mu,(p)}_{\Lambda_\mu}$ are bounded, and Proposition 3.10 is equivalent to the statement that $\delta^{*_\mu,(p)}_{\Lambda_\mu}$ is the adjoint of $\delta^{(p)}_{\Lambda_\mu}$ for every $p \in \mathbb{N}_0$ and lattice graph Λ_μ.

Proposition 3.13 (Complex property for δ^{*_μ}).

For every $p \in \mathbb{N}_0$

$$\delta^{*_\mu,(p)}\delta^{*_\mu,(p+1)} \equiv 0 \quad .$$

Proof. As in the case of the complex property of δ (see Proposition 2.6), the complex property of $\delta^{*\mu}$ is a consequence of the "Schwarz Lemma",

$$\mathcal{D}^{2,(p)}_{w_1,w_2} \;=\; \mathcal{D}^{2,(p)}_{w_1,w_2} \quad ,$$

valid for every $(w_1, w_2) \in V^2$. This implies for an alternating α

$$D^{2,(p)}_{w_1,w_2}\alpha(\zeta, w_2, w_1, \mathbf{v}) \;=\; -\mathcal{D}^{2,(p)}_{w_2,w_1}\alpha(\zeta, w_1, w_2, \mathbf{v}) \quad .$$

Therefore

$$\delta^{*_\mu,(p)}\delta^{*_\mu,(p+1)}\;\alpha(\zeta,\mathbf{v}) \;=$$

$$= \;-\frac{1}{2}\int_V \;\mathcal{D}^{(p+1)}_{w_1}\delta^{*_\mu,(p+1)}\alpha\;(\zeta, w_1, \mathbf{v})\;\mu(dw_1) \;=$$

$$= \;-\frac{1}{2}\int_V \;\mathcal{D}^{(p+1)}_{w_1}\Big(\; -\frac{1}{2}\int_V \;\mathcal{D}^{(p+2)}_{w_2}\alpha\;(\zeta, w_2, w_1, \mathbf{v})\;\mu(dw_2)\;\Big)\;\mu(dw_1) \;=$$

$$= \;\frac{1}{4}\int_{V^2}\mathcal{D}^{2,(p)}_{w_1,w_2}\alpha\;(\zeta, w_2, w_1, \mathbf{v})\;\mu(dw_1)\otimes\mu(dw_2) \;=\; 0 \quad .$$

$\square$

Remark 3.14. *The complex property for $\delta^{*\mu}$ could also be derived from the complex property of δ (see Prop. 2.6) and from Prop. 3.10.*

Remark 3.15. *A simple geometric interpretation can also be given for $\delta^{*\mu}$. In fact, from the discussion on oriented cells and their boundaries given in Remark 2.7 it follows that $\delta^{*_\mu,(p)}\alpha(\zeta, \mathbf{v})$ equals the sum of the weighted values of α on the oriented $p+1$-cells having the p-cell $\mathrm{Cell}_{\mathrm{sign}}(\zeta, [\mathbf{v}])$ as part of their boundary. So $\delta^{*_\mu,(0)}$ resembles the usual discrete divergence operator, which sums over the incoming edges at a point.*

4. The discrete Hodge Laplacian $\mathcal{L}_\mu$

In this section we introduce on an affine space with discrete geometry a Hodge-type Laplacian acting on the algebra of antisymmetric functions.

Definition 4.1 (**Discrete Hodge Laplacians).**

Let M be an n-dimensional affine space and μ a discrete geometry. For $p \in \mathbb{N}_0$ the p-th (formal) discrete Hodge Laplacian $\mathcal{L}_\mu^{(p)} : F_a(M \times V^p) \to F_a(M \times V^p)$ is defined by setting

$$\mathcal{L}_\mu^{(p)} \;:=\; \delta^{*_\mu,(p)}\delta^{(p)} \;+\; \delta^{(p-1)}\delta^{*_\mu,(p-1)} \quad .$$

Moreover we let $\mathcal{L}_\mu := \oplus_{p=0}^{\infty}\mathcal{L}_\mu^{(p)}$

The following proposition gives a representation of $\mathcal{L}_\mu^{(p)}$ which is analogous to the representation of the standard infinitesimal Hodge Laplacian in Euclidean space, expressing exact equality between the Hodge Laplacian and the covariant Laplacian. We state the proposition in a compact notation, which will be particularly useful in later, more involved sections, exploiting the trace operator with respect to a discrete geometry μ. More precisely, given $P := \{P_{w_1,w_2}\}_{w_1,w_2 \in V}$ with $P_{w_1,w_2} : F(M \times V^p) \to F(M \times V^p)$ for every $w_1, w_2 \in V$ we define

$$\operatorname{Tr}_\mu^{(p)} P : F(M \times V^p) \to F(M \times V^p)$$

by setting

$$\operatorname{Tr}_\mu P \;\alpha\; (\zeta, \mathbf{v}) \;:=\; \frac{1}{2}\int_V P_{w,w} \;\alpha\; (\zeta, \mathbf{v}) \;\mu(dw) \quad . \tag{4.1}$$

Observe that if for every $w_1, w_2 \in V$ the operator P_{w_1,w_2} leaves invariant the space of alternating functions, then so does $\operatorname{Tr}_\mu P$.

Proposition 4.2.

For every discrete geometry μ on M the discrete Hodge Laplacian is given by

$$\mathcal{L}_\mu \;=\; \operatorname{Tr}_\mu \mathcal{D}^\star\mathcal{D} \quad .$$

More explicitly we have

$$\mathcal{L}_\mu^{(p)}\alpha\ (\zeta,\mathbf{v}) \ = \ -\frac{1}{2}\int_V \mathcal{D}^{2,(p)}_{w,w}\ \alpha(\zeta,\mathbf{v})\ \mu(dw) \ =$$

$$= \ \frac{1}{2}\int_V \big[\ 2\alpha(\zeta,\mathbf{v})-\alpha(\zeta+w,\mathbf{v})-\alpha(\zeta-w,\mathbf{v})\ \big]\ \mu(dw) \ =$$

$$= \ \frac{1}{2}\sum_{w\in E}\big[\ 2\alpha(\zeta,\mathbf{v})-\alpha(\zeta+w,\mathbf{v})-\alpha(\zeta-w,\mathbf{v})\ \big]\ \mu(\{w\}) \quad .$$

The second equality above follows from (2.5), the third from the definition of μ.

By symmetry one also gets

$$\mathcal{L}_\mu^{(p)}\alpha\ (\zeta,\mathbf{v}) \ = \ \int_V \big[\ \alpha(\zeta,\mathbf{v})-\alpha(\zeta+w,\mathbf{v})\ \big]\ \mu(dw) \quad .$$

Remark 4.3. *The previous proposition states in particular that* $\mathcal{L}_\mu^{(p)}$ *is a* **scalar operator**. *Here we call an operator* $T : F(M\times V^p)\to F(M\times V^p)$ *a scalar operator if there exists an operator* $T_0 : F(M)\to F(M)$ *such that for every* $\alpha\in F(M\times V^p)$, $\mathbf{v}\in V^p$, *denoting by* $\alpha_{\mathbf{v}}$ *the function* $\zeta\mapsto\alpha(\zeta,\mathbf{v})$ *one has*

$$T\alpha\ (\zeta,\mathbf{v}) \ = \ T_0\alpha_{\mathbf{v}}(\zeta) \qquad \textit{for every } \zeta\in M \quad .$$

Otherwise we say that T *is a* **matrix operator**.

Proof of Proposition 4.2. This is a straightforward computation. We give here the details for completeness.

Recalling (see (2.7) and (3.12)) that

$$\delta^{(p)}\alpha\ (\zeta,\mathbf{v}_{+(w,j)}) \ = \ \sum_{l=1}^{p+1}(-1)^{l+1}\ \mathcal{D}_{v_l}\ \alpha(\zeta,\mathbf{v}_{\substack{+(w,j)\\-(l)}})$$

and

$$\delta^{*_\mu,(p)}\alpha(\zeta,\mathbf{v}) \ = \ \frac{1}{2(p+1)}\sum_{j=1}^{p+1}(-1)^{j+1}\int_{V\setminus\pm\mathbf{v}}\mathcal{D}^{\star}_w\ \alpha(\zeta,\mathbf{v}_{+(w,j)})\ \mu(dw)$$

one gets

$$\delta^{*_\mu,(p)}\delta^{(p)}\ \alpha(\zeta,\mathbf{v}) \ = \ \frac{1}{2(p+1)}\sum_{l,j=1}^{p+1}(-1)^{j+l}\int_{V\setminus\pm\mathbf{v}}\mathcal{D}^\star_w\mathcal{D}_{(\mathbf{v}_{+(w,j)})_l}\ \alpha(\zeta,\mathbf{v}_{\substack{+(w,j)\\-(l)}})\ \mu(dw) \ =$$

$$= \ \frac{1}{2(p+1)}\sum_{j}^{p+1}\int_{V\setminus\pm\mathbf{v}}\mathcal{D}^\star_w\mathcal{D}_w\ \alpha(\zeta,\mathbf{v})\ \mu(dw) \ +$$

$$+\ \frac{1}{2(p+1)}\sum_{\substack{j,l=1\\j<l}}^{p+1}(-1)^{j+l}\int_{V\setminus\pm\mathbf{v}}\mathcal{D}^\star_w\mathcal{D}_{(\mathbf{v}_{+(w,j)})_l}\ \alpha(\zeta,\mathbf{v}_{\substack{+(w,j)\\-(l)}})\ \mu(dw) \ +$$

$$+\ \frac{1}{2(p+1)}\sum_{\substack{j,l=1\\j>l}}^{p+1}(-1)^{j+l}\int_{V\setminus\pm\mathbf{v}}\mathcal{D}^\star_w\mathcal{D}_{(\mathbf{v}_{+(w,j)})_l}\ \alpha(\zeta,\mathbf{v}_{\substack{+(w,j)\\-(l)}})\ \mu(dw) \quad .$$

Using that

$$\alpha(\zeta,\mathbf{v}_{\substack{+(w,j)\\-(l)}}) \ = \ \begin{cases}(-1)^j\ \alpha(\zeta,\mathbf{v}_{\substack{+(w,1)\\-(l+1)}}) & \text{if } j>l\\ (-1)^{j+1}\ \alpha(\zeta,\mathbf{v}_{\substack{+(w,1)\\-(l)}}) & \text{if } j<l\end{cases}$$

gives

$$\delta^{*_\mu,(p)}\delta^{(p)}\ \alpha(\zeta,\mathbf{v}) \ = \ \frac{1}{2}\int_{V\setminus\pm\mathbf{v}}\mathcal{D}^\star_w\mathcal{D}_w\ \alpha(\zeta,\mathbf{v})\ \mu(dw) \ +$$

$$+\ \frac{1}{2(p+1)}\sum_{l=2}^{p+1}\sum_{j=1}^{l-1}(-1)^{l+1}\int_{V\setminus\pm\mathbf{v}}\mathcal{D}^\star_w\mathcal{D}_{v_{l-1}}\ \alpha(\zeta,\mathbf{v}_{\substack{+(w,1)\\-(l)}})\ \mu(dw) \ + \tag{4.2}$$

$$+\ \frac{1}{2(p+1)}\sum_{l=1}^{p}\sum_{j=l+1}^{p+1}(-1)^{l}\int_{V\setminus\pm\mathbf{v}}\mathcal{D}^\star_w\mathcal{D}_{v_l}\ \alpha(\zeta,\mathbf{v}_{\substack{+(w,1)\\-(l+1)}})\ \mu(dw) \quad .$$

A change of the summation variable in the summand (4.2) yields

$$\frac{1}{2(p+1)}\sum_{l=2}^{p+1}\sum_{j=1}^{l-1}(-1)^{l+1}\int_{V\setminus\pm\mathbf{v}}\mathcal{D}^\star_w\mathcal{D}_{v_{l-1}}\ \alpha(\zeta,\mathbf{v}_{\substack{+(w,1)\\-(l)}})\ \mu(dw) \ =$$

$$= \ \frac{1}{2(p+1)}\sum_{l=1}^{p}\sum_{j=1}^{l}(-1)^{l}\int_{V\setminus\pm\mathbf{v}}\mathcal{D}^\star_w\mathcal{D}_{v_l}\ \alpha(\zeta,\mathbf{v}_{\substack{+(w,1)\\-(l+1)}})\ \mu(dw) \quad ,$$

so

$$\delta^{*_\mu,(p)}\delta^{(p)}\ \alpha(\zeta,\mathbf{v}) \ = \ \frac{1}{2}\int_{V\setminus\pm\mathbf{v}}\mathcal{D}^\star_w\mathcal{D}_w\ \alpha(\zeta,\mathbf{v})\ \mu(dw) \ +$$

$$+\ \frac{1}{2}\sum_{l=1}^{p}(-1)^{l}\int_{V\setminus\pm\mathbf{v}}\mathcal{D}^\star_w\mathcal{D}_{v_l}\ \alpha(\zeta,\mathbf{v}_{\substack{+(w,1)\\-(l+1)}})\ \mu(dw) \quad .$$

Similarly, recalling that

$$\delta^{*_\mu,(p-1)}\alpha(\zeta,\mathbf{v}_{-(l)}) \;=\; \frac{1}{2p}\sum_{j=1}^{p}(-1)^{j+1}\int_{V\setminus\pm\mathbf{v}_{-(l)}} \mathcal{D}^\star_w\;\alpha(\zeta,\mathbf{v}_{\substack{-(l)\\+(w,j)}})\;\mu(dw)$$

$$\delta^{(p-1)}\alpha\;(\zeta,\mathbf{v}) \;=\; \sum_{l=1}^{p}(-1)^{l+1}\;\mathcal{D}_{v_l}\;\alpha(\zeta,\mathbf{v}_{-(l)})$$

and observing that $V\setminus\pm\mathbf{v}_{-(l)}=\{v_l,-v_l\}\cup V\setminus\pm\mathbf{v}$, we get

$$\delta^{(p-1)}\delta^{*_\mu,(p-1)}\alpha(\zeta,\mathbf{v}) \;=\; \frac{1}{2p}\sum_{j,l=1}^{p}(-1)^{j+l}\int_{V\setminus\pm\mathbf{v}_{-(l)}}\mathcal{D}_{v_l}\mathcal{D}^\star_w\;\alpha(\zeta,\mathbf{v}_{\substack{-(l)\\+(w,j)}})\;\mu(dw) \;=$$

$$=\;\frac{1}{2p}\sum_{j=1}^{p}\sum_{l=1}^{p}(-1)^{j+l}\Big\{\;\mathcal{D}_{v_l}\mathcal{D}^\star_{v_l}\;\alpha(\zeta,\mathbf{v}_{\substack{-(l)\\+(v_l,j)}})\;\mu(\{v_l\})+\mathcal{D}_{v_l}\mathcal{D}^\star_{-v_l}\;\alpha(\zeta,\mathbf{v}_{\substack{-(l)\\+(-v_l,j)}})\;\mu(\{v_l\})\;\Big\}\;+$$

$$+\;\frac{1}{2p}\sum_{\substack{j,l=1\\j\le l}}^{p}(-1)^{j+l}\int_{V\setminus\pm\mathbf{v}}\mathcal{D}_{v_l}\mathcal{D}^\star_w\;\alpha(\zeta,\mathbf{v}_{\substack{-(l)\\+(w,j)}})\;\mu(dw)\;+$$

$$+\;\frac{1}{2p}\sum_{\substack{j,l=1\\j>l}}^{p}(-1)^{j+l}\int_{V\setminus\pm\mathbf{v}}\mathcal{D}_{v_l}\mathcal{D}^\star_w\;\alpha(\zeta,\mathbf{v}_{\substack{-(l)\\+(w,j)}})\;\mu(dw)\quad.$$

Using

$$\alpha(\zeta,\mathbf{v}_{\substack{-(l)\\+(v_l,j)}})=(-1)^{j+l}\alpha(\zeta,\mathbf{v})$$

for the first summand and

$$\alpha(\zeta,\mathbf{v}_{\substack{-(l)\\+(w,j)}})\;=\;\begin{cases}(-1)^{j+1}\;\alpha(\zeta,\mathbf{v}_{\substack{+(w,1)\\-(l+1)}}) & \text{if } j>l\\[2mm] (-1)^{j+1}\;\alpha(\zeta,\mathbf{v}_{\substack{+(w,1)\\-(l+1)}}) & \text{if } j\le l\end{cases}$$

for the second and third summands gives

$$
\begin{aligned}
\delta^{(p-1)}\delta^{*_\mu,(p-1)}\alpha(\zeta,\mathbf{v}) \;&=\; \frac{1}{2}\int_{\pm\mathbf{v}} \mathcal{D}_w\mathcal{D}_w^\star\ \alpha(\zeta,\mathbf{v})\ \mu(dw) \;+ \\
&+\frac{1}{2p}\sum_{j=1}^{p}\sum_{l=j}^{p}(-1)^{l+1}\ \int_{V\setminus\pm\mathbf{v}} \mathcal{D}_{v_l}\mathcal{D}_w^\star\ \alpha(\zeta,\mathbf{v}_{\substack{+(w,1)\\-(l+1)}})\ \mu(dw)\;+ \\
&+\frac{1}{2p}\sum_{j=1}^{p}\sum_{l=1}^{j-1}(-1)^{l+1}\ \int_{V\setminus\pm\mathbf{v}} \mathcal{D}_{v_l}\mathcal{D}_w^\star\ \alpha(\zeta,\mathbf{v}_{\substack{+(w,1)\\-(l+1)}})\ \mu(dw)\;= \\
&=\;\frac{1}{2}\int_{\pm\mathbf{v}} \mathcal{D}_w\mathcal{D}_w^\star\ \alpha(\zeta,\mathbf{v})\ \mu(dw)\;+ \\
&-\frac{1}{2}\sum_{l=1}^{p}(-1)^{l}\ \int_{V\setminus\pm\mathbf{v}} \mathcal{D}_{v_l}\mathcal{D}_w^\star\ \alpha(\zeta,\mathbf{v}_{\substack{+(w,1)\\-(l+1)}})\ \mu(dw)\quad .
\end{aligned}
$$

□

A fundamental property of the Hodge Laplacian is that it commutes with its differential.

Proposition 4.4 (Intertwining relations).
For every $p\in\mathbb{N}_0$, $\alpha\in F_a(M\times V^p)$

$$
\mathcal{L}_\mu^{(p+1)}\ \delta^{(p)}\alpha \;=\; \delta^{(p)}\mathcal{L}_\mu^{(p)}\alpha
$$

and for every $\alpha\in F_a(M\times V^{p+1})$

$$
\mathcal{L}_\mu^{(p)}\delta^{*_\mu,(p)}\alpha \;=\; \delta^{*_\mu,(p)}\mathcal{L}_\mu^{(p+1)}\alpha \quad .
$$

Proof. This is an immediate consequence of the definition of $\mathcal{L}_\mu^{(p)}$ and the complex properties stated in Propositions 2.6 and 3.13. □

Observe that for every lattice graph Λ_μ and for every $p\in\mathbb{N}_0$

$$
\alpha\in L_a^2(M\times V^p,\Lambda_\mu)\qquad\Rightarrow\qquad \mathcal{L}_\mu^{(p)}\alpha \text{ is well-defined in } L_a^2(M\times V^p,\Lambda_\mu)\quad .
$$

The restriction of $\mathcal{L}_\mu^{(p)}$ to $L_a^2(M\times V^p,\Lambda_\mu)$ will be denoted by $\mathcal{L}_{\Lambda_\mu}^{(p)}$. Recall from Remark 3.5 that $L_a^2(M\times V^p,\Lambda_\mu)=\{0\}$ if $p>N$, where $N\geq n$ is the size of μ.

Remark 4.5. *In coordinates adapted to* Λ_μ *(see page 55) one has for every* $I \in \mathcal{M}_N^p$ *and* $x \in \mathbb{Z}^n$

$$\left(\mathcal{L}_{\Lambda_\mu}^{(p)} \, \alpha \right)_I (x) \;=\; \mathcal{L}_{\Lambda_\mu}^{(0)} \, \alpha_I \,(x) \;=\; \sum_{j=1}^{N} \mu_j \,[\, 2\alpha_I(x) - \alpha_I(x+e_j) - \alpha_I(x-e_j) \,] \;\;,$$

where $\mu_j := \mu(\{e_j\})$ *in accordance with the definition given in* (3.8)*.*

Proposition 4.6.

Let M *be an* n*-dimensional affine space with discrete geometry* μ *of size* $N \geq n$ *and let* $p = 0, \ldots, N$*. Then for every lattice graph* Λ_μ *the operator* $\mathcal{L}_{\Lambda_\mu}^{(p)}$ *is bounded, selfadjoint and positive. Moreover there exists a constant* $K_\mu > 0$ *independent of* Λ*, s.t.*

$$\mathrm{Spec}(\mathcal{L}_{\Lambda_\mu}^{(p)}) = [0, K_\mu] \quad .$$

In the case $N = n$

$$K_\mu = 2 \sum_{v \in E} \mu(v) = 4 \sum_{j=1}^{n} \mu_j \quad .$$

Proof. Boundedness follows from the fact that translations are bounded operators. Selfadjointness follows immediately from the definition of $\mathcal{L}_\mu$ and from Proposition 3.10. Moreover

$$\langle \alpha, \mathcal{L}_\mu \alpha \rangle_{\Lambda_\mu} \;=\; \|\delta\alpha\|_{\Lambda_\mu}^2 + \|\delta^{*\mu}\alpha\|_{\Lambda_\mu}^2 \geq 0 \quad ,$$

so $\mathcal{L}_{\Lambda_\mu}^{(p)}$ is positive. The statement regarding the spectrum is obtained by passing to the Fourier representation and analyzing the range of the symbol of $\mathcal{L}_{\Lambda_\mu}$.

□

5. Inhomogeneous discrete geometries

In this section we generalize the previous discussions by introducing a weight function ρ on M describing possible inhomogeneities in space and thus possibly breaking the translation invariance.

More precisely we consider here an n-dimensional affine space M together with a discrete geometry μ and a function $\rho : M \to (0, \infty)$. We call the couple (μ, ρ) an **inhomogeneous discrete geometry** and write for short $\rho\mu$.

As in the homogeneous case, once an inhomogeneous geometry $\rho\mu$ is given, a corresponding notion of lattice graph can be introduced. The only difference with the homogeneous case is that now also the vertices of the graph have a weight attached, given precisely by ρ. More formally, we call $\Lambda_{\rho\mu}$ a **lattice graph** (in M associated to $\rho\mu$) if it is a weighted undirected graph with the following properties: its vertices Λ are the elements of an equivalence class in M under the relation $\sim_\Gamma$. The weight of the vertex $\zeta \in \Lambda$ is defined to be $\rho(\zeta)$. A pair $\{\zeta, \eta\}$ of vertices is an edge if and only if there exists an $e \in E$ such that $\zeta = \eta + e$. The weight of this edge is defined to be $\mu(\{e\})$.

Definition 5.1 (Weighted scalar products).

Let M be an n-dimensional affine space with inhomogeneous discrete geometry $\rho\mu$. For every $p \in \mathbb{N}_0$ and lattice graph $\Lambda_{\rho\mu}$, define $\|\cdot\|^{(p)}_{\Lambda_{\rho\mu}} : F(M \times V^p) \to [0, \infty]$ by setting

$$\|\alpha\|^{(p)}_{\Lambda_{\rho\mu}} \;:=\; \|\sqrt{\rho}\alpha\|^{(p)}_{\Lambda_\mu} \quad .$$

On $L^2(M\times V^p, \Lambda_{\rho\mu}) \;:=\; \{\alpha \in F(M\times V^p) : \|\alpha\|^{(p)}_{\Lambda_{\rho\mu}} < \infty\}$ the (degenerate) scalar product $\langle\cdot,\cdot\rangle^{(p)}_{\Lambda_{\rho\mu}}$ is defined via

$$\langle\alpha, \beta\rangle^{(p)}_{\Lambda_{\rho\mu}} \;:=\; \langle\alpha, \rho\beta\rangle^{(p)}_{\Lambda_\mu} \quad .$$

As before we will henceforth consider $L^2(M \times V^p, \Lambda_{\rho\mu})$ as a set of equivalence classes of functions, and set

$$L^2_a(M \times V^p, \Lambda_{\rho\mu}) \;:=\; L^2(M \times V^p, \Lambda_{\rho\mu}) \bigcap F_a(M \times V^p)$$

and

$$L^2_s(M \times V^p, \Lambda_{\rho\mu}) \;:=\; L^2(M \times V^p, \Lambda_{\rho\mu}) \bigcap F_s(M \times V^p) \quad .$$

The operator $\delta^{*_{\rho\mu}}$.

The metric distorsion through the inhomogeneity ρ leads to a distorted adjoint operator of δ.

Definition 5.2.
Let M be an affine space with inhomogeneous discrete geometry $\rho\mu$. For $p \in \mathbb{N}_0$ define the formal operator $\delta^{*_{\rho\mu},(p)} : F_a(M \times V^{p+1}) \to F_a(M \times V^p)$ by setting

$$\delta^{*_{\rho\mu},(p)} \ \alpha(\zeta, \mathbf{v}) \ := \ \frac{1}{\rho(\zeta)} \ \delta^{*_{\mu},(p)}[\rho\alpha](\zeta, \mathbf{v}) \quad .$$

Moreover let $\delta^{*_{\rho\mu}} := \oplus_{p=0}^{\infty} \delta^{*_{\rho\mu},(p)}$.

It will be convenient to introduce the notation

$$\mathcal{D}^{\star\rho,(p)} \ := \ \frac{1}{\rho} \ \mathcal{D}^{\star,(p)} \ \rho \quad . \tag{5.1}$$

As usual we shall drop the superscript (p) when the corresponding direct sum is considered.

The following three more explicit expressions for $\delta^{*_{\rho\mu},(p)}$ are a direct consequence of the analogous formulae (3.11),(3.12) and (3.13) for $\delta^{*_{\mu},(p)}$.

$$\delta^{*_{\rho\mu},(p)} \ \alpha(\zeta, \mathbf{v}) \ = \ \frac{1}{2} \int_{V \setminus \pm \mathbf{v}} \mathcal{D}_w^{\star\rho,(p+1)} \alpha \ (\zeta, w, \mathbf{v}) \ \mu(dw) \qquad ,$$

$$\delta^{*_{\rho\mu},(p)} \ \alpha(\zeta, \mathbf{v}) \ = \tag{5.2}$$

$$= \ \frac{1}{2(p+1)} \sum_{j=1}^{p+1} (-1)^{j+1} \int_{V \setminus \pm \mathbf{v}} \mathcal{D}_w^{\star\rho,(p+1)} \ \alpha \ (\zeta, \mathbf{v}_{+(w,j)}) \ \mu(dw)$$

and

$$\delta^{*_{\rho\mu},(p)} \ \alpha(\zeta, \mathbf{v}) \ = \ \frac{1}{2} \sum_{w \in E \setminus \pm \mathbf{v}} \mathcal{D}_w^{\star\rho,(p+1)} \alpha \ (\zeta, w, \mathbf{v}) \ \mu(\{w\}) \quad .$$

The analogue to Proposition 3.10 is given by the following. Here it is convenient to introduce spaces of functions with compact support. More precisely we let

$$F_{0,a}(M \times V^p) \ := $$
$$\{\alpha \in F_a(M \times V^p) : \exists \text{ a compact } K \subset M \text{ s.t. } \alpha(\zeta, \mathbf{v}) = 0 \ \forall \zeta \in K^c, \mathbf{v} \in V^p\} \ .$$

Proposition 5.3.

Let $p \in \mathbb{N}_0$ and $\alpha \in F_a(M \times V^p)$, $\beta \in F_a(M \times V^{p+1})$. If at least one of α and β has compact support then

$$\langle \delta^{(p)} \alpha, \beta \rangle^{(p+1)}_{\Lambda_{\rho\mu}} \ = \ \langle \alpha, \delta^{*_{\rho\mu},(p)} \ \beta \rangle^{(p)}_{\Lambda_{\rho\mu}} \ .$$

Proof. This follows immediately from Prop. 3.10. Indeed

$$\langle \delta^{(p)} \alpha, \beta \rangle^{(p+1)}_{\Lambda_{\rho\mu}} \ = \ \langle \delta^{(p)} \alpha, \rho\beta \rangle^{(p+1)}_{\Lambda_{\mu}} \ =$$
$$= \ \langle \alpha, \delta^{*_{\mu},(p)} [\rho\beta] \rangle^{(p)}_{\Lambda_{\rho\mu}} \ = \ \langle \alpha, \delta^{*_{\rho\mu},(p)} \ \beta \rangle^{(p)}_{\Lambda_{\rho\mu}} \ .$$

□

In accordance with Remark 3.12 we attach the subscript $\Lambda_{\rho\mu}$ to δ and $\delta^{*_{\rho\mu},(p)}$ if we consider them as operators in the L^2 space corresponding to the (inhomogeneous) lattice graph $\Lambda_{\rho\mu}$. More precisely, for every lattice graph $\Lambda_{\rho\mu}$ and for $p \in \mathbb{N}_0$ we define

$$\delta^{(p)}_{\Lambda_{\rho\mu}} : F_{0,a}(M \times V^p) \to L^2_a(M \times V^{p+1}, \Lambda_{\rho\mu})$$

and

$$\delta^{*_{\rho\mu},(p)}_{\Lambda_{\rho\mu}} : F_{0,a}(M \times V^{p+1}) \to L^2_a(M \times V^p, \Lambda_{\rho\mu})$$

by restricting respectively $\delta^{(p)}$ to $F_{0,a}(M \times V^p)$ and $\delta^{*_{\rho\mu},(p)}$ to $F_{0,a}(M \times V^{p+1})$. Here (and in the sequel) we do not distinguish between $F_{0,a}(M \times V^p)$ and the set of its equivalence classes under the equivalence relation induced by $\| \cdot \|_{\Lambda_{\rho\mu}}$. Observe that $\delta^{(p)}_{\Lambda_{\rho\mu}}$ and $\delta^{*_{\rho\mu},(p)}_{\Lambda_{\rho\mu}}$ are densely defined. In general they are unbounded. The previous proposition affirms that they are formally adjoint for every $p \in \mathbb{N}_0$ and lattice graph $\Lambda_{\rho\mu}$.

As an immediate consequence of Proposition 3.13 we also have

Proposition 5.4 (Complex property for $\delta^{*_{\rho\mu}}$).

For every $p \in \mathbb{N}_0$

$$\delta^{*_{\rho\mu}(p)} \ \delta^{*_{\rho\mu}(p+1)} \equiv 0 \ .$$

6. The inhomogeneous discrete Hodge Laplacian $\mathcal{L}_{\rho\mu}$

We introduce a Hodge-type Laplacian acting on the algebra of antisymmetric functions in the case of an underlying inhomogeneous discrete geometry.

Definition 6.1 (Discrete Hodge Laplacians: inhomogeneous case).
Let M be an n-dimensional affine space and $\rho\mu$ an inhomogeneous discrete geometry. For $p \in \mathbb{N}_0$ the p-th (formal) discrete Hodge Laplacian $\mathcal{L}^{(p)}_{\rho\mu}$: $F_a(M \times V^p) \to F_a(M \times V^p)$ is defined by setting

$$\mathcal{L}^{(p)}_{\rho\mu} \ := \ \delta^{*_{\rho\mu}(p)}\delta^{(p)} \ + \ \delta^{(p-1)}\delta^{*_{\rho\mu}(p-1)} \quad .$$

Moreover we let $\mathcal{L}_{\rho\mu} := \oplus_{p=0}^{\infty}\mathcal{L}^{(p)}_{\rho\mu}$.

The following Proposition 6.2 gives a representation of $\mathcal{L}_{\rho\mu}$ which splits it into two parts: one acting as a scalar operator and another acting as a matrix. The scalar term is described in terms of the trace operator, defined in (4.1). The matrix term is described most conveniently by introducing the following operations.

Given $P := \{P_{w_1,w_2}\}_{w_1,w_2\in V^2}$ with $P_{w_1,w_2} : F(M) \to F(M)$ for every $w_1, w_2 \in V$, we define for every discrete geometry μ the operator

$$P^{\ \sharp\mu} : F(M \times V) \to F(M \times V)$$

by setting

$$\big(\ P^{\ \sharp\mu}\ \alpha\ \big)_v \ := \ \frac{1}{2}\int_V P_{v,w}\ \alpha_w\ \mu(dw) \quad . \tag{6.1}$$

Moreover, every $A : F(M \times V) \to F(M \times V)$ induces for every $p \in \mathbb{N}_*$ a $d\Gamma^{(p)}A : F(M \times V^p) \to F(M \times V^p)$ defined in the following way. Given $\alpha \in F(M \times V^p)$, $j = 1, \ldots, p$ and $\mathbf{v} \in V^{p-1}$, denote by $\alpha_{\mathbf{v},j}$ the 1-function

$$(\zeta, w) \mapsto \alpha(\zeta, v_1, \ldots, v_{j-1}, w, v_j, \ldots, v_{p-1}) \quad .$$

Then

$$\big(\ d\Gamma^{(p)}A\ \alpha\ \big)_{\mathbf{v}} \ := \ \sum_{j=1}^{p}\big(\ A\ \alpha_{\mathbf{v}_{-j},j}\ \big)_{v_j} \quad . \tag{6.2}$$

In particular $d\Gamma^{(1)}A = A$. For convenience we set $d\Gamma^{(0)}A$ to be zero and define $d\Gamma A := \oplus_{p=0}^{\infty}\ d\Gamma^{(p)}A$. Notice the identity

$$\big(\ d\Gamma^{(p)}A\ \alpha\ \big)_{\mathbf{v}} \ = \ \sum_{j=1}^{p}(-1)^{j+1}\big(\ A\ \alpha_{\mathbf{v}_{-j},1}\ \big)_{v_j}$$

and observe that in the case $A = P^{\ \sharp\mu}$, with $P := \{P_{w_1,w_2}\}_{w_1,w_2\in V^2}$ and $P_{w_1,w_2} : F(M) \to F(M)$ for every $w_1, w_2 \in V$, one gets the expression

$$\left(\, d\Gamma^{(p)} A \ \alpha \, \right)_{\mathbf{v}} \ = \ \sum_{j=1}^{p} (-1)^{j+1} \frac{1}{2} \int_V P_{v_j,w} \ \alpha_{w,\mathbf{v}_{-j}} \ \mu(dw) \quad .$$

Finaly, assume given $p \in \mathbb{N}_0$, $P := \{P_w\}_{w\in V}$ and $Q := \{Q_w\}_{w\in V}$ with $P_w, Q_w : F(M \times V^p) \to F(M \times V^p)$ for every $w \in V$. Then the commutator $[P, Q] \ := \ \{[P, Q]_{w_1,w_2}\}_{w_1,w_2\in V}$,

$$[P, Q]_{w_1,w_2} : F(M \times V^p) \to F(M \times V^p)$$

for every $(w_1, w_2) \in V^2$, is defined by setting

$$[P, Q]_{w_1,w_2} \ := \ P_{w_1} Q_{w_2} \ - \ Q_{w_2} P_{w_1} \quad .$$

Recall that in (5.1) we defined $\mathcal{D}^{\star\rho} := \ \frac{1}{\rho} \ \mathcal{D}^{\star} \ \rho$.

Proposition 6.2.

For every inhomogeneous discrete geometry $\rho\mu$ on M the discrete Hodge Laplacian is given by

$$\mathcal{L}_{\rho\mu} \ = \ \mathrm{Tr}_{\mu} \ \mathcal{D}^{\star\rho}\mathcal{D} \ + \ d\Gamma \ [\mathcal{D}, \mathcal{D}^{\star\rho}]^{\ \sharp\mu} \quad .$$

More explicitly we have for $\alpha \in F_a(M \times V^p)$

$$\mathrm{Tr}_{\mu} \ \mathcal{D}^{\star\rho}\mathcal{D} \ \alpha \ (\zeta, \mathbf{v}) \ = \ \frac{1}{2} \int_V \mathcal{D}^{\star\rho}_w \mathcal{D}_w \ \alpha \ (\zeta, \mathbf{v}) \ \mu(dw)$$

and in the case $p = 1$

$$[\mathcal{D}, \mathcal{D}^{\star\rho}]^{\ \sharp\mu} \ \alpha \ (\zeta, v) \ = \ \frac{1}{2} \ \int_V \ \left[\ \mathcal{D}_v \mathcal{D}^{\star\rho}_w - \mathcal{D}^{\star\rho}_w \mathcal{D}_v \ \right] \ \alpha \ (\zeta, w) \ \mu(dw) \quad .$$

So, on the level of 1-functions, Proposition 6.2 gives

$$\mathcal{L}^{(1)}_{\rho\mu} \ \alpha \ (\zeta, v) \ =$$

$$= \ \frac{1}{2} \int_V \mathcal{D}^{\star\rho}_w \mathcal{D}_w \ \alpha \ (\zeta, v) \ \mu(dw) \ + \ \frac{1}{2} \ \int_V \ \left[\ \mathcal{D}_v \mathcal{D}^{\star\rho}_w - \mathcal{D}^{\star\rho}_w \mathcal{D}_v \ \right] \ \alpha \ (\zeta, w) \ \mu(dw) \quad .$$

Before giving the proof of Proposition 6.2, we collect in the following two remarks some further useful representations of $\mathcal{L}_{\rho\mu}$, which are a consequence of it.

For this purpose we use the following notation, which will be useful also in the sequel.

Given $P := \{P_{w_1,w_2}\}_{w_1,w_2 \in V^2}$ and $a := \{a_{w_1,w_2}\}_{w_1,w_2 \in V^2}$ with $P_{w_1,w_2} : F(M \times V^p) \to F(M \times V^p)$ and with $a_{w_1,w_2} \in F(M)$ for every $w_1, w_2 \in V$, we define $aP := \{aP_{w_1,w_2}\}_{w_1,w_2 \in V^2}$, with $aP_{w_1,w_2} : F(M \times V^p) \to F(M \times V^p)$ by setting for $\alpha \in F(M \times V^p)$

$$\left(aP_{w_1,w_2} \ \alpha \right)_{\mathbf{v}} (x) \ = \ a_{w_1,w_2}(x) \left(P_{w_1,w_2} \ \alpha \right)_{\mathbf{v}} (x) \quad .$$

Moreover, we define for every $\mathbf{s} \in \{-1,1\}^2$

$$P_{\mathbf{s}} \ := \{P_{s_1 w_1, s_2 w_2}\}_{w_1,w_2 \in V^2} \quad .$$

Remark 6.3. *It follows from Proposition 6.2 using* (2.4) *that*

$$\mathcal{L}_{\rho\mu} \ = \sum_{\mathbf{s} \in \{-1,1\}^2} \operatorname{sign}(\mathbf{s}) \left\{ \ \mathrm{Tr}_\mu \ (\mathfrak{a}_\rho \mathcal{T}^2)_{\mathbf{s}} \ + \ d\Gamma \ \ (\bar{\mathfrak{a}}_\rho \mathcal{T}^2)_{\mathbf{s}}{}^{\sharp\mu} \ \right\} \quad ,$$

where $\mathfrak{a}_\rho \ := \{\mathfrak{a}_{\rho;w_1,w_2}\}_{w_1,w_2 \in V^2}$, $\bar{\mathfrak{a}}_\rho \ := \{\bar{\mathfrak{a}}_{\rho;w_1,w_2}\}_{w_1,w_2 \in V^2}$ *and* $\mathfrak{a}_{\rho;w_1,w_2}, \bar{\mathfrak{a}}_{\rho;w_1,w_2} \in F(M)$ *are given by*

$$\mathfrak{a}_{\rho;w_1,w_2} \ := \ - \ \frac{1}{\rho} \ \mathcal{T}_{w_1} \ \rho \qquad i.e. \quad \mathfrak{a}_{\rho;w_1,w_2}(\zeta) \ = \ - \ \frac{\rho(\zeta + w_1/2)}{\rho(\zeta)}$$

and

$$\bar{\mathfrak{a}}_{\rho;w_1,w_2} \ := \ \mathcal{T}_{w_1} \mathfrak{a}_{\rho;w_2,w_1} \ - \ \mathfrak{a}_{\rho;w_2,w_1} \quad .$$

Note that $\mathfrak{a}_{\rho;w_1,w_2}$ *does in fact not depend on* w_2*.*

Remark 6.4. *Let*

$$\mathfrak{r}_{\rho,w} \ := \ -\mathfrak{a}_{\rho,w,w} \ = \ \frac{\mathcal{T}_w \rho}{\rho} \quad i.e. \quad \mathfrak{r}_{\rho,w}(\zeta) \ = \ \frac{\rho(\zeta + w/2)}{\rho(\zeta)} \quad . \tag{6.3}$$

A simple computation gives

$$\mathrm{Tr}_\mu \ \mathcal{D}^{\star\rho}\mathcal{D} \ \alpha \ (\zeta, \mathbf{v}) \ = \ \int_V \mathfrak{r}_{\rho,w}(\zeta) \ \left[\ \alpha(\zeta, \mathbf{v}) - \alpha(\zeta + w, \mathbf{v}) \ \right] \ \mu(dw) \quad .$$

It follows from Proposition 6.2 that for every $\alpha \in F(M)$

$$\mathcal{L}_{\rho\mu}^{(0)} \ \alpha \ (\zeta) \ = \ \int_V \mathfrak{r}_{\rho,w}(\zeta) \ \left[\alpha(\zeta) - \alpha(\zeta + w)\right] \ \mu(dw) \quad .$$

Proof of Proposition 6.2. This is a straightforward computation, analogous to the one shown in the proof of Proposition 4.2.

Indeed, proceeding exactly as in the proof of Proposition 4.2 with $\mathcal{D}^{\star\rho}$ instead of $\mathcal{D}^{\star}$ gives

$$\delta^{*_{\rho\mu}(p)}\delta^{(p)}\ \alpha(\zeta,\mathbf{v}) \ = \ \frac{1}{2}\int_{V\setminus\pm\mathbf{v}} \mathcal{D}^{\star\rho}_{w}\mathcal{D}_{w}\ \alpha\ (\zeta,\mathbf{v})\ \mu(dw)\ +$$

$$-\ \frac{1}{2}\sum_{l=1}^{p}(-1)^{l+1}\int_{V\setminus\pm\mathbf{v}} \mathcal{D}^{\star\rho}_{w}\mathcal{D}_{v_l}\ \alpha\ (\zeta,\mathbf{v}_{\substack{+(w,1)\\-(l+1)}})\ \mu(dw)$$

and

$$\delta^{(p-1)}\delta^{*_{\rho\mu},(p-1)}\alpha(\zeta,\mathbf{v}) \ = \ \frac{1}{2}\int_{\pm\mathbf{v}} \mathcal{D}_{w}\mathcal{D}^{\star\rho}_{w}\ \alpha\ (\zeta,\mathbf{v})\ \mu(dw)\ +$$

$$+\ \frac{1}{2}\sum_{l=1}^{p}(-1)^{l+1}\ \int_{V\setminus\pm\mathbf{v}} \mathcal{D}_{v_l}\mathcal{D}^{\star\rho}_{w}\alpha\ (\zeta,\mathbf{v}_{\substack{+(w,1)\\-(l+1)}})\ \mu(dw)\quad ,$$

i.e.

$$\begin{aligned}
\mathcal{L}^{(p)}_{\rho\mu}\ \alpha\ (\zeta,\mathbf{v}) \ &= \ \delta^{*_{\rho\mu}(p)}\delta^{(p)}\ \alpha(\zeta,\mathbf{v})\ +\ \delta^{(p-1)}\delta^{*_{\rho\mu},(p-1)}\alpha(\zeta,\mathbf{v})\ = \\
&= \ \frac{1}{2}\int_{V} \mathcal{D}^{\star\rho}_{w}\mathcal{D}_{w}\ \alpha\ (\zeta,\mathbf{v})\ \mu(dw)\ \ + \\
&+\ \frac{1}{2}\int_{\pm\mathbf{v}}\ \left[\ \mathcal{D}_{w}\mathcal{D}^{\star\rho}_{w} - \mathcal{D}^{\star\rho}_{w}\mathcal{D}_{w}\ \right]\ \alpha\ (\zeta,\mathbf{v})\ \mu(dw)\ \ + \\
&+\ \frac{1}{2}\sum_{l=1}^{p}\ \int_{V\setminus\pm\mathbf{v}}(-1)^{l+1}\ \left[\ \mathcal{D}_{v_l}\mathcal{D}^{\star\rho}_{w} - \mathcal{D}^{\star\rho}_{w}\mathcal{D}_{v_l}\ \right]\ \alpha\ (\zeta,\mathbf{v}_{\substack{+(w,1)\\-(l+1)}})\ \mu(dw)\quad .
\end{aligned}$$

This gives the desired result, by observing that

$$\begin{aligned}
\left(\ d\Gamma\ [\mathcal{D},\mathcal{D}^{\star\rho}]^{\ \sharp\mu}\ \alpha\ \right)_{\mathbf{v}} \ &= \ \frac{1}{2}\int_{V}\sum_{j=1}^{p}(-1)^{j+1}\ [\mathcal{D}_{v_j}\mathcal{D}^{\star\rho}_{w} - \mathcal{D}^{\star\rho}_{w}\mathcal{D}_{v_j}]\ \alpha_{w,\mathbf{v}_{-j}}\ \mu(dw)\ \ = \\
&= \ \frac{1}{2}\sum_{j=1}^{p}\ \int_{V\setminus\pm\mathbf{v}}(-1)^{j+1}\ \left[\ \mathcal{D}_{v_j}\mathcal{D}^{\star\rho}_{w} - \mathcal{D}^{\star\rho}_{w}\mathcal{D}_{v_j}\ \right]\ \alpha_{\mathbf{v}_{\substack{+(w,1)\\-(j+1)}}}\ \mu(dw)\ \ + \\
&+\ \frac{1}{2}\sum_{j=1}^{p}\sum_{l=1}^{p}\ \left\{\ \left[\ \mathcal{D}_{v_j}\mathcal{D}^{\star\rho}_{v_l} - \mathcal{D}^{\star\rho}_{v_l}\mathcal{D}_{v_j}\ \right]\ \alpha_{\mathbf{v}_{\substack{+(v_l,1)\\-(j+1)}}}\ -\ \left[\ \mathcal{D}_{v_j}\mathcal{D}^{\star\rho}_{-v_l} - \mathcal{D}^{\star\rho}_{-v_l}\mathcal{D}_{v_j}\ \right]\alpha_{\mathbf{v}_{\substack{+(v_l,1)\\-(j+1)}}}\ \right\}\ = \\
&= \ \frac{1}{2}\sum_{j=1}^{p}\ \int_{V\setminus\pm\mathbf{v}}(-1)^{j+1}\ \left[\ \mathcal{D}_{v_j}\mathcal{D}^{\star\rho}_{w} - \mathcal{D}^{\star\rho}_{w}\mathcal{D}_{v_j}\ \right]\ \alpha_{\mathbf{v}_{\substack{+(w,1)\\-(j+1)}}}\ \mu(dw)\ \ + \\
&+\ \frac{1}{2}\int_{\pm\mathbf{v}}\ \left[\ \mathcal{D}_{w}\mathcal{D}^{\star\rho}_{w} - \mathcal{D}^{\star\rho}_{w}\mathcal{D}_{w}\ \right]\ \alpha_{\mathbf{v}}\ \mu(dw)\quad .
\end{aligned}$$

$\square$

Observe that the intertwining relations for the Hodge Laplacian, established in Prop. 4.4 for the homogeneous case, continue to hold in the inhomogeneous case thanks to Prop. 5.4. More precisely we have for every $p \in \mathbb{N}_0$, $\alpha \in F_a(M \times V^p)$

$$\mathcal{L}_{\rho\mu}^{(p+1)} \; \delta^{(p)} \; \alpha \; = \; \delta^{(p)} \; \mathcal{L}_{\rho\mu}^{(p)} \; \alpha$$

and for every $\alpha \in F_a(M \times V^{p+1})$

$$\mathcal{L}_{\rho\mu}^{(p)} \; \delta^{*_{\rho\mu}(p)} \; \alpha \; = \; \delta^{*_{\rho\mu}(p)} \; \mathcal{L}_{\rho\mu}^{(p+1)} \; \alpha \quad .$$

Consider the restriction $\mathcal{L}_{0,\rho\mu}^{(p)}$ of $\mathcal{L}_{\rho\mu}^{(p)}$ on $F_{0,a}(M \times V^p)$, the space of alternating p-functions with compact support. By definition of $\mathcal{L}_{\rho\mu}^{(p)}$ and Proposition 5.3, $\mathcal{L}_{0,\rho\mu}^{(p)}$ is a well-defined nonnegative and symmetric operator in $L_a^2(M \times V^p, \Lambda_{\rho\mu})$ for every lattice graph $\Lambda_{\rho\mu}$. In general $\mathcal{L}_{0,\rho\mu}^{(p)}$ is unbounded and may be even not essentially selfadjoint.[27] A canonical selfadjoint extension is given by the Friedrichs extension (see [88] Vol.II, Theorem X.23).

Definition 6.5. *For every lattice graph $\Lambda_{\rho\mu}$ we denote by $\mathcal{L}_{\Lambda_{\rho\mu}}^{(p)}$ the Friedrichs extension of $\mathcal{L}_{0,\rho\mu}^{(p)}$, considered as an operator in $L_a^2(M \times V^p, \Lambda_{\rho\mu})$. Moreover we set $\mathcal{L}_{\Lambda_{\rho\mu}} := \oplus_{p=0}^{\infty} \mathcal{L}_{\Lambda_{\rho\mu}}^{(p)}$.*

Recall that the Friedrichs extension is constructed via the associated symmetric bilinear form

$$F_{0,a}(M \times V^p) \ni \alpha, \beta \mapsto \langle \alpha, \mathcal{L}_{\rho\mu}^{(p)} \beta \rangle_{\Lambda_{\rho\mu}}^{(p)} \quad ,$$

whose closure[28] we shall denote by $\mathcal{E}_{\Lambda_{\rho\mu}}^{(p)}$, with domain $D(\mathcal{E}_{\Lambda_{\rho\mu}}^{(p)})$. The Friedrichs extension is then characterized by the property that for $\alpha, \beta \in D(\mathcal{E}_{\Lambda_{\rho\mu}}^{(p)})$

$$\mathcal{E}_{\Lambda_{\rho\mu}}^{(p)}(\alpha, \beta) = \langle \sqrt{\mathcal{L}_{\Lambda_{\rho\mu}}^{(p)}} \alpha, \sqrt{\mathcal{L}_{\Lambda_{\rho\mu}}^{(p)}} \beta \rangle_{\Lambda_{\rho\mu}}^{(p)} \quad . \tag{6.4}$$

Observe that $\mathcal{L}_{\Lambda_{\rho\mu}}^{(p)}$ is a nonnegative, selfadjoint and in general unbounded operator in $L_a^2(M \times V^p, \Lambda_{\rho\mu})$. Moreover it agrees on its domain $D(\mathcal{L}_{\Lambda_{\rho\mu}}^{(p)})$

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[27] Take dimension $n = 1$, a nearest neighbour discrete geometry μ and fix a lattice Λ. Take the inhomogeneity ρ satisfying $\rho(\zeta) = \frac{1}{\zeta^2}$ for large $\zeta \in \Lambda$ and $\rho(\zeta + v/2) = \zeta^3$ for large $\zeta \in \Lambda$ and for every v with $\mu(\{v\}) > 0$. Then one can show that $\mathcal{L}_{\Lambda_{\rho\mu}}^{(0)}$ is not essentially selfadjoint. For more details see [20], in particular Example 5.3.1.

[28] A bilinear form arising from a nonegative symmetric operator is always closable, see [88] Vol.II, Theorem X.23 for the abstract result, or [63] in our concrete setting.

with the formal operator, i.e. for every $\alpha \in D(\mathcal{L}^{(p)}_{\Lambda_{\rho\mu}})$

$$\mathcal{L}^{(p)}_{\Lambda_{\rho\mu}}\ \alpha = \mathcal{L}^{(p)}_{\rho\mu}\ \alpha \quad . \tag{6.5}$$

To see this observe that for every test function $\varphi \in F_{0,a}(M \times V^p)$, dropping for notational simplicity the superscripts (p), we have

$$\langle \mathcal{L}_{\Lambda_{\rho\mu}} \alpha, \varphi \rangle_{\Lambda_{\rho\mu}} = \langle \alpha, \mathcal{L}_{\Lambda_{\rho\mu}} \varphi \rangle_{\Lambda_{\rho\mu}} = \langle \alpha, \mathcal{L}_{0,\rho\mu} \varphi \rangle_{\Lambda_{\rho\mu}} = \langle \mathcal{L}_{\rho\mu} \alpha, \varphi \rangle_{\Lambda_{\rho\mu}} \quad ,$$

where in the last equality Proposition 5.3 was used.

By means of the spectral theorem one can check that $\mathcal{L}^{(p)}_{\Lambda_{\rho\mu}}$ generates an analytic contraction semigroup of angle $\pi/2$ on $L^2_a(M \times V^p, \Lambda_{\rho\mu})$, which we shall denote by

$$t \mapsto e^{-t\mathcal{L}^{(p)}_{\Lambda_{\rho\mu}}} \quad . \tag{6.6}$$

For more details on this see for example [31], in particular Example 3.27 and Corollary 4.7 therein.

7. Probabilistic interpretation of $\mathcal{L}^{(0)}_{\rho\mu}$

Assume given an inhomogeneous discrete geometry $\rho\mu$. In the present section we focus our attention on $\mathcal{L}^{(0)}_{\rho\mu}$, the restriction of the discrete Hodge Laplacian to the level of functions. We shall consider the families of generators $\{ \mathcal{L}^{(0)}_{\Lambda_{\rho\mu}} \}$, of semigroups $\{t \mapsto e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}\}$ and of bilinear forms $\{ \mathcal{E}^{(0)}_{\Lambda_{\rho\mu}} \}$ indexed by the set of lattice graphs corresponding to $\rho\mu$, as defined in Definition 6.5 and in (6.4), (6.6).

In the first subsection we will state some basic properties linked to the Markovian character of these families. In particular each $\mathcal{E}^{(0)}_{\Lambda_{\rho\mu}}$ turns out to be a regular Dirichlet form (see Proposition (7.4)); each semigroup $t \mapsto e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}$ is Markovian, irreducible (see Remark 7.5) and is obtained through an approximation involving a sequence of compacta exhausting M (see Remark 7.6).

In the second subsection we introduce the (in general substochastic) transition function $P^{\rho\mu}$ induced by the discrete geometry $\rho\mu$ (see (7.18)).[29] Assuming that the transition function is stochastic, i.e. no loss of mass occurs, we shall associate to it a Markovian family of probability measures $(\mathbb{P}^{\rho\mu}_{\zeta})$ on a suitable path space [30], see (7.21). Its link to the operator $\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}$ is made explicit in formula (7.22). The corresponding canonical Markov process evolves in continuous time and is of pure jump type.

The considerations in this section are known or even standard. Moreover they are not strictly needed for the subsequent sections. Nevertheless it is useful to clarify the probabilistic framework in the present context and to

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[29]We use here the following standard terminology: a function $P : [0,\infty) \times A \times \mathcal{A} \to [0,\infty)$ is a (time-homogeneous) substochastic transition function on the measurable space $(A, \mathcal{A})$ if

(i) $(t,\zeta) \mapsto P(t,\zeta,\cdot)$ is a measure with $P(t,\zeta,A) \le 1$ for every $t \in (0,\infty)$, $\zeta \in A$.
(ii) $(t,S) \mapsto P(t,\cdot,S)$ is measurable for every $t \in [0,\infty)$, $S \in \mathcal{A}$
(iii) $P(t+s,\zeta,S) = \int_A P(t,\zeta,d\eta)\ P(s,\eta,S)$ for every $t,s \in [0,\infty)$, $\zeta \in A$ and $S \in \mathcal{A}$

If equality holds in (i) P is called stochastic.

[30]In fact there are standard procedures to associate a Markovian family to the transition function even in the more general substochastic case. A way is to extend the state space to the set $M \cup \dagger$ where the additional point $\dagger$ represents the "cemetery" for the process. We restrict to the nonexplosive (i.e. stochastic) case to avoid unnecessary technical and notational complications.

fix some notation for occasional reference to it. Indeed the main motivation for this work and most of the heuristics behind it originate from this probabilistic metaphor. We follow here basically [62],[63] for the considerations concerning Dirichlet forms. For more background on continuous time Markov chains see also [74], [84], [93] and [16].

Remark 7.1. *An analogous probabilistic interpretation for $\mathcal{L}^{(p)}_{\Lambda_{\rho\mu}}$ in the case $p > 0$ is not attempted in this work and postponed to subsequent research. For probabilisitc interpretations of (inhomogeneous) Hodge Laplacians in continuous space setting and $p > 0$ we refer the reader to* [99]*. See also* [56]*.*

Markovian properties of $\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}$, $t \mapsto e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}$ and $\mathcal{E}^{(0)}_{\Lambda_{\rho\mu}}$.

Fix an inhomogeneous discrete geometry $\rho\mu$ on the affine space M. Recall that in (6.3) we defined for $\zeta \in M$ and $v \in V$

$$\mathfrak{r}_\rho(\zeta, v) \;:=\; \frac{\rho(\zeta + v/2)}{\rho(\zeta)} \quad .$$

We shall henceforth refer to $\mathfrak{r}_\rho(\zeta, v)\ \mu(\{v\})$ as the **(jump) rate** from ζ to $\zeta + v$ induced by the discrete geometry $\rho\mu$. By Remark 6.4

$$\mathcal{L}^{(0)}_{\rho\mu}\ \alpha\ (\zeta) \;=\; \int_V \mathfrak{r}_\rho(\zeta, w)\ \left[\alpha(\zeta) - \alpha(\zeta + w)\right] \mu(dw) \quad . \tag{7.1}$$

Remark 7.2. *Observe that the jump rates obey the following* **detailed balance condition** *with respect to ρ: for every $\zeta \in M$ and $v \in V$*

$$\rho(\zeta)\ \mathfrak{r}_\rho(\zeta, v)\ \mu(\{v\}) \;=\; \rho(\zeta + v)\ \mathfrak{r}_\rho(\zeta + v, -v)\ \mu(\{-v\}) \quad . \tag{7.2}$$

We shall also introduce some notation making precise the notion of being local with respect to the discrete geometry μ. Given $\zeta_0 \in M$, we denote by $\mathcal{U}_\mu(\zeta_0)$ the set of neighbours of ζ_0 relative to μ: i.e. $\zeta \in \mathcal{U}_\mu(\zeta_0)$ if and only if $\mu(\{\zeta - \zeta_0\}) > 0$. We say that a property holds μ-locally at $\zeta_0 \in M$ if it holds true for every $\zeta \in \mathcal{U}_\mu(\zeta_0)$.

An important feature of $\mathcal{L}^{(0)}_{\rho\mu}$ is expressed by the following (versions of the) minimum principle. First of all, since the jump rates are nonnegative, it is clear by looking at (7.1) that for $\alpha : M \to \mathbb{R}$

$$\left\{\ \zeta_0 \text{ is a } \mu\text{-local minimum of } \alpha\ \right\} \implies \mathcal{L}_{\rho\mu}\alpha\ (\zeta_0) \leq 0 \quad . \tag{7.3}$$

Indeed, the following refinement is easily seen to hold true. Let ζ_0 be a μ-local minimum of α. Then we have the two implications

$$\begin{aligned} &\left\{\ \zeta_0 \text{ also is a } \mu\text{-local maximum of } \alpha \text{ (i.e. } \alpha \text{ is locally constant at } \zeta_0)\ \right\} \\ &\qquad\qquad\Longrightarrow \left\{\ \mathcal{L}_{\rho\mu}\alpha\ (\zeta_0) = 0\ \right\} \end{aligned} \tag{7.4}$$

and

$$\left\{\ \zeta_0 \text{ is not a } \mu\text{-local maximum of } \alpha\ \right\} \Longrightarrow \left\{\ \mathcal{L}_{\rho\mu}\alpha\ (\zeta_0) < 0\ \right\}\ . \tag{7.5}$$

Recall from Section 3 that the (finite) support of μ generates a lattice in V, which is denoted bt Γ. This ellipticity assumption leads to the following global statement.

Proposition 7.3 (Elliptic minimum principle)**.**
Let $\alpha : M \to \mathbb{R}$ and $\Lambda \in M/\Gamma$.

(i) *Assume $\mathcal{L}_{\rho\mu}\alpha \geq 0$ on Λ and that α admits a global minimum on Λ. Then α is constant on Λ.*

(ii) *Let $z > 0$. Assume $(\mathcal{L}_{\rho\mu} + z)\ \alpha \geq 0$ on Λ and that α admits a nonpositive global minimum on Λ. Then α is constant on Λ. In fact $\alpha \equiv 0$ on Λ.*

Proof. (i): Let ζ_0 be a global minimum of α. Then by (7.5), the assumption $\mathcal{L}_{\rho\mu}\alpha(\zeta_0) \geq 0$ implies

$$\alpha(\zeta_1) = \alpha(\zeta_0) \text{ for every } \zeta_1 \in \mathcal{U}_\mu(\zeta_0)\ \ .$$

In particular every $\zeta_1 \in \mathcal{U}_\mu(\zeta_0)$ also is a global minimum for α in Λ. For generic $\zeta \in \Lambda$ take a sequence $\{\zeta_0, \zeta_1, \ldots, \zeta_p = \zeta\}$ with $\zeta_{i+1} \in \mathcal{U}_\mu(\zeta_i)$ and $\mu(\{\zeta_{i+1} - \zeta_i\}) > 0$. Then repeating the above argument step after step for the whole sequence gives $\alpha(\zeta) = \alpha(\zeta_0)$.

The argument for (ii) is analogous. We report it for completeness. Observe that (7.5) gives

$$\begin{aligned} &\left\{\ (\mathcal{L}_{\rho\mu} + z)\ \alpha\ (\zeta) \geq z\alpha(\zeta)\ \right\} \\ &\Longrightarrow \left\{\ \zeta \text{ is not a } \mu\text{-local minimum of } \alpha \text{ or } \alpha \text{ is locally constant at } \zeta\ \right\}\ . \end{aligned} \tag{7.6}$$

Let ζ_0 be a nonpositive global minimum of α. Then (7.6) together with the assumption

$$(\mathcal{L}_{\rho\mu} + z)\ \alpha\ (\zeta_0) \geq 0 \tag{7.7}$$

implies again

$$\alpha(\zeta_1) = \alpha(\zeta_0) \text{ for every } \zeta_1 \in \mathcal{U}_\mu(\zeta_0)\ \ .$$

In particular every $\zeta_1 \in \mathcal{U}_\mu(\zeta_0)$ also is a nonpositive global minimum for α in Λ. Moreover $\alpha(\zeta_0) = 0$, since by (7.4) $\alpha(\zeta_0) = \frac{1}{z}(\mathcal{L}_{\rho\mu} + z)\ \alpha\ (\zeta_0)$, and the latter is nonnegative by (7.7). The conclusion is achieved by proceeding iteratively as in (i). $\square$

Consider the family of closed nonnegative symmetric bilinear forms $\{\ \mathcal{E}^{(0)}_{\Lambda_{\rho\mu}}\ \}$ indexed by the set of lattice graphs in M corresponding to the discrete geometry $\rho\mu$, as defined in (6.4). Observe that for $\alpha \in F_0(M)$ (recall that the latter denotes the set of real functions on M which vanish outside a compact set of M) and every lattice graph $\Lambda_{\rho\mu}$

$$\mathcal{E}^{(0)}_{\Lambda_{\rho\mu}}(\alpha,\alpha)\ =\ \langle \alpha, \mathcal{L}_{\rho\mu}\alpha\rangle^{(0)}_{\Lambda_{\rho\mu}}\ =\ \langle \delta\alpha, \delta\alpha\rangle^{(0)}_{\Lambda_{\rho\mu}}\ =$$
$$\int_M \int_V \big[\alpha(\zeta + w/2) - \alpha(\zeta - w/2)\big]^2\ \rho(\zeta)\ \mu(dw)\ \Lambda(d\zeta)\ =$$
$$\int_M \int_V \big[\alpha(\zeta + w) - \alpha(\zeta)\big]^2\ \rho(\zeta + w/2)\ \mu(dw)\ \Lambda(d\zeta)$$

or, using the jump rates,

$$\mathcal{E}^{(0)}_{\Lambda_{\rho\mu}}(\alpha,\alpha)\ =\ \int_M \int_V \big[\alpha(\zeta + w) - \alpha(\zeta)\big]^2\ \mathfrak{r}_\rho(\zeta, w)\ \mu(dw)\ \ \rho(\zeta)\ \Lambda(d\zeta)\ \ . \tag{7.8}$$

In the sequel we use standard terminology and results in the theory of Dirichlet forms. For more informations see in particular [35], [75] [62] and [63].

Proposition 7.4. *$\mathcal{E}^{(0)}_{\Lambda_{\rho\mu}}$ is a regular Dirichlet form for every lattice graph $\Lambda_{\rho\mu}$.*

Proof. The Markovian property follows from the representation (7.8). In fact standard arguments imply that it is sufficient to check the Markovian property on the smaller domain $F_0(M)$. Regularity is straightforward by construction. For more details see [62]. $\square$

Since $\mathcal{E}^{(0)}_{\Lambda_{\rho\mu}}$ is a Dirichlet form it follows by standard arguments (see [35]) that the semigroup $t \mapsto e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}$ is Markovian for every lattice graph $\Lambda_{\rho\mu}$, i.e. for $\alpha \in L^2(M, \Lambda_{\rho\mu})$

$$0 \le \alpha \le 1\ \ \Rightarrow\ \ 0 \le e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}\ \alpha \le 1\ \ ,$$

with the inequalitites to be understood to hold $d\Lambda$-almost everywhere. In particular for every $t \in [0,\infty)$ the operator $e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}$ is positivity preserving, i.e.

$$\Big(\;\alpha \in L^2(M,\Lambda_{\rho\mu}) \;\text{ and }\; \alpha \geq 0 \;\Big) \;\;\Rightarrow\;\; e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}\alpha \geq 0 \;\; . \tag{7.9}$$

This is easily seen by applying the semigroup to the sequence $\big(\frac{1}{k}(\alpha \wedge k) \big)_{k\in\mathbb{N}_*}$, where $\wedge$ denotes the pointwise minimum between two functions. Equivalent to property (7.9) is

$$|e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}\;\alpha| \;\leq\; e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}\;|\alpha| \tag{7.10}$$

for every $\alpha \in L^2(M,\Lambda_{\rho\mu})$ (consider $|\alpha| \pm \alpha$).

The Markovian property permits to extend (uniquely) each $e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}$ so that it can be considered as a contraction on the space $L^1(M,\Lambda_{\rho\mu})$. In fact, for every $\alpha \in L^1(M,\Lambda_{\rho\mu}) \cap L^2(M,\Lambda_{\rho\mu})$ and compact set $K \subset M$, using also the selfadjoitness of $e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}$ and (7.10), we have

$$\begin{aligned}\int_K |e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}\;\alpha|\;\rho\; d\Lambda \;&\leq\; \int_K (e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}\;|\alpha|)\;\rho\; d\Lambda \;= \\ =\; \int_M |\alpha|\; (e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}\;\mathbb{1}_K)\;\rho\; d\Lambda &\leq \int_M |\alpha|\;\rho\; d\Lambda \;\; .\end{aligned} \tag{7.11}$$

Taking a sequence $\{K_m\}$ of compacta exhausting M gives the claimed property.[31] If the contrary is not explicitly mentioned we will always mean by $t \mapsto e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}$ the semigroup on $L^2(M,\Lambda_{\rho\mu})$.

In the next subsection we shall exploit further important properties of $t \mapsto e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}$, which we collect in the following two remarks.

Remark 7.5. *The semigroup $t \mapsto e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}$ is not only positive but also irreducible (or ergodic in the terminology of* [88]*). Recall that a positive semigroup is irreducible if its resolvent is positivity improving (i.e. mapping nontrivial $d\Lambda$-a.e. nonnegative functions to $d\Lambda$-a.e. strictly positive functions) for sufficiently big real values in the resolvent set. The Markovian property is in general not sufficient for this. To show irreducibility in the case of $t \mapsto e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}$ one can use the elliptic minimum principle (see Proposition 7.3). More precisely: let $\beta \in L^2(M,\Lambda_{\rho\mu})$ with $\beta \geq 0$ and β not identically zero. Fix $z \geq 0$ and let $\alpha := (\mathcal{L}_{\Lambda_{\rho\mu}} + z)^{-1}\;\beta$. Since $t \mapsto e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}$*

[31] It is well-known that the Markovian property permits to define contraction semigroups $t \mapsto e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}$ on $L^q(M;\Lambda_{\rho\mu})$ for every $q \in [1,\infty]$. These semigroups agree on their common domain and are in general strongly continuous only for $q \in [1,\infty)$ For details see [24], in particular Theorem 1.4.1, or [88] Theorem XIII.51.

is positive it follows that $\alpha \geq 0$. Moreover using (6.5) *we have for every $\zeta \in \Lambda$*

$$(\mathcal{L}_{\rho\mu} + z)\ \alpha\ (\zeta)\ =\ \beta(\zeta)\ \geq\ 0\ \ . \tag{7.12}$$

If there did exist a $\zeta_0 \in \Lambda$ with $\alpha(\zeta_0) = 0$, Proposition 7.3 (ii) would force $\alpha \equiv 0$ on Λ. It would follow from (7.12) *that $\beta \equiv 0$ which is in contradiction with the definition of β.*

Using analyticity of the semigroup, it follows from general principles (see for example [80]*, Theorem 3.2, p.306) that irreducibility of the semigroup implies automatically the stronger property that $e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}$ is positivity improving for every $t \in (0, \infty)$.*

Remark 7.6. *Let $\{\mathcal{K}_n\}$ be an increasing sequence of compact subsets of M such that $M = \cup \mathcal{K}_n$. We shall consider for every n the Hilbert space $L^2(\mathcal{K}_n, \Lambda_{\rho\mu})$ consisting of real functions on $\mathcal{K}_n$, with scalar product given by*

$$\langle \alpha, \beta \rangle_n\ :=\ \sum_{\zeta \in \Lambda \cap \mathcal{K}_n} \alpha(\zeta)\ \beta(\zeta)\ \rho(\zeta)\ \ .$$

Notice that through zero extension outside $\mathcal{K}_n$ each $L^2(\mathcal{K}_n, \Lambda_{\rho\mu})$ is canonically embedded into $L^2(M, \Lambda_{\rho\mu})$. Denote by $i_{\mathcal{K}_n} : L^2(\mathcal{K}_n, \Lambda_{\rho\mu}) \to L^2(M, \Lambda_{\rho\mu})$ this embedding and by $\pi_{\mathcal{K}_n} : L^2(M, \Lambda_{\rho\mu}) \to L^2(\mathcal{K}_n, \Lambda_{\rho\mu})$ its adjoint, i.e. the canonical projection onto $L^2(\mathcal{K}_n, \Lambda_{\rho\mu})$.

For every $\mathcal{K}_n$ we consider the (bounded) operator $\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}, \mathcal{K}_n}$ on $L^2(\mathcal{K}_n, \Lambda_{\rho\mu})$ obtained from $\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}$ by incorporating Dirichlet boundary conditions, i.e.

$$\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}, \mathcal{K}_n} := \pi_{\mathcal{K}_n}\ \mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}\ i_{\mathcal{K}_n}\ \ .$$

Observe that $\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}, \mathcal{K}_n}$ is nonnegative and selfadjoint, so the semigroup $t \mapsto e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}, \mathcal{K}_n}}$ is well-defined.

In [62, Prop. 2.7] *it is proven that for any $\alpha \in F_0(M)$ and $t \in [0, \infty)$*

$$\lim_{n \to \infty} i_{\mathcal{K}_n}\ e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}, \mathcal{K}_n}}\ \pi_{\mathcal{K}_n}\ \alpha = e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}\ \ .\ \alpha \tag{7.13}$$

For this result, which again does not hold in general for Markovian semigroups (for example it can not hold if we consider other selfadjoint extensions of $\mathcal{L}^{(0)}_{0,\rho\mu}$), it is crucial that we defined $\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}$ as the Friedrichs extension of an operator defined on $F_0(M)$.

The transition function $P_t^{\rho\mu}$.

We shall consider the Cauchy problem associated with $\mathcal{L}^{(0)}_{\rho\mu}$. In the sequel the dot over a function denotes as usual differentiation with respect to the variable t.

Definition 7.7 (**Cauchy problem associated with $\mathcal{L}^{(0)}_{\rho\mu}$).** *We say that a function $[0,\infty)\times M \ni (t,\zeta) \mapsto u_t(\zeta) \in \mathbb{R}$ is a solution of the Cauchy problem associated with $\mathcal{L}^{(0)}_{\rho\mu}$, corresponding to the initial value $f : M \to \mathbb{R}$, if for every $\zeta \in M$ the function $t \mapsto u_t(\zeta)$ is continuous on $[0,\infty)$, differentiable on $(0,\infty)$ and if*

$$\begin{cases} \dot{u}_t(\zeta) &= -\mathcal{L}^{(0)}_{\rho\mu}\ u_t\ (\zeta) \quad \text{for } t>0, \zeta \in M \\ u_0(\zeta) &= f(\zeta) \quad \text{for } \zeta \in M \end{cases} . \tag{7.14}$$

We look at the Cauchy problem above as a family of ordinary differential equations. Note that the equation for $t \mapsto u_t(\zeta)$ is coupled to the equation of $t \mapsto u_t(\eta)$ if and only if $\zeta - \eta \in \Gamma$.

Observe also that for a solution u as defined in Definition 7.7 the time derivative $t \mapsto \dot{u}_t(\zeta)$ can be extended by continuity to $t = 0$ using just the continuity of $t \mapsto u_t(\zeta)$ and the first equation in (7.14).

Remark 7.8. *If the initial value f in* (7.14) *is nonnegative, then any corresponding solution u of the Cauchy problem remains nonnegative for every $t \in (0,\infty)$. This is an easy consequence of* (7.3)*. In fact, assume on the contrary the existence of t, ζ such that $u_t(\zeta) < 0$. Then, with*

$$t_0 := \inf\ \{t > 0 : \text{ there exists } \zeta \in M \text{ s.t. } u_t(\zeta) < 0\} \quad ,$$

we have the existence of a point ζ_0 with $u_{t_0}(\zeta_0) = 0$, $u_{t_0}(\zeta) \geq 0$ for $\zeta \in M$ and $\dot{u}_{t_0}(\zeta_0) < 0$. On the other hand Property (7.3) *together with the first equation in* (7.14) *imply that $\dot{u}_{t_0}(\zeta_0) \geq 0$, giving a contradiction.*

The following result is a consequence of (7.3). A proof can be found in [57, Theorem 1.3.2]

Proposition 7.9 (Parabolic minimum principle)**.**

Let $\Lambda \in M/\Gamma$, $\mathcal{K}$ a finite subset of Λ, $T > 0$ and consider a function $[0,T] \times \Lambda \ni (t,\zeta) \mapsto u_t(\zeta) \in \mathbb{R}$ such that $t \mapsto u_t(\zeta)$ is continuous and *differentiable in* $[0,T]$ *for every* $\zeta \in \mathcal{K}$*. If*

$$\begin{cases} \dot{u}_t(\zeta) \geq -\mathcal{L}_{\rho\mu} u_t\ (\zeta) & \text{for } t \in (0,T], \zeta \in \mathcal{K} \\ u_0(\zeta) \geq 0 & \text{for } \zeta \in \mathcal{K} \\ u_t(\zeta) \geq 0 & \text{for } (t,\zeta) \in [0,T] \times (\Lambda \setminus \mathcal{K}) \end{cases} \quad . \tag{7.15}$$

Then $u \geq 0$ *on* Λ*.*

Fix an initial value $f : M \to \mathbb{R}$. A solution u of (7.14) corresponding to f is called minimal if $u \leq v$ for every other solution corresponding to f. Observe that a minimal solution is by definition unique. We denote in the sequel for every $\zeta \in M$ by $\mathbb{1}_\zeta$ the indicator function of the set $\{\zeta\}$ and by Λ_ζ the lattice $\zeta + \Gamma$.

Theorem 7.10 (Existence of the fundamental solution)**.**
There exists a function $p_{\rho\mu} : [0,\infty) \times M \times M \to \mathbb{R}$ *such that for every* $\eta \in M$ $(t,\zeta) \mapsto p_{\rho\mu}(t,\zeta,\eta)$ *is a minimal solution of the Cauchy problem* (7.7) *associated with* $\mathcal{L}^{(0)}_{\rho\mu}$ *corresponding to the initial function* $\mathbb{1}_\eta$*. Moreover* $p_{\rho\mu}$ *has the following properties:*

(i) $p_{\rho\mu} \geq 0$

(ii) *for every* $t \geq 0$ *and* $\zeta \in M$

$$\int_M p_{\rho\mu}(t,\zeta,\eta)\ \Lambda_\zeta(d\eta)) \leq 1 \quad .$$

(iii) *for every* $t, s \geq 0$ *and* $\zeta, \eta \in M$

$$p_{\rho\mu}(t+s,\zeta,\eta) = \int_M p_{\rho\mu}(t,\zeta,\zeta')\ p_{\rho\mu}(s,\zeta',\eta)\ \Lambda_\zeta(d\zeta') \quad .$$

(iv) *for every* $t \geq 0$ *and* $\zeta, \eta \in M$

$$\rho(\zeta)\ p_{\rho\mu}(t,\zeta,\eta) = \rho(\eta)\ p_{\rho\mu}(t,\eta,\zeta) \quad .$$

(v) *for every* $t > 0$ *and* $\zeta, \eta \in M$

$$\begin{cases} p_{\rho\mu}(t,\zeta,\eta) > 0 & \text{if } \zeta - \eta \in \Gamma \\ p_{\rho\mu}(t,\zeta,\eta) = 0 & \text{otherwise} \end{cases} \quad .$$

Moreover $p_{\rho\mu}$ *has the representation*

$$p_{\rho\mu}(t,\zeta,\eta) = \begin{cases} e^{-t\mathcal{L}_{\Lambda\rho\mu}}\mathbb{1}_\eta(\zeta) & \text{if } \zeta,\eta \in \Lambda \text{ for some } \Lambda \in M/\Gamma \\ 0 & \text{otherwise} \end{cases} \quad . \tag{7.16}$$

The function $p_{\rho\mu}$ is called the **fundamental solution** of the Cauchy problem (7.14). In another current terminology $p_{\rho\mu}$ is referred to as the heat kernel, and the name heat equation is used for the Cauchy problem. In the language of probability the Cauchy problem takes the name of Kolmogorov's backward[32] equation. There are several well known strategies to prove the above theorem. For completeness we report here one, which exploits the L^2 semigroup $e^{-t\mathcal{L}^{(0)}_{\Lambda_{\rho\mu}}}$ and its basic properties derived in the last subsection using the Dirichlet form $\mathcal{E}^{(0)}_{\Lambda_{\rho\mu}}$. This has the advantage of giving immediately the representation (7.16).

Proof of Theorem 7.10.

Define $p_{\rho\mu}$ as in (7.16). Then standard semigroup theory (see for example [31, Prop. 6.2, p.45]) together with (6.5) give that $p_{\rho\mu}$ is a solution of the considered Cauchy problem.

Property (i) is clear since $t \mapsto e^{-t\mathcal{L}_{\Lambda_{\rho\mu}}}$ is positivity preserving for every lattice graph $\Lambda_{\rho\mu}$, see (7.9). (In fact (i) must hold a priori due to Remark 7.8.)

Property (ii) follows since $t \mapsto e^{-t\mathcal{L}_{\Lambda_{\rho\mu}}}$ is a contraction in $L^1(M;\Lambda_{\rho\mu})$ for every lattice graph $\Lambda_{\rho,\mu}$, see (7.11) . In fact, denoting by $\Lambda_{\zeta,\rho\mu}$ the lattice graph with vertices Λ_ζ, we have

$$\int_M p_{\rho\mu}(t,\zeta,\eta)\ \Lambda_\zeta(d\eta)\ =\ \int_M e^{-t\mathcal{L}_{\Lambda_{\zeta,\rho\mu}}}\mathbb{1}_\eta\ (\zeta)\ \Lambda_\zeta(d\eta)\ =$$

$$=\ \int_M (e^{-t\mathcal{L}_{\Lambda_{\zeta,\rho\mu}}}\frac{\mathbb{1}_\eta}{\rho(\eta)})\ (\zeta)\ \rho(\eta)\ \Lambda_\zeta(d\eta)\ \le\ \int_M \frac{\mathbb{1}_\eta(\zeta)}{\rho(\eta)}\ \rho(\eta)\ \Lambda_\zeta(d\eta)\ =\ 1\ \ .$$

(iii) is due to the semigroup property of $t \mapsto e^{-t\mathcal{L}_{\Lambda_{\rho\mu}}}$, and (iv) to its selfadjointness:

$$\begin{aligned}\rho(\zeta)\ p_{\rho\mu}(t,\zeta,\eta) &= \int_M (e^{-t\mathcal{L}_{\Lambda_{\eta,\rho\mu}}}\mathbb{1}_\eta)\ \mathbb{1}_\zeta\ \rho\ d\Lambda_\zeta = \\ &= \int_M \mathbb{1}_\eta\ (e^{-t\mathcal{L}_{\Lambda_{\eta,\rho\mu}}}\mathbb{1}_\zeta)\ \rho\ d\Lambda_\zeta = \\ &\quad p_{\rho\mu}(t,\eta,\zeta)\ \rho(\eta)\ \ .\end{aligned}$$

[32]Backward hints to the fact that the transition function is reconstructed from the infinitesimal properties by fixing the arrival state η and determining the starting states of the particles which reached η in short time t.

Property (v) is implied by the irreducibility of $t \mapsto e^{-t\mathcal{L}_{\Lambda_{\rho\mu}}}$, see Remark 7.5.

To prove minimality, fix $\eta \in M$ and let $\tilde{p}$ be another solution of the considered Cauchy problem. If $\zeta \notin \Lambda_\eta$ there is nothing to prove, since by Remark 7.8 $\tilde{p}(t,\zeta) \geq 0 = p_{\rho\mu}(t,\zeta)$.

So it is enough to consider ζ variable in Λ_η. Recall the notation of Remark 7.6 and define for $\zeta \in \Lambda_\eta$, $t \in [0,\infty)$

$$p_n(t,\zeta) := i_{\mathcal{K}_n} \; e^{-t\mathcal{L}_{\Lambda_\eta,\rho\mu,\mathcal{K}_n}} \; \pi_{\mathcal{K}_n} \; \mathbb{1}_\eta(\zeta)$$

for an increasing sequence $\{\mathcal{K}_n\}$ of compact subsets of M such that $M = \cup\mathcal{K}_n$. Again by general principles it follows that p_n satisfies the Cauchy problem with Dirichlet boundary conditions, i.e. $t \mapsto p_n(t,\zeta)$ is differentiable for every $\zeta \in \Lambda_\eta$ and

$$\begin{cases} \dot{p}_n(t,\zeta) = -\mathcal{L}_{\rho\mu} \; p_n \; (t,\zeta) \quad \text{ for } t \in (0,\infty), \zeta \in \mathcal{K}_n \\ p_n(0,\zeta) = \mathbb{1}_\eta(\zeta) \quad \text{ for } \zeta \in \Lambda_\eta \\ p_n(t,\zeta) = 0 \quad \text{ for } (t,\zeta) \in [0,\infty) \times (\Lambda_\eta \cap \mathcal{K}_n^c) \end{cases} . \tag{7.17}$$

It follows that $u_n := \tilde{p} - p_n$ satisfies the assumptions of Proposition 7.9 with $\Lambda = \Lambda_\eta$, so $\tilde{p} \geq p_n$. Finally, using the approximation (7.13) gives $\tilde{p} \geq p_{\rho\mu}(\cdot,\cdot,\eta)$ as claimed. □

For every $t \in [0,\infty)$, $\zeta \in M$ and $S \subset M$ we define

$$P_t^{\rho\mu}(\zeta, S) := \int_S p_{\rho\mu}(t,\zeta,\eta) \; \Lambda_\zeta(d\eta) \; . \tag{7.18}$$

Properties (i) to (iii) in Theorem 7.10 imply that $(t,\zeta,S) \mapsto P_t^{\rho\mu}(\zeta,S)$ is a substochastic transition function on $(M,\mathcal{S})$, where $\mathcal{S}$ denotes the set of all subsets of M. We refer to it as the **transition function associated with** $\rho\mu$.[33] It shall be interpreted as giving the probability to reach the set S at time t when starting at ζ. Since

$$\int_{\{\eta\}} p_{\rho\mu}(t,\zeta,\zeta') \; \Lambda_\zeta(d\zeta') = \begin{cases} p_{\rho\mu}(t,\zeta,\eta) & \text{if } \zeta - \eta \in \Gamma \\ 0 & \text{otherwise} \end{cases}$$

and since, by Property (v), $p_{\rho\mu}(t,\zeta,\eta) = 0$ if $\zeta - \eta \neq \Gamma$, we have that $p_{\rho\mu}(t,\zeta,\eta)$ gives the probability to reach η at time t when starting at ζ.

[33] By Property (v) in Theorem (7.10), we see that $\zeta \mapsto P_t^{\rho\mu}(\zeta,S)$ is measurable also with respect to the Borel sigma algebra $\mathcal{B}$ of M. It follows that the restriction of $P^{\rho\mu}$ to $[0,\infty) \times M \times \mathcal{B}$ is a substochastic transition function on $(M,\mathcal{B})$.

Fix a lattice $\Lambda \in M/\Gamma$. Property (v) asserts that starting from $\zeta \in \Lambda$ the probability to leave Λ at some time t is zero (i.e Λ is an absorbing class). Moreover for every $\zeta, \eta \in \Lambda$ there exists a $t \geq 0$ (in fact every $t \geq 0$ does well) such that one can go in time t from ζ to η with positive probability (i.e. Λ is a communicating class). Therefore the partitioning $M = \sqcup_{\Lambda \in M/\Gamma} \Lambda$ decomposes the state space into absorbing communicating classes. This is not surprising and just reflects our choice of the support of μ. It is therefore natural to consider for every lattice Λ and $t \geq 0$ the restriction $P_t^{\Lambda_{\rho\mu}}$ of $P_t^{\rho\mu}$ to $(\Lambda, \mathcal{S} \cap \Lambda)$. We call $P^{\Lambda_{\rho\mu}} : t \mapsto P_t^{\Lambda_{\rho\mu}}$ the **transition function associated with the lattice graph** $\Lambda_{\rho\mu}$. Observe that $P^{\Lambda_{\rho\mu}}$ is irreducible, i.e. the whole state space Λ is a communicating class with respect to it. Moreover by Property (iv) it is reversible with respect to the measure given by the restriction of ρ to Λ.

In general the Cauchy problem (7.14) does not have unique solutions. In fact (see [62, Theorem 1]) unique solvability for bounded initial data is equivalent to $P^{\rho\mu}$ being stochastic, i.e. to

$$\int_M p_{\rho\mu}(t, \zeta, \eta)\ \Lambda_\zeta(d\eta) = 1 \tag{7.19}$$

for every $\zeta \in M$.

A sufficient condition for (7.19) to hold is given by (see [74, Corollary 2.34, p.76])

$$\sup_{\zeta \in M} \int_V \mathfrak{r}_\rho(\zeta, w)\ \mu(dw) < \infty$$

with $\mathfrak{r}_\rho$ as defined in (6.3).

In the rest of this section we shall make for simplicity the following assumption.

Assumption I.1. *The transition function $P^{\rho\mu}$ associated to $\rho\mu$ is stochastic.*

Consider the set $M^{[0,\infty)}$ equipped with the smallest sigma algebra such that for every $t \in [0, \infty)$ the canonical projection $\tilde{X}_t : M^{[0,\infty)} \to (M, \mathcal{B})$ given by $\tilde{X}_t(\omega) := \omega_t$ is measurable. Under the above assumption, by the classical Kolmogorov extension theorem there exists for every $\zeta \in M$ a unique probability measure $\tilde{\mathbb{P}}_\zeta^{\rho\mu}$ on $M^{[0,\infty)}$ satisfying

$$\begin{aligned} &\tilde{\mathbb{P}}_\zeta^{\rho\mu}(\tilde{X}_{t_1} = \zeta_1, \dots, \tilde{X}_{t_n} = \zeta_n) = \\ &= P_{t_1}^{\rho\mu}(\zeta, \zeta_1)\ P_{t_2-t_1}^{\rho\mu}(\zeta_1, \zeta_2)\ \dots\ P_{t_n-t_{n-1}}^{\rho\mu}(\zeta_{n-1}, \zeta_n) \end{aligned} \tag{7.20}$$

for every $n \in \mathbb{N}_*$ and $t_1 \leq \dots \leq t_n \in [0, \infty)$.

In fact standard arguments (see [74, Theorem 2.37, p.77]) show that it is possible to construct probability measures satisfying (7.20) on a much more regular path space. More precisley, fix $\Lambda \in M/\Gamma$ and let

$$\begin{aligned} \Omega_\Lambda := \{\omega : [0, \infty) \to \Lambda \text{ s. t. } \omega \text{ is right continuous} \\ \text{with finitely many jumps in any finite interval}\} \quad , \end{aligned}$$

equipped with the smallest sigma algebra such that for every $t \in [0, \infty)$ the canonical projection $X_t^\Lambda : \Omega_\Lambda \to (\Lambda, \mathcal{S} \cap \Lambda)$ given by $X_t^\Lambda(\omega) = \omega_t$ is measurable. Then for every $\zeta \in \Lambda$ there exists a unique measure $\mathbb{P}_\zeta^{\rho\mu}$ on Ω_Λ satisfying

$$\begin{aligned} &\mathbb{P}_\zeta^{\rho\mu}(X_{t_1}^\Lambda = \zeta_1, \dots, X_{t_n}^\Lambda = \zeta_n) = \\ &= P_{t_1}^{\rho\mu}(\zeta, \zeta_1)\ P_{t_2-t_1}^{\rho\mu}(\zeta_1, \zeta_2)\ \dots\ P_{t_n-t_{n-1}}^{\rho\mu}(\zeta_{n-1}, \zeta_n) \end{aligned} \tag{7.21}$$

for every $n \in \mathbb{N}_*$ and $t_1 \leq \dots \leq t_n \in [0, \infty)$.

We shall denote by $\mathbb{E}_\zeta^{\rho\mu}$ the expectation with respect to $\mathbb{P}_\zeta^{\rho\mu}$ and refer to the family of probability measures $(\mathbb{P}_\zeta^{\rho\mu})_{\zeta \in M}$ as **the Markovian family associated with** $\rho\mu$.

Recalling formula (7.16), observing that in the above fromula $P^{\rho\mu}$ can be substituted with $P^{\Lambda_{\rho\mu}}$, and using Property (iv) of Theorem 7.10 gives for every bounded $\alpha : \Lambda \to \mathbb{R}$, with $\sum_{\zeta \in \Lambda} \alpha^2(\zeta)\ \rho(\zeta) < \infty$ and every $\zeta \in \Lambda$

$$\begin{aligned} \mathbb{E}_\zeta^{\rho\mu} \alpha(X_t^\Lambda) \ &= \ \int_M \alpha(\eta)\ \frac{\rho(\eta)}{\rho(\zeta)} e^{-t\mathcal{L}_{\Lambda_{\rho\mu}}} \mathbb{1}_\zeta\ (\eta)\ \Lambda(d\eta) \ = \\ &\frac{1}{\rho(\zeta)} \int_M (e^{-t\mathcal{L}_{\Lambda_{\rho\mu}}} \alpha)\ (\eta)\ \mathbb{1}_\zeta(\eta)\ \rho(\eta)\ \Lambda(d\eta) \quad , \end{aligned}$$

i.e.

$$\mathbb{E}_\zeta^{\rho\mu} \alpha(X_t^\Lambda) \ = \ e^{-t\mathcal{L}_{\Lambda_{\rho\mu}}}\ \alpha\ (\zeta) \quad . \tag{7.22}$$

Standard arguments permit to extend the above formula to every bounded α.

Remark 7.11. *For every Λ and $\zeta \in \Lambda$ we have that $X^\Lambda = (X^\Lambda)_{t\in[0,\infty)}$ is by construction a Markov process with respect to the probability space $(\Omega_\Lambda, \mathbb{P}^{\rho\mu}_\zeta)$ with initial value ζ, i.e.*

(i) $\mathbb{P}^{\rho\mu}_\zeta(X^\Lambda = \zeta) = 1$.

(ii) *for every $t, s > 0$ one has $\mathbb{P}^{\rho\mu}_\zeta$-almost surely*

$$\mathbb{P}^{\rho\mu}_\zeta(X^\Lambda_{t+s} \mid \mathcal{F}_s(X^\Lambda)) = \mathbb{P}^{\rho\mu}_{X^\Lambda_s}(X^\Lambda_t) \quad ,$$

where $\mathcal{F}_s(X^\Lambda)$ is the sigma algebra generated by $(X^\Lambda_{s'})_{s'\in[0,s]}$.

The transition function of X_Λ is given by $P^{\Lambda_{\rho\mu}}$ for every choice of $\zeta \in \Lambda$. It follows that X^Λ is irreducible. Moreover it satisfies the strong Markov property (see for example [84]).

Observe also that X^Λ is a pure jump process. Let $X^\Lambda_t = \zeta$ for some $\zeta \in M$ and $t \geq 0$. Then, by construction, for every $t' > t$ the process has positive probability to jump in direction $v \in V$ at time t' if and only if $\mu(\{v\}) > 0$, independently of ζ (and of t). This means that the support of the jump measure is finite and homogeneous in space.

Remark 7.12. *For every probability measure $\tilde{\rho}$ on Λ one can define the probability $\mathbb{P}^{\rho\mu}_{\tilde{\rho}}$ on the path space Ω_Λ by setting for every measurable B*

$$\mathbb{P}^{\rho\mu}_{\tilde{\rho}}(B) := \sum_{\zeta\in\Lambda} \mathbb{P}^{\rho\mu}_\zeta(B)\ \rho(\zeta) \quad .$$

In particular, if $\sum_{\zeta\in\Lambda} \rho(\zeta) = 1$, one can consider $\mathbb{P}^{\rho\mu}_\rho$. With respect to the probability space $(\Omega_\Lambda, \mathbb{P}^{\rho\mu}_\rho)$ the process X^Λ has the property to be reversible (in particular stationary).

Remark 7.13. *If ρ is such that*

$$\int_V \mathfrak{r}_\rho(\zeta, w)\ \mu(dw) \ = \ 1$$

for every $\zeta \in M$ (i.e. the rates are normalized), one could consider $\mathcal{L}^{(0)}_{\rho\mu}$ as the generator of a discrete time Markov chain.

8. The discrete Witten Laplacian $\mathcal{H}_{\rho,\mu}$

Assume given an n-dimensional affine space M together with a discrete geometry μ and a function $\rho : M \to (0, \infty)$, as in the preceding sections. In some situations it is more natural or useful to change point of view and think of ρ not as an inhomogeneity perturbing the discrete geometry μ, but rather as a deformation parameter of the operators δ and $\delta^{*\mu}$. This different point of view turns out to be unitarily equivalent to the previous one (see in particular Proposition 8.5 below).

The deformation of δ we are going to introduce in Definition 8.1 below is the discrete analogue of the deformation of the classical de Rham exterior differential on manifolds introduced by Witten: in his famous paper [103] a supersymmetric proof of the Morse inequalities is given using the mentioned deformation and semiclassical analysis.

Definition 8.1 (**Discrete Witten complexes and Witten Laplacians).** *Let M be an affine space with inhomogeneous discrete geometry $\rho\mu$. For every $p \in \mathbb{N}_0$ define the formal operators*

$$\delta_\rho \;:=\; \sqrt{\rho}\;\delta\;\frac{1}{\sqrt{\rho}}\quad ,$$

$$\delta_\rho^{*\mu} \;:=\; \frac{1}{\sqrt{\rho}}\;\delta^{*\mu}\;\sqrt{\rho}$$

and

$$\mathcal{H}_{\rho,\mu} \;:=\; \delta_\rho^{*\mu}\delta_\rho \;+\; \delta_\rho\delta_\rho^{*\mu}\quad .$$

The corresponding restrictions to the space of p-functions are denoted respectively by $\delta_\rho^{(p)}$, $\delta_\rho^{*\mu,(p-1)}$ and $\mathcal{H}_{\rho,\mu}^{(p)}$.

Complex properties, duality properties, intertwining relations, etc. follow easily from the definitions and previously established facts. We collect them in the next proposition for future reference.

Proposition 8.2. *For every inhomogeneous discrete geometry $\rho\mu$*

(i) $\delta_\rho\delta_\rho \;\equiv\; \delta_\rho^{*\mu}\delta_\rho^{*\mu} \;\equiv\; 0.$
(ii) $\mathcal{H}_{\rho,\mu}\;\delta_\rho = \delta_\rho\;\mathcal{H}_{\rho,\mu}$ *and* $\mathcal{H}_{\rho,\mu}\;\delta_\rho^{*\mu} = \delta_\rho^{*\mu}\;\mathcal{H}_{\rho,\mu}$

Moreover for every $p \in \mathbb{N}_0$, lattice graph Λ_μ and $\alpha, \alpha' \in F_{0,a}(M \times V^p)$, $\beta \in F_{0,a}(M \times V^{p+1})$

(iii) $\langle \delta_\rho^{(p)} \alpha, \beta \rangle_{\Lambda_\mu}^{(p+1)} = \langle \alpha, \delta_\rho^{*_\mu,(p)} \beta \rangle_{\Lambda_\mu}^{(p)}$

(iv) $\langle \mathcal{H}_{\rho,\mu}^{(p)} \alpha, \alpha' \rangle_{\Lambda_\mu}^{(p)} = \langle \alpha, \mathcal{H}_{\rho,\mu}^{(p)} \alpha' \rangle_{\Lambda_\mu}^{(p)}$

(v) $\langle \mathcal{H}_{\rho,\mu}^{(p)} \alpha, \alpha' \rangle_{\Lambda_\mu}^{(p)} \geq 0$

Notice that properties (iii) - (v) hold with respect to every *homogeneous* lattice graph Λ_μ, while the corresponding properties for δ, $\delta^{*_{\rho\mu}}$ and $\mathcal{L}_{\rho\mu}$ hold for every *inhomogeneous* lattice graph $\Lambda_{\rho\mu}$ (see Proposition 5.3).

In fact the Hilbert spaces on which the above defined formal Witten operators naturally act are the "flat" L^2 spaces corresponding to homogeneous lattice graphs. More precisely we give the following definition, which will be fundamental for the sequel. Here we use the symbol $\mathcal{H}_{0,\rho,\mu}^{(p)}$ for the restriction of $\mathcal{H}_{\rho,\mu}^{(p)}$ to $F_{0,a}(M \times V^p)$, the space of alternating p-functions with compact support.

Definition 8.3. *For every lattice graph Λ_μ we denote by $\mathcal{H}_{\rho,\Lambda_\mu}^{(p)}$ the Friedrichs extension of $\mathcal{H}_{0,\rho,\mu}^{(p)}$, considered as an operator in $L_a^2(M \times V^p, \Lambda_\mu)$. Moreover we set $\mathcal{H}_{\rho,\Lambda_\mu} := \oplus_{p=0}^{\infty} \mathcal{H}_{\rho,\Lambda_\mu}^{(p)}$.*

Observe that $\mathcal{H}_{\rho,\Lambda_\mu}^{(p)}$ is a nonnegative, selfadjoint and in general unbounded operator in $L_a^2(M \times V^p, \Lambda_\mu)$. Moreover it agrees on its domain $D(\mathcal{H}_{\rho,\Lambda_\mu}^{(p)})$ with the formal Witten Laplacian, i.e. for every $\alpha \in D(\mathcal{H}_{\rho,\Lambda_\mu}^{(p)})$

$$\mathcal{H}_{\rho,\Lambda_\mu}^{(p)} \ \alpha = \mathcal{H}_{\rho,\mu}^{(p)} \ \alpha \quad . \tag{8.1}$$

The following version of the intertwining relations, involving spectral projections of $H_{\rho,\Lambda_\mu}^{(p)}$, will be a key ingredient in Section 16 for the sake of comparing exact and approximate eigenvalues.

Proposition 8.4. *Fix $p \in \mathbb{N}_0$. Let $c > 0$ and consider the interval $E := [0, c]$. Assume that*

$$[c, c+\gamma] \ \cap \ \mathrm{Spec}\left(\ \mathcal{H}_{\rho,\Lambda_\mu}^{(q)} \ \right) \ = \ \emptyset \tag{8.2}$$

for some $\gamma > 0$ and for $q = p, p+1$. Then for every $\alpha \in F_{0,a}(M \times V^p)$

$$1_E \ \left(\mathcal{H}_{\rho,\Lambda_\mu}^{(p+1)}\right) \ \delta_\rho^{(p)} \ \alpha \ = \ \delta_\rho^{(p)} \ 1_E \ \left(\mathcal{H}_{\rho,\Lambda_\mu}^{(p)}\right) \ \alpha \quad . \tag{8.3}$$

Similarly, for every $\alpha \in F_{0,a}(M \times V^{p+1})$

$$1_E\ \left(\mathcal{H}^{(p)}_{\rho,\Lambda_\mu}\right)\ \delta^{*\mu,(p)}_\rho\ \alpha\ =\ \delta^{*\mu,(p)}_\rho\ 1_E\ \left(\mathcal{H}^{(p+1)}_{\rho,\Lambda_\mu}\right)\ \alpha\quad .$$

Proof. Let $z \in \mathbb{C}\backslash[0,\infty)$. Then using Proposition 8.2 (ii) we get immediately the intertwining relations for the resolvents:

$$\left(\ z - \mathcal{H}^{(p+1)}_{\rho,\Lambda_\mu}\ \right)^{-1}\ \delta^{(p)}_\rho\ \alpha\ =\ \delta^{(p)}_\rho\ \left(\ z - \mathcal{H}^{(p)}_{\rho,\Lambda_\mu}\ \right)^{-1}\ \alpha\quad . \tag{8.4}$$

Statement (8.3) follows now from Stone's formula (see [88, Theorem VII.13]) applied with the interval $[0-\gamma', c+\gamma']$, with $0 < \gamma' < \gamma$, and from the observation that, due to assumption (8.2),

$$1_E\ \left(\mathcal{H}^{(q)}_{\rho,\Lambda_\mu}\right)\ =\ 1_{[0-\gamma',c+\gamma']}\ \left(\mathcal{H}^{(q)}_{\rho,\Lambda_\mu}\right)\ =\ 1_{(0-\gamma',c+\gamma')}\ \left(\mathcal{H}^{(q)}_{\rho,\Lambda_\mu}\right)$$

for $q = p, p+1$.

The case with $\delta^{*\mu,(p)}_\rho$ instead of $\delta^{(p)}_\rho$ is analogous. □

The link between the present point of view à la Witten and the one developed in Sections 5 and 6 is given by the so-called **ground state transformation**. To make this precise, observe that, once a lattice $\Lambda \in M/\Gamma$ is selected, there is a canonical Hilbert space isomorphism

$$L^2_a(M \times V^p, \Lambda_{\rho\mu})\ \overset{\Phi_\rho}{\simeq}\ L^2_a(M \times V^p, \Lambda_\mu)\quad ,$$

the isomorphism Φ_ρ (the ground state transformation) being the multiplication with $\sqrt{\rho}$. In other terms, for $\alpha \in L^2_a(M \times V^p, \Lambda_{\rho\mu})$ and $\beta \in L^2_a(M \times V^p, \Lambda_\mu)$

$$\Phi_\rho(\alpha)\ :=\ \sqrt{\rho}\alpha \quad \text{and} \quad \Phi^{-1}_\rho(\beta)\ =\ \frac{1}{\sqrt{\rho}}\beta\quad . \tag{8.5}$$

A simple computation shows that the formal operators are related as follows.

$$\mathcal{H}_{\rho,\mu}\ =\ \sqrt{\rho}\ \mathcal{L}_{\rho\mu}\ \frac{1}{\sqrt{\rho}}\quad . \tag{8.6}$$

As a consequence, the L^2 realizations of the Witten and inhomogeneous Hodge Laplacians we are considering, are unitarily equivalent.

Proposition 8.5.
$\mathcal{H}^{(p)}_{\rho,\Lambda_\mu}$ is unitarily equivalent to $\mathcal{L}^{(p)}_{\Lambda_{\rho\mu}}$ for every $p \in \mathbb{N}_0$ and $\Lambda \in M/\Gamma$. In particular $\operatorname{Spec} \mathcal{H}^{(p)}_{\rho,\Lambda_\mu} = \operatorname{Spec} \mathcal{L}^{(p)}_{\Lambda_{\rho\mu}}$.

Proof. By (8.1) and (8.6) we just have to verify that $D(\mathcal{H}^{(p)}_{\rho,\Lambda_\mu})$ transforms into $D(\mathcal{L}^{(p)}_{\Lambda_{\rho\mu}})$ under the ground state transformation Φ_ρ defined in (8.5).

To see this observe that $\alpha \in D(\mathcal{L}^{(p)}_{\Lambda_{\rho\mu}})$ if and only if there exists a sequence $\{\alpha_n\} \subset F_{0,a}(M \times V^p)$ such that $\lim_{n,m} \|\delta\, (\alpha_n - \alpha_m)\|^{(p)}_{\Lambda_{\rho\mu}} = 0$ and $\lim_n \|(\alpha_n - \alpha)\|^{(p)}_{\Lambda_{\rho\mu}} = 0$. Using the analogous characterization for $D(\mathcal{H}^{(p)}_{\rho,\Lambda_\mu})$ gives that $\beta = \sqrt{\rho}\alpha \in D(\mathcal{H}^{(p)}_{\rho,\Lambda_\mu})$ if and only if $\alpha = \frac{1}{\sqrt{\rho}}\beta \in D(\mathcal{L}^{(p)}_{\Lambda_{\rho\mu}})$: just consider $\beta_n = \sqrt{\rho}\alpha_n$. $\square$

Remark 8.6. *Since the ground state transformation preserves the space of functions with compact support it follows from* (8.6) *that also $\mathcal{L}^{(p)}_{0,\rho\mu}$ and $\mathcal{H}^{(p)}_{0,\rho,\mu}$ are unitarily equivalent. Since essential selfadjointness is preserved under unitarily transformations we have that $\mathcal{L}^{(p)}_{0,\rho\mu}$ is essentially selfadjoint in $L^2_a(M \times V^p, \Lambda_{\rho\mu})$ if and only if it is the case for $\mathcal{H}^{(p)}_{0,\rho,\mu}$ in $L^2_a(M \times V^p, \Lambda_\mu)$. As we already remarked in Footnote 27 at the end of Section 6, essential selfadjointness is not fullfilled automatically if no further assumptions are imposed on $\rho\mu$.*

Next we give a representation of the formal Witten Laplacian analogous to the one given in Proposition 6.2 for the inhomogeneous Hodge Laplacian, by splitting it into a scalar operator and a matrix operator.

We shall use in the sequel the notation $\mathcal{D}^{(p)}_\rho$ and $\mathcal{D}^{\star,(p)}_\rho$ to indicate the ground state transformations of $\mathcal{D}^{(p)}$ and $\mathcal{D}^{\star\rho,(p)}$ (the latter being defined in (5.1)) respectively. That is

$$\mathcal{D}^{(p)}_\rho \;:=\; \sqrt{\rho}\; \mathcal{D}^{(p)}\; \frac{1}{\sqrt{\rho}}$$

and

$$\mathcal{D}^{\star,(p)}_\rho \;:=\; \sqrt{\rho}\; \mathcal{D}^{\star\rho,(p)}\; \frac{1}{\sqrt{\rho}} \left(\;=-\frac{1}{\sqrt{\rho}}\; \mathcal{D}^{(p)}\; \sqrt{\rho}\; \right) \;.$$

The superscript (p) is dropped when the corresponding direct sum is considered.

Recall also the definitions of Tr_μ, $d\Gamma$ given in (4.1), (6.2) and of the sharp operator $\sharp\mu$ in (6.1). Proposition 6.2 and (8.6) give immediately:

Proposition 8.7.
For every discrete inhomogeneous geometry $\rho\mu$ on the affine space M the following representation holds for the discrete Witten Laplacian.

$$\mathcal{H}_{\rho,\mu} \;=\; \mathrm{Tr}_\mu \;\mathcal{D}_\rho^\star \mathcal{D}_\rho \;+\; d\Gamma \;[\mathcal{D}_\rho, \mathcal{D}_\rho^\star]^{\;\sharp\mu} \quad .$$

The analogue of Remark 6.3 is

Remark 8.8. *It follows from Proposition 8.7 using* (2.4) *that*

$$\mathcal{H}_{\rho,\mu} \;=\; \sum_{\mathbf{s}\in\{-1,1\}^2} \mathrm{sign}(\mathbf{s}) \left\{ \;\mathrm{Tr}_\mu \;(\mathfrak{b}_\rho \mathcal{T}^2)_\mathbf{s} \;+\; d\Gamma \;\;(\bar{\mathfrak{b}}_\rho \mathcal{T}^2)_\mathbf{s}^{\;\;\sharp\mu} \;\right\} \quad ,$$

where $\mathfrak{b}_\rho := \{\mathfrak{b}_{\rho;w_1,w_2}\}_{w_1,w_2\in V^2}$, $\bar{\mathfrak{b}}_\rho := \{\bar{\mathfrak{b}}_{\rho;w_1,w_2}\}_{w_1,w_2\in V^2}$ *and* $\mathfrak{b}_{\rho;w_1,w_2}, \bar{\mathfrak{b}}_{\rho;w_1,w_2} \in F(M)$ *are given by*

$$\mathfrak{b}_{\rho;w_1,w_2} \;:=\; -\,\frac{1}{\sqrt{\rho}}\,\mathcal{T}_{w_1}\,\rho\,\mathcal{T}_{w_2}\,\frac{1}{\sqrt{\rho}} \quad i.e. \quad \mathfrak{b}_{\rho;w_1,w_2}(\zeta) \;=\; -\,\frac{\rho(\zeta+w_1/2)}{\sqrt{\rho(\zeta)\rho(\zeta+w_1/2+w_2/2)}}$$

and

$$\bar{\mathfrak{b}}_{\rho;w_1,w_2} \;:=\; \mathfrak{b}_{\frac{1}{\rho};w_1,w_2} \;-\; \mathfrak{b}_{\rho;w_2,w_1} \quad .$$

The analogue of Remark 6.4 is

Remark 8.9. *Let*

$$\mathfrak{g}_{\rho,w} \;:=\; -\mathfrak{b}_{\rho,w,w} \;=\; \frac{1}{\sqrt{\rho}}\,\mathcal{T}_w\;\rho\;\mathcal{T}_w\,\frac{1}{\sqrt{\rho}} \quad ,$$

i.e.

$$\mathfrak{g}_{\rho,w}(\zeta) \;=\; \frac{\rho(\zeta+w/2)}{\sqrt{\rho(\zeta)\rho(\zeta+w)}} \;=\; \mathfrak{r}_\rho(\zeta,w)\sqrt{\frac{\rho(\zeta)}{\rho(\zeta+w)}} \quad ,$$

with the rates $\mathfrak{r}_\rho$ as defined in (6.3)*. A simple computation gives for $\alpha \in F_a(M\times V^p)$*

$$\mathrm{Tr}_\mu \;\mathcal{D}_\rho^\star\mathcal{D}_\rho\;\alpha\;\;(\zeta,\mathbf{v}) \;=\;=\; \int_V \big[\,\mathfrak{r}_{\rho,w}(\zeta)\;\alpha(\zeta,\mathbf{v}) - \mathfrak{g}_{\rho,w}(z)\;\alpha(\zeta{+}w,\mathbf{v})\,\big]\;\mu(dw) \quad .$$

Proposition 8.7 gives therefore for every $\alpha\in F(M)$

$$\mathcal{H}^{(0)}_{\rho,\mu}\;\alpha\;(\zeta) \;=\; \int_V \big[\;\mathfrak{r}_{\rho,w}(\zeta)\;\alpha(\zeta) \;-\; \mathfrak{g}_{\rho,w}(z)\;\alpha(\zeta+w)\;\big]\;\mu(dw) \quad .$$

Note that $\mathcal{H}^{(0)}_{\rho,\mu}$ does not annihilate constants as is the case for $\mathcal{L}^{(0)}_{\rho\mu}$. Separating the "kinetic part" (which annihilates constants) from the "potential parts", which are obtained by applying the operator to the function with constant value one, gives the following representation: for every $\alpha \in F(M)$

$$\mathcal{H}^{(0)}_{\rho,\mu}\ \alpha\ (\zeta)\ =$$

$$= \int_V \mathfrak{g}_\rho(\zeta, w)\ \big[\ \alpha(\zeta) - \alpha(\zeta + w)\ \big]\ \mu(dw)\ +\ \Big(\ \int_V \big[\ \mathfrak{r}_\rho(\zeta, w) - \mathfrak{g}_\rho(\zeta, w)\ \big]\ \mu(dw)\ \Big)\ \alpha(\zeta)\quad .$$

This can be seen as a discrete Schrödinger operator, with kinetic term

$$\int_V \mathfrak{g}_{\rho,w}(\zeta)\ \big[\ \alpha(\zeta) - \alpha(\zeta + w)\ \big]\ \mu(dw)$$

and potential

$$\int_V \big[\ \mathfrak{r}_{\rho,w}(\zeta) - \mathfrak{g}_{\rho,w}(\zeta)\ \big]\ \mu(dw)\quad .$$

Therefore we shall refer to the Witten point of view presented in this section also as the Schrödinger point of view, as opposed to the probabilistic one which is more natural for $\mathcal{L}^{(0)}_{\rho\mu}$ as explained in Section 7.

Part II. Semiclassical discrete Witten Laplacians

In this second part we consider on the affine space M inhomogeneous discrete geometries, which are rescaled via a small parameter $\varepsilon > 0$. Basic asymptotic spectral properties of the corresponding rescaled Witten Laplacians are derived. The scaling we consider is analogous to the semiclassical limit for Schrödinger operators.

9. Semiclassical scaling

As in Part I we consider here throughout an n-dimensional affine space M with underlying vector space V. Moreover we assume given an inhomogeneous discrete geometry $\rho\mu$ on M. Recall from Section 5 in Part I, that $\rho\mu$ consists of a function $\rho : M \to (0, \infty)$ and a symmetric measure μ on V with a finite support which generates a lattice Γ in V. Recall also that $E = \operatorname{supp} \mu \setminus \{0\}$ is referred to as the set of admissible jumps.

The aim of this section is to introduce a scaling of $\rho\mu$ and to establish useful representation formulas for the leading symbols of the corresponding rescaled Witten Laplacians. Moreover we declare the assumptions we shall adopt throughout the rest of this part (see Assumptions II.1, II.2 below).

Let $\varepsilon > 0$ be a small parameter (the "semiclassical" parameter), and let $f : M \to \mathbb{R}$ (the "energy") be given by

$$f \ := \ -\frac{1}{2} \log \rho \ \ .$$

For $\varepsilon > 0$ the **rescaled inhomogeneous geometry** $\rho_\varepsilon\mu_\varepsilon := (\rho_\varepsilon, \mu_\varepsilon)$, with $\rho_\varepsilon : M \to (0, \infty)$ and μ_ε a measure on V, is defined by setting for every $\zeta \in M$

$$\rho_\varepsilon(\zeta) \ := \ e^{-2f(\zeta)/\varepsilon}$$

and for every measurable set S in V

$$\mu_\varepsilon(S) \ := \ \mu(\varepsilon^{-1} S) \ \ .$$

Observe that $\rho_\varepsilon\mu_\varepsilon$ is an inhomogeneous discrete geometry for every $\varepsilon > 0$. Moreover the set of admissible jumps (respectively the generated lattice) of μ_ε is given by εE (respectively $\varepsilon\Gamma$).

As in Part I we shall consider lattice graphs in M associated with discrete geometries: we fix for $\varepsilon > 0$ an equivalence class in M under $\sim_{\varepsilon\Gamma}$ and denote by Λ_ε the elements of the chosen equivalence class. The weighted graph with vertices Λ_ε, edges determined by εE and weight μ_ε on the edges will be denoted by $\Lambda_{\mu_\varepsilon}$; if we consider the vertices weighted with ρ_ε the symbol $\Lambda_{\rho_\varepsilon \mu_\varepsilon}$ will be used.

We call $\mathcal{H}_{\rho_\varepsilon,\mu_\varepsilon} = \oplus_{p=0}^{\infty} \mathcal{H}^{(p)}_{\rho_\varepsilon,\mu_\varepsilon}$ the (formal) **rescaled Witten Laplacian** and shall consider its realizations $\mathcal{H}^{(p)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$ as operators in $L^2_a(M \times V^p, \Lambda_{\mu_\varepsilon})$: recall from Section 8 that

$$\mathcal{H}_{\rho_\varepsilon,\mu_\varepsilon} \ := \ \delta^{*\mu_\varepsilon}_{\rho_\varepsilon} \delta_{\rho_\varepsilon} \ + \ \delta_{\rho_\varepsilon} \delta^{*\mu_\varepsilon}_{\rho_\varepsilon}$$

and that $\mathcal{H}^{(p)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$ is defined as Friedrichs extension of the restriction of $\mathcal{H}^{(p)}_{\rho_\varepsilon,\mu_\varepsilon}$ to p-functions with compact support.

For the sequel it is sometimes convenient not to work in $L^2_a(M \times V^p; \Lambda_{\mu_\varepsilon})$ but in a suitable $L^2_a(M \times V^p, \Lambda_{\varepsilon,\mu})$, where $\Lambda_{\varepsilon,\mu}$ is a lattice graph differing from $\Lambda_{\mu_\varepsilon}$ by the fact that its edges have weight μ instead of μ_ε. To be precise we define the **scalar product** in $L^2_a(M \times V^p, \Lambda_{\varepsilon,\mu})$ as

$$\langle \alpha, \beta \rangle^{(p)}_{\Lambda_{\varepsilon,\mu}} \ := \ \int_M \langle \tau_{\varepsilon *} \alpha(\zeta), \tau_{\varepsilon *} \beta(\zeta) \rangle^{(p)}_\mu \ \Lambda_\varepsilon(d\zeta) \quad , \tag{9.1}$$

where

$$(\tau_{\varepsilon *} \alpha)_{\mathbf{v}}(\zeta) \ := \ \alpha_{\mathbf{v}}(\zeta + \varepsilon \mathbf{v}/2)$$

is the **scaled shift operator**, $d\Lambda_\varepsilon$ denotes the counting measure on Λ_ε and $\langle \cdot, \cdot \rangle_\mu$ is defined as in (3.5). The superscript (p) in (9.1) will be frequently omitted. To see the relation to $L^2_a(M \times V^p; \Lambda_{\mu_\varepsilon})$ we introduce for $\varepsilon > 0$ the **scaling operator** $\Psi_\varepsilon : F(M \times V^p) \to F(M \times V^p)$, defined as

$$\Psi_\varepsilon \ \alpha \ (\zeta, \mathbf{v}) \ := \ \alpha(\zeta, \varepsilon \mathbf{v}) \quad . \tag{9.2}$$

Note that the restriction of Ψ_ε to $L^2_a(M \times V^p, \Lambda_{\mu_\varepsilon})$ gives a Hilbert space isomorphism between the latter and $L^2_a(M \times V^p, \Lambda_{\varepsilon,\mu})$. Indeed

$$\langle \alpha, \beta \rangle^{(p)}_{\Lambda_{\varepsilon,\mu}} \ = \ \langle \Psi_\varepsilon^{-1} \alpha, \Psi_\varepsilon^{-1} \beta \rangle^{(p)}_{\Lambda_{\mu_\varepsilon}} \quad .$$

We can therefore equivalently consider instead of $\mathcal{H}_{\rho_\varepsilon,\mu_\varepsilon}$ the formal operator

$$\tilde{\mathcal{H}}_{\rho_\varepsilon,\varepsilon,\mu} \ := \Psi_\varepsilon \ \mathcal{H}_{\rho_\varepsilon,\mu_\varepsilon} \ \Psi_\varepsilon^{-1} \tag{9.3}$$

and the operator

$$\tilde{\mathcal{H}}_{\rho_\varepsilon,\Lambda_{\varepsilon,\mu}} \ := \Psi_\varepsilon \ \mathcal{H}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}} \ \Psi_\varepsilon^{-1}$$

acting in $L^2_a(M \times V^p, \Lambda_{\varepsilon,\mu})$.

Throughout this part we make the following smoothness assumption.

Assumption II.1.

(i) $f \in C^\infty(M)$

(ii) *There exists a point* $O \in M$ *such that* $O \in \Lambda_\varepsilon$ *for* $\varepsilon > 0$.

The smoothness of f together with Remark 8.8 leads through a simple Taylor expansion to the following representation of $\tilde{\mathcal{H}}_{\rho_\varepsilon,\varepsilon,\mu}$:

$$\tilde{\mathcal{H}}_{\rho_\varepsilon,\varepsilon,\mu} \;=\; \mathcal{L}_{\varepsilon,\mu} \;+\; U_{f,\mu} \;+\; \varepsilon\, \mathcal{M}_{\varepsilon,f,\mu} \;+\; \varepsilon^2\, \mathcal{N}_{\varepsilon,f,\mu} \quad , \tag{9.4}$$

where

- $\mathcal{L}_{\varepsilon,\mu} := \mathcal{L}_{\mu_\varepsilon}$ is the discrete Hodge Laplacian corresponding to the discrete geoemtry μ_ε as introduced in Section 4, i.e.

$$\mathcal{L}_{\varepsilon,\mu}\, \alpha\, (\zeta, \mathbf{v}) \;=\; \int_V \big[\, \alpha(\zeta,\mathbf{v}) - \alpha(\zeta+\varepsilon w, \mathbf{v}) \,\big]\; \mu(dw) \quad .$$

- $U_{f,\mu} \in C^\infty(M;\mathbb{R})$ is given by

$$U_{f,\mu}(\zeta) \;:=\; \|2 \sinh \frac{\nabla f(\zeta)}{2}\|_\mu^2 \tag{9.5}$$

  and acts as a multiplication operator.

- $\mathcal{M}_{\varepsilon,f,\mu}$ is a translation operator given by

$$\mathcal{M}_{\varepsilon,f,\mu} \;:=\; \frac{1}{4} \sum_{\mathbf{s}\in\{-1,1\}^2} \operatorname{sign}(\mathbf{s}) \Big\{ \;-\; \operatorname{Tr}_\mu\, (\mathfrak{m}_f \mathcal{T}_\varepsilon^2)_{\mathbf{s}} \;+\; d\Gamma\;\; 2(\mathfrak{m}_f \mathcal{T}_\varepsilon^2)_{\mathbf{s}}{}^{\sharp\mu} \Big\} \quad , \tag{9.6}$$

  where $\mathfrak{m}_f := \{\mathfrak{m}_{f;w_1,w_2}\}_{w_1,w_2\in V^2}$ and $\mathfrak{m}_{f;w_1,w_2} \in C^\infty(M;\mathbb{R})$ is given by

$$\mathfrak{m}_{f;w_1,w_2} \;:=\; e^{\frac{1}{2}\nabla_{w_1-w_2} f}\;\; \nabla^2_{w_1,w_2} f$$

  and $\mathcal{T}_\varepsilon := (\mathcal{T}_{\varepsilon w})_{w\in V}$.

- $\mathcal{N}_{\varepsilon,f,\mu}$ is a translation operator of the form

$$\mathcal{N}_{\varepsilon,f,\mu} \;=\; \frac{1}{4} \sum_{\mathbf{s}\in\{-1,1\}^2} \operatorname{sign}(\mathbf{s}) \Big\{ \operatorname{Tr}_\mu\, (\mathfrak{n}_{\varepsilon,f} \mathcal{T}_\varepsilon^2)_{\mathbf{s}} \;+\; d\Gamma\;\; (\bar{\mathfrak{n}}_{\varepsilon,f} \mathcal{T}_\varepsilon^2)_{\mathbf{s}}{}^{\sharp\mu} \Big\} \quad ,$$

where $\mathfrak{n}_{\varepsilon,f} := \{\mathfrak{n}_{\varepsilon,f;w_1,w_2}\}_{w_1,w_2\in V^2}$, $\bar{\mathfrak{n}}_f := \{\bar{\mathfrak{n}}_{\varepsilon,f;w_1,w_2}\}_{w_1,w_2\in V^2}$ and $\mathfrak{n}_{\varepsilon,f;w_1,w_2}, \bar{\mathfrak{n}}_{f;w_1,w_2} \in C^\infty(M;\mathbb{R})$ satisfy for $\varepsilon \to 0$

$$\mathfrak{n}_{\varepsilon,f;w_1,w_2} = \mathcal{O}(1) \quad \text{and} \quad \bar{\mathfrak{n}}_{\varepsilon,f;w_1,w_2} = \mathcal{O}(1) \ . \tag{9.7}$$

Remark 9.1. *Property* (9.7) *means that for every $w_1, w_2 \in V^2$, every $j \in \mathbb{N}_0$, every compact $K \subset M$ and every $\mathbf{v} \in V^j$ there exist constants $C_1, C_2 > 0$ such that*

$$|\nabla^j_{\mathbf{v}} \mathfrak{n}_{\varepsilon,f;w_1,w_2}(\zeta)| + |\nabla^j_{\mathbf{v}} \bar{\mathfrak{n}}_{\varepsilon,f;w_1,w_2}(\zeta)| \ \le \ C_1 \quad \textit{for every } \varepsilon \in (0, C_2) \ \textit{ and every } \zeta \in K \ .$$

Remark 9.2. *More explicitly,* (9.6) *says that in the case $p = 1$, for $\alpha \in F_a(M \times V)$*

$$\mathcal{M}_{\varepsilon,f,\mu}\ \alpha\ (\zeta, v) \ =$$

$$= \frac{1}{4} \sum_{\mathbf{s}\in\{-1,1\}^2} \Big\{ -\frac{1}{2}\int_V e^{\frac{1}{2}\nabla_{(s_1-s_2)w} f(\zeta)} \ \nabla^2_{w,w} f(\zeta)\ \alpha(\zeta + \varepsilon(s_1+s_2)w, v)\ \mu(d_w) \ +$$

$$+ \frac{1}{2}\int_V 2e^{\frac{1}{2}\nabla_{s_1 v - s_2 w} f(\zeta)} \ \nabla^2_{v,w} f(\zeta)\ \alpha(\zeta + \varepsilon(s_1+s_2)v, w)\ \mu(dw) \Big\} \ .$$

Remark 9.3. *Using the identity* $\cosh x - 1 = 2\sinh^2 \frac{x}{2}$ *one gets from* (9.5)

$$U_{f,\mu}(\zeta) \ := \ \frac{1}{2}\int_V 4\sinh^2 \frac{\nabla_w f(\zeta)}{2}\ \mu(dw) \ = \ \int_V [\cosh \nabla_w f(\zeta) - 1]\ \mu(dw) \ .$$

Remark 9.4.

Let $p \in \mathbb{N}_0$, $\alpha \in F_a(M \times V^p)$ and let $\Omega \subset M$. The representation (9.4) *implies that there exist ε-independent constants $R, C > 0$ such that for every $\zeta \in \Omega$ and $\varepsilon > 0$*

$$\|\tilde{\mathcal{H}}_{\rho_\varepsilon,\varepsilon,\mu}\ \alpha\ (\zeta)\|_\mu \ \le C \sup_{\eta\in B_R(\Omega)} \|\alpha(\eta)\|_\mu \ ,$$

where B_R denotes a ball of radius R around Ω (say with respect to the distance induced by μ).

Formula (9.4) represents the rescaled Witten Laplacian as a perturbation of the discrete Schrödinger operator $\mathcal{L}_{\varepsilon,\mu} + U_{f,\mu}$. For the semiclassical analysis in the next two sections it will be convenient to introduce the symbol of $\mathcal{L}_{\varepsilon,\mu} + U_{f,\mu}$ and of $\mathcal{M}_{\varepsilon,f,\mu}$, which gives the leading term of the perturbation. More precisely, denoting by V^* the dual vector space of V we define the

kinetic energy $K_\mu : V^* \to \mathbb{R}$ as the symbol of $\mathcal{L}_{\varepsilon,\mu}$, i.e. for every $\xi \in V^*$ (denoting by ξ_w the value of ξ on $w \in V$)

$$K_\mu(\xi) \;:=\; \int_V [1 - e^{-\mathrm{i}\xi_w}]\;\mu(dw) \;=\; \|2\sin\frac{\xi}{2}\|_\mu^2 \;\;,$$

so that formally

$$K_\mu(\varepsilon \mathrm{i}\nabla) \;=\; \mathcal{L}_{\varepsilon,\mu} \;\;.$$

The **Hamiltonian** $H_{f,\mu} : M \times V^* \to \mathbb{R}$ is then defined as the symbol of $\mathcal{L}_{\varepsilon,\mu} + U_{f,\mu}$, i.e.

$$H_{f,\mu}(\zeta,\xi) \;:=\; K_\mu(\xi) \;+\; U_{f,\mu}(\zeta) \;=\; \|2\sin\frac{\xi}{2}\|_\mu^2 \;+\; \|2\sinh\frac{\nabla f(\zeta)}{2}\|_\mu^2 \;\;. \quad (9.8)$$

Similarly, denoting by $\mathrm{End}(F(V^p))$ the set of linear operators from $F(V^p)$ to itself, we introduce the **subleading symbol** $M_{f,\mu} : M \times V^* \to \mathrm{End}(F(V^p))$ as the symbol of $\mathcal{M}_{\varepsilon,f,\mu}$, given by

$$M_{f,\mu}(\zeta,\xi) \;:=\; -\;\mathrm{Tr}_\mu\;\mathring{\mathfrak{m}}_f(\zeta,\xi) \;+\; d\Gamma\;\; 2\,\mathring{\mathfrak{m}}_f(\zeta,\xi)\;\;^{\sharp\mu} \;\;, \qquad (9.9)$$

where

$$\mathring{\mathfrak{m}}_{f;w_1,w_2}(\zeta,\xi) \;:=\; \frac{1}{4}\sum_{\mathbf{s}\in\{-1,1\}^2} \mathrm{sign}(\mathbf{s})\;\mathfrak{m}_{f;s_1w_1,s_2w_2}(\zeta)\;e^{-\frac{1}{2}\mathrm{i}\xi_{s_1w_1+s_2w_2}} \;\;.$$

Note that a straightforward calculation (see Lemma E.2 in the appendix for details) gives

$$\mathring{\mathfrak{m}}_{f;w_1,w_2}(\zeta,\xi) \;=\; \nabla^2_{w_1,w_2} f(\zeta)\;\cosh\frac{\nabla_{w_1} f - \mathrm{i}\xi_{w_1}}{2}\;\;\cosh\frac{\nabla_{w_2} f + \mathrm{i}\xi_{w_2}}{2}$$

and in particular

$$\mathring{\mathfrak{m}}_{f;w,w}(\zeta,\xi) \;=\; \nabla^2_w f(\zeta)\;\Big(\;-\sin^2\frac{\xi_w}{2} + \cosh^2\frac{\nabla_w f(\zeta)}{2}\;\Big) \;\;.$$

Remark 9.5. *For the WKB Ansatz which will be developed in Section 11 we will use the following formulas.*

Let $\varphi \in C^\infty(M;\mathbb{R})$. It follows from the identity $\sin ix = i\sinh x$ that

$$H_{f,\mu}(\zeta, -i\nabla\varphi(\zeta)) \;=\; H_{f,\mu}(\zeta, i\nabla\varphi(\zeta)) \;=$$
$$=\; -\|2\sinh\frac{\nabla\varphi(\zeta)}{2}\|_\mu^2 \;+\; \|2\sinh\frac{\nabla f(\zeta)}{2}\|_\mu^2$$

and

$$\mathring{\mathfrak{m}}_{f;w_1,w_2}(\zeta, -i\nabla\varphi(\zeta)) \;=\; \nabla^2_{w_1,w_2} f(\zeta)\;\cosh\frac{\nabla_{w_1}(f-\varphi)}{2}\cosh\frac{\nabla_{w_2}(f+\varphi)}{2} \;\;.$$

In particular, for $w_1 = w_2$,

$$\mathring{\mathfrak{m}}_{f;w,w}(\zeta, -i\nabla\varphi(\zeta)) \;=\; \nabla_w^2 f(\zeta) \;\Big(\; \sinh^2 \frac{\nabla_w \varphi(\zeta)}{2} + \cosh^2 \frac{\nabla_w f(\zeta)}{2} \;\Big) \quad .$$

In the next two sections we shall assume besides Assumption II.1:

Assumption II.2.

(i) *f is a Morse function.*

(ii) *There exists a compact $K \subset \mathbb{R}^n$ and coordinates $z = (z_1, \ldots, z_n)$ on M such that for $z \in \mathbb{R}^n \setminus K$*

$$f(z) \;=\; \sum_i z_i^2 \quad .$$

Recall that the Morse property means that for every critical point $\bar{\zeta}$ of f the matrix

$$(\partial_{z_i,z_j} f)_{i,j}(\bar{\zeta})$$

of second derivatives with respect to one (and therefore any) coordinate system is nondegenerate. The number of negative eigenvalues of $\partial_{z_i,z_j} f(\bar{\zeta})$ which is also invariant, is called the index of $\bar{\zeta}$. Note that since critical points of a Morse function can not accumulate, it follows from Assumption II.2(ii) that f has only finitely many critical points.

Assumption II.2(i) is not very restrictive, in the sense that Morse functions are generic in the category of smooth functions. We assume it here to avoid further technical complications, but in principle the type of results we shall obtain should be extendable with suitable modifications also by allowing degenerate critical points.

Assumption II.2(ii) is used (as far this Part II is concerned) only in Section 10. Indeed some condition on f at infinity has to be assumed in order to guarantee that the bottom of the essential spectrum of the Witten Laplacian $\mathcal{H}^{(p)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$ is bounded away from zero. This is for example not the case if f is constant. Of course, assuming exactly quadratic grow, is by no means optimal. We have chosen this case as a paradigmatic example, which facilitates some rather nasty computations, without pushing here much further in investigating the interesting problem of the relation between the behaviour of f at infinity and the spectrum of the discrete Witten Laplacian. The search for more satisfactory assumptions to localize the essential spectrum is postponed until further research. But we mention that the arguments we use in our proofs work at least also in the case of bounded second derivative and gradient bounded away from zero. More precisely one could assume with no harm instead of Assumption II.2(ii) the following:

There exists a compact $K \subset \mathbb{R}^n$, constants $C', C'' > 0$ and coordinates $z = (z_1, \ldots, z_n)$ on M such that for $z \in \mathbb{R}^n \setminus K$

(ii'.a)

$$\sum_{i=1}^{n} |\frac{\partial}{\partial z_i} f(z)|^2 \ \geq \ C' \quad .$$

(ii'.b)

$$\sum_{i,j=1}^{n} |\frac{\partial^2}{\partial z_i \partial z_j} f(z)|^2 \ \leq \ C'' \quad .$$

$\tilde{\mathcal{H}}_{\rho_\varepsilon, \Lambda_{\varepsilon,\mu}}$ in coordinates adapted to the lattice.

In some situations we shall work in a suitable coordinate system adapted to the present setting. To be precise, when referring in the sequel to **coordinates adapted to the lattice**, we will mean coordinates on M with respect to the point O appearing in Assumption II.1 and to an arbitrary basis $\mathscr{B}_\Gamma$ of the lattice $\Gamma \subset V$.

Recall also from Section 3 (see in particular Remark 3.7) that the choice of such a basis $\mathscr{B}_\Gamma$ associates to the set E of admissible jumps an array $\overrightarrow{E} = (e_1, \ldots, e_N)$, where N is half the cardinality of E (i.e. the size of μ) and $e_j \in E$ for every $j = 1, \ldots, N$. It follows (see in particular (3.10)) that the choice of $\mathscr{B}_\Gamma$ defines a canonical isomorphism

$$L^2_a(M \times V^p, \Lambda_{\mu_\varepsilon}) \ \simeq \ L^2(\varepsilon\mathbb{Z}^n; \mathbb{R}^{\mathcal{M}^p_N, \mu}) \quad ,$$

where $\mathcal{M}^p_N$ is the set of increasing multiindices of length p defined in (3.6). We shall refer for short to $L^2(\varepsilon\mathbb{Z}^n; \mathbb{R}^{\mathcal{M}^p_N, \mu})$ as coordinate space.

Equations (9.10) and (9.12) below give representations in coordinate space of $\tilde{\mathcal{H}}^{(p)}_{\rho_\varepsilon, \Lambda_{\varepsilon,\mu}}$ for $p = 0, 1$. Analogous formulas are also valid for $p > 1$ and we stick to the cases $p = 0, 1$ just for notational simplicity.

As in Section 3 we use the notation $\mu_j := \mu\{e_j\}$ and write $\alpha = (\alpha_j)_{j=1,\ldots,N}$ for the elements of $L^2(\varepsilon\mathbb{Z}^n; \mathbb{R}^{\mathcal{M}^1_N, \mu}) = L^2(\varepsilon\mathbb{Z}^n; \mathbb{R}^{N,\mu})$. For every $j = 1, \ldots, N$ the coordinate vector of e_j with respect to the basis $\mathscr{B}_\Gamma$ is denoted by $(e^i_j)_i \in \mathbb{R}^n$. Moreover we abuse notation as follows: we do not distinguish between functions on M and the corresponding function on coordinate space and denote by the same symbol $\tilde{\mathcal{H}}^{(p)}_{\rho_\varepsilon,\Lambda_{\varepsilon,\mu}}$ both the operator in $L^2_a(M \times V^p, \Lambda_{\varepsilon,\mu})$ and in $L^2(\varepsilon\mathbb{Z}^n; \mathbb{R}^{\mathcal{M}^p_N,\mu})$.

With these conventions a straightforward computation (see Lemma E.3 and Lemma E.6 for more details) yields that in $L^2(\varepsilon\mathbb{Z}^n;\mathbb{R})$ $\big(= L^2(\varepsilon\mathbb{Z}^n;\mathbb{R}^{\mathcal{M}^0_N,\mu})\big)$

$$\tilde{\mathcal{H}}^{(0)}_{\rho_\varepsilon,\Lambda_{\varepsilon,\mu}} \quad = \tag{9.10}$$

$$= \; - \sum_{\gamma\in\mathbb{Z}^n} \mu(\{\gamma\}) \; \big[\; \tau_{\varepsilon\gamma} - 1 \;\big] \; + \; \sum_{j=1}^{N} 4\mu_j \;\sinh^2 \frac{\nabla_{e_j} f}{2} \; + \; \varepsilon \sum_{\gamma\in\mathbb{Z}^n} q_{\varepsilon,\gamma} \; \tau_{\varepsilon\gamma} \quad ,$$

where τ_γ denotes translation in direction $\gamma \in \mathbb{R}^n$, i.e.

$$\tau_\gamma \;\alpha\; (x) \;:=\; \alpha(x+\gamma)$$

and for $\varepsilon > 0$ and $\gamma \in \mathbb{R}^n$ we have $q_{\varepsilon,\gamma} \in C^\infty(\mathbb{R}^n;\mathbb{R})$ and satisfying

$$q_{\varepsilon,\gamma} \;=\; q_\gamma \;+\; \mathcal{O}(\varepsilon) \quad ,$$

with

$$q_\gamma \;:=\; \begin{cases} -\;\frac{1}{4}\;\mu(\{\gamma\})\;\nabla^2_\gamma f & \text{if } \gamma = \pm(e^i_1)_i, \ldots, \pm(e^i_N)_i \\ -\;\frac{1}{2}\;\sum_{j=1}^N \mu_j\;\nabla^2_{e_j} f\;\;\cosh \nabla_{e_j} f & \text{if } \gamma = 0 \\ 0 & \text{otherwise} \end{cases} \quad . \tag{9.11}$$

For $p = 1$ we have in $L^2(\varepsilon\mathbb{Z}^n;\mathbb{R}^{N,\mu})$

$$\tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\Lambda_{\varepsilon,\mu}} \quad = \tag{9.12}$$

$$= \; - \sum_{\gamma\in\mathbb{Z}^n} \mu(\{\gamma\}) \; \big[\; \tau_{\varepsilon\gamma} - 1 \;\big] \; + \; \sum_{j=1}^{N} 4\mu_j \;\sinh^2 \frac{\nabla_{e_j} f}{2} \; + \; \varepsilon \sum_{\gamma\in\mathbb{Z}^n} Q_{\varepsilon,\gamma} \; \tau_{\varepsilon\gamma} \quad ,$$

where for $\varepsilon > 0$ and $\gamma \in \mathbb{R}^n$ we have $Q_{\varepsilon,\gamma} = (Q_{\varepsilon,\gamma;i,j})_{i,j=1,\ldots,N}$ with each $Q_{\varepsilon,\gamma;i,j} \in C^\infty(\mathbb{R}^n;\mathbb{R})$ and

$$Q_{\varepsilon,\gamma} \;=\; D_\gamma \;+\; G_\gamma \;+\; \mathcal{O}(\varepsilon) \quad . \tag{9.13}$$

Here $D_\gamma(x) = (D_{\gamma;i,j}(x))_{i,j=1,\ldots,N}$ is a diagonal matrix for every $\gamma, x \in \mathbb{R}^n$ and

$$D_{\gamma;i,i} \;:=\; \begin{cases} q_\gamma & \text{if } \gamma = \pm(e^i_1)_i, \ldots, \pm(e^i_N)_i \\ q_\gamma \;+\; \sum_{k=1}^N \mu_k\;\nabla^2_{e_k,e_i} f\;\;\sinh \nabla_{e_k} f & \text{if } \gamma = 0 \\ 0 & \text{otherwise} \end{cases} \quad . \tag{9.14}$$

Moreover $G_\gamma(x) = (G_{\gamma;i,j}(x))_{i,j=1,\dots,N}$ for every $\gamma \in \mathbb{R}^n$ and [34]

$$G_{\gamma;i,j} \ := \tag{9.15}$$

$$\begin{cases} \frac{1}{2}\mu_j \ \nabla^2_{e_i,e_j} f \ \big(\ 1_{\gamma,e_i} \ e^{\frac{1}{2}\nabla_{e_i-e_j} f} \ + \ 1_{\gamma,-e_j} \ e^{-\frac{1}{2}\nabla_{e_i-e_j} f} \ \big) & \text{if } \gamma = \pm(e_1^k)_k, \dots, \pm(e_N^k)_k \\ \frac{1}{2}\mu_j \ \nabla^2_{e_i,e_j} f \ e^{-\frac{1}{2}\nabla_{e_i+e_j} f} + \frac{1}{8}\mu_j \big(\ \nabla^2_{e_i} f + \nabla^2_{e_j} f \ \big) \sinh \frac{1}{2}\nabla_{e_i+e_j} f & \text{if } \gamma = 0 \\ \frac{1}{2}\mu_j \ \nabla^2_{e_i,e_j} f \ e^{\frac{1}{2}\nabla_{e_i+e_j} f} & \text{if } \gamma = (e_i^k)_k - (e_j^k)_k \\ 0 & \text{otherwise} \end{cases} .$$

Standard inequalities together with Assumption II.2 (ii) (see Lemma E.7 for more details) give for $q_{\varepsilon,\gamma}$ and $Q_{\varepsilon,\gamma}$ also the following estimates: there exists a constant $C > 0$ and a compact $K \subset \mathbb{R}^n$ such that for $x \in \mathbb{R}^n \setminus K$

$$\sum_{\gamma \in \mathbb{Z}^n} \big(\ |q_{\varepsilon,\gamma}(x)| \ + \ \|Q_{\varepsilon,\gamma}(x)\| \ \big) \ \leq \ C \ V(x) \quad , \tag{9.16}$$

where V is the “potential” appearing both in (9.10) and (9.12) , i.e.

$$V(x) \ := \ \sum_{j=1}^N 4\mu_j \ \sinh^2 \frac{\nabla_{e_j} f(x)}{2} \quad .$$

Remark 9.6. *A word of caution may be said about the relation between the potential $U_{f,\mu}$ appearing in the coordinate-free representation* (9.4) *and the potential V appearing in the above coordinate representations of the Witten Laplacian: if seen as functions, V is just the coordinate expression of $U_{f,\mu}$. But the multiplication operator induced by V is not the coordinate expression of the multiplication operator induced by $U_{f,\mu}$ when $p > 0$! Indeed when expressed in coordinates the multiplication operator $U_{f,\mu}$ on* 1*-functions becomes ε-dependent:*

$$\big(\ U_{f,\mu} \ \alpha \ \big)_i \ (x) \ = \ U_{f,\mu}(x + \varepsilon \frac{1}{2} e_i) \ \alpha_i(x) \quad . \tag{9.17}$$

This is why in (9.13) *the matrix D_γ appears instead of q_γ (the difference is exactly the ε order term in the expansion of the right hand side of* (9.17)*). Note also that the difference between D_γ and q_γ is zero at critical points.*

Remark 9.7. *It is worth to notice that in the case of a nearest neighbour geometry μ (i.e. $N = n$, see Remark 3.1) we have*

$$V(x) \ = \ \sum_{j=1}^n 4 \sinh^2 \frac{\partial_j f}{2} \quad .$$

[34] For $\gamma \in \mathbb{R}^n$ and $v \in V$ we define $1_{\gamma,v}$ to be equal to 1 if γ are the coordinates of v with respect to $\mathscr{B}_\Gamma$ and 0 otherwise.

We work here under Assumptions II.1 and II.2 and denote for every $p = 0, \ldots, n$ by m_p the (finite) number of critical points of f having index p. For the sake of the reader we recall here that n is the dimension of the affine space we are working on and that $N > n$ denotes the size of the discrete geometry μ (see Section 3). For simplicity we restrict here to the Witten Laplacians with $p = 0, 1$. But note that the following discussion could also be extended (mutatis mutandis) to $p > 1$.

The aim of this section is to prove Theorem 10.1 below which provides existence of a certain number (related to m_0, m_1, n and N) of "small" eigenvalues of $\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$ and $\mathcal{H}^{(1)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$. This is an important preliminary result for the analysis which will be developed in Part III, more specifically, for the reduction of the problem of the spectral asymptotics of small eigenvalues of $\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$ to a finite dimensional linear algebra problem (see also Remark 10.5 below and Section 16 in Part III). We stress that both the statements for $p = 0$ *and* $p = 1$ of Theorem 10.1 are used in Part III.

Theorem 10.1.
There exists a constant $c > 0$ such that for $p = 0, 1$ and $\varepsilon > 0$ sufficiently small

$$\mathrm{Spec}_{\mathrm{ess}}\left(\mathcal{H}^{(p)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}\right) \ \subset \ [c, \infty) \quad . \tag{10.1}$$

Moreover for $\varepsilon > 0$ sufficiently small

$$\dim \mathrm{Ran}\, 1_{[0,\varepsilon^{6/5})}(\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}) \ = \ m_0 \tag{10.2}$$

and

$$\dim \mathrm{Ran}\, 1_{[0,\varepsilon^{6/5})}(\mathcal{H}^{(1)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}) \ = \ \tilde{m}_1 \quad , \tag{10.3}$$

where $\tilde{m}_1 \ := \ m_1 \ + \ m_0 \ (N - n)$.

Remark 10.2. *Note that in the case of a nearest neighbour geometry μ (i.e. $N = n$) Theorem 10.1 implies*

$$\dim \mathrm{Ran}\, 1_{[0,\varepsilon^{6/5})}(\mathcal{H}^{(1)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}) \ = \ m_1 \quad ,$$

as in the case of the continuous Witten Laplacian.

Remark 10.3. *The theorem above gives a rather rough bound from above on the small eigenvalues. With some more effort one could show as in the theory of the continuous Witten Laplacian, that the small eigenvalues are actually exponentially small in ε. More precisely, there exists a constant $c > 0$ such that for $\varepsilon > 0$ sufficiently small*

$$\dim \operatorname{Ran} 1_{[0,e^{-c/\varepsilon})}(\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}) \;=\; m_0 \tag{10.4}$$

and

$$\dim \operatorname{Ran} 1_{[0,e^{-c/\varepsilon})}(\mathcal{H}^{(1)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}) \;=\; \tilde{m}_1 \quad .$$

Statement (10.4) *can be obtained as in the continuous case by the min-max theorem, using as test functions in the variational principle $\chi_1 e^{-f/\varepsilon}, \ldots, \chi_k e^{-f/\varepsilon}$ where the χ_k's are suitable cutoff functions each one localized around a minimum of f. We shall not go along this strategy, since in in Part III we will follow another approach, providing much stronger results than* (10.4) *on the small eigenvalues.*

Statement (10.3) *could be obtained by combining the constructions of WKB expansions of the next sections with suitable Agmon estimates on the semiclassical decay of eigenfunctions (see* [64] *for Agmon estimates in the present lattice setting, but note that formally only scalar functions are considered therein).*

Note also that from the proof of Theorem 10.1 given below one can deduce that in both cases $p = 0, 1$ the rest of the spectrum (i.e. the spectrum apart from the low-lying spectrum consisting of the small eigenvalues) is bounded form below by εC with $C > 0$ a constant.

Remark 10.4. *It follows from Assumption II.2(ii) that $e^{-f/\varepsilon} \in L^2(M, d\Lambda_\varepsilon)(\simeq L^2(\varepsilon\mathbb{Z}^n;\mathbb{R}))$ for $\varepsilon > 0$. Since by Proposition B.2 in the appendix $\mathcal{H}^{(0)}_{\rho_\varepsilon,\mu_\varepsilon}$ is essentially selfadjoint for ε sufficiently small when restricted to the space of functions with compact support, we can conclude that $e^{-f/\varepsilon} \in D(\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}})$. It follows that 0 is an eigenvalue of $\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$. This is in accordance with the fact that by Assumption II.2(ii) $m_0 > 0$.*

Remark 10.5. *We shall use Theorem 10.1 in Part III of this work as follows. Let for $p = 0, 1$ and $\varepsilon > 0$*

$$F^{(p)}_\varepsilon \;:=\; \operatorname{Ran} 1_{[0,\varepsilon^{6/5})}(\mathcal{H}^{(p)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}) \quad .$$

Then by Proposition 8.4 we have

$$\delta^{(0)}_{\rho_\varepsilon}\; F^{(0)}_\varepsilon \;\subset\; F^{(1)}_\varepsilon$$

and Theorem 10.1 gives that $\Theta_\varepsilon : F_\varepsilon^{(0)} \to F_\varepsilon^{(1)}$, defined as

$$\Theta_\varepsilon \ := \ \delta^{(0)}_{\rho_\varepsilon}\big|_{F_\varepsilon^{(0)}} \quad ,$$

is for $\varepsilon > 0$ an operator between finite dimensional Hilbert spaces, of dimension m_0 and $\tilde m_1$.

The strategy of the proof of Theorem 10.1 is the same as in the continuous space setting, namely to compare the spectrum of the Witten Laplacian with the spectrum of the harmonic oscillators sitting at the wells of the potential $U_{f,\mu} = \|2\sinh\frac{\nabla f}{2}\|^2_\mu$ appearing in 9.4.

Proof of Theorem 10.1.
We shall work in coordinates $(\mathcal{O}, \mathscr{B}_\Gamma)$ adapted to the lattice. Note first that, due to the coordinate representations (9.10), (9.12) and the estimate (9.16) we are in the setting of Section B in the appendix. The localization (10.1) of the essential spectrum is therefore a consequence of Proposition B.3.

The rest of Theorem 10.1 follows from an application of Theorem B.5. To see this, we introduce first some notation to describe the approximating harmonic oscillators: we denote by D^2 the matrix of second partial derivatives in $\mathbb{R}^n$; after arbitrary ordering of the critical points of f we let $x^{(p,k)}$ be the coordinate vector of the k-th critical point of index p of f; moreover we define the matrix $a = (a_{i,j})_{i,j=1,\dots,n}$ via

$$a_{i,j} \ := \ \frac{1}{2}\sum_{\gamma\in\mathbb{Z}^n} \mu(\{\gamma\})\ \gamma_i\gamma_j \ = \ \sum_{r=1}^{N} \mu_r\ e_r^i e_r^j \quad .$$

Observe that a and $D^2 f(x^{(p,k)})$ commute since both a and $D^2 f(x^{(p,k)})$ are symmetric matrices and a is positive definite.

Recall now equation (9.10) and note that

$$\frac{1}{2}D^2\ \|2\sinh\frac{\nabla f}{2}\|_\mu\ (x^{(p,k)}) \ = \ \big[\ a\ D^2 f(x^{(p,k)})\ \big]^2$$

and that for every $p = 1,\dots,n$ and $k = 1,\dots,m_p$

$$\sum_{\gamma\in\mathbb{Z}^n} q_\gamma(x^{(p,k)}) \ = \ -\ \mathrm{tr}\ aD^2 f(x^{(p,k)}) \quad ,$$

where tr stands for the trace of a matrix.

Recalling (9.12) and (9.13), observe that

$$\sum_{\gamma\in\mathbb{Z}^n} D_\gamma(x^{(p,k)}) \;=\; -\ \mathrm{tr}\left[\ a\ D^2 f\ (x^{(p,k)})\ \right]$$

and define for short for every $p = 1,\dots,n$ and $k = 1,\dots,m_p$ the $N\times N$ matrix $A^{(p,k)}$ as

$$A^{(p,k)} \;:=\; \sum_{\gamma\in\mathbb{Z}^n} G_\gamma(x^{(p,k)}) \quad .$$

From the definition of G_γ (see (9.15)) it follows that

$$A^{(p,k)}_{i,j} \;:=\; 2\ \mu_j\ \nabla^2_{e_i,e_j} f(x^{(p,k)}) \;=\; 2\ \sum_{r',r=1}^{n} \mu_j\ e_i^{r'}\ e_j^{r}\ D^2_{r',r} f(x^{(p,k)})$$

and $A^{(p,k)}$ can be rewritten as

$$A^{(p,k)} \;=\; 2\ E\ D^2 f(x^{(p,k)})\ E^t\ \Lambda_\mu \quad , \tag{10.5}$$

where Λ_μ is the diagonal $N\times N$ matrix with $(\mu_1,\dots,\mu_N)$ on the diagonal and E is an $N\times n$ matrix with $E_{i,j} \;=\; e_i^j$. Note that $A^{(p,k)}$ is in general not a symmetric matrix, but it induces a symmetric operator in $\mathbb{R}^N$ with scalar product given by Λ_μ (i.e. in what we call $\mathbb{R}^{N,\mu}$). We shall denote by $\tilde\lambda_1^{(p,k}, \dots, \tilde\lambda_N^{(p,k)}$ the eigenvalues of $A^{(p,k)}$. It follows from (10.5) that at least $N-n$ eigenvalues of $A^{(p,k)}$ vanish. The remaining eigenvalues coincide (counting multiplicity) with the eigenvalues of $D^2 f(x^{(p,k)})a$. Indeed, E has 0-dimensional kernel, and from $E^t\Lambda_\mu E = a$ and (10.5) it follows that

$$A^{(p,k)}\ E \;=\; E\ D^2 f(x^{(p,k)})a \quad .$$

Now consider for every every $p = 1,\dots,n$ and $k = 1,\dots,m_p$ in $L^2(\mathbb{R}^n, dx;\mathbb{R})$

$$H^{\mathrm{osc},(0)}_{p,k} \;:=\; -\ \mathrm{tr}\, D^2 \;+\; \langle x, \left[\ a\ D^2 f(x^{(p,k)})\ \right]^2 x\rangle \;-\; \mathrm{tr}\left[\ a\ D^2 f\ (x^{(p,k)})\ \right]$$

and in $L^2(\mathbb{R}^n, dx; \mathbb{R}^N, \Lambda_\mu)$

$$H^{\mathrm{osc},(1)}_{p,k} \;:= \mathrm{Id}_N\ H^{\mathrm{osc},(0)}_{p,k} \;+\; 2\ A^{(p,k)} \quad .$$

Thanks to Theorem B.5, to prove (10.2) it is enough to show that $\bigcup_{p,k} \mathrm{Spec}\left(H^{\mathrm{osc},(0)}_{p,k}\right)$ contains only nonnegative numbers and contains 0 with multiplicity m_0.

This can be easily checked, observing that

$$\mathrm{Spec}\left(H^{\mathrm{osc},(0)}_{p,k}\right) \;=\; \left\{\ \sum_{i=1}^{n} |\lambda_i^{(p,k)}|\ (2r_i+1) \;-\; \sum_{i=1}^{n} \lambda_i^{(p,k)}\ \right\}_{r_1,\dots,r_n\in\mathbb{N}_0} \quad ,$$

where $\lambda_1^{(p,k)},\dots,\lambda_n^{(p,k)}$ are the eigenvalues of $aD^2 f(x^{(p,k)})$, and observing that the expression within braces is always nonnegative and 0 only if $k = 1,\dots,m_0$ and $r_1 = \cdots = r_n = 0$ and $p = 0$.

Similarly, again by Theorem B.5, to prove (10.2) it is enough to show that $\bigcup_{p,k} \mathrm{Spec}\left(H^{\mathrm{osc},(1)}_{p,k}\right)$ contains only nonnegative numbers and contains 0 with multiplicity $\tilde{m}_1$.

Indeed, we have now

$$\mathrm{Spec}\left(H^{\mathrm{osc},(1)}_{p,k}\right) \;=\; \Big\{ \;\sum_{i=1}^{n} |\lambda_i^{(p,k)}|\;(2r_i+1) \;-\; \sum_{i=1}^{n} \lambda_i^{(p,k)} \;+\; 2\tilde{\lambda}_j^{(p,k)} \;\Big\}_{\substack{r_1,\dots,r_n\in\mathbb{N}_0\\ j=1,\dots,N}}$$

and the expression within braces is always nonnegative and 0 only in the following cases:

1) $r_1 = \cdots = r_n = 0$ and $p = 0$ and $k = 1, \dots, m_0$ and j is such that $\tilde{\lambda}_j^{(0,k)} = 0$ (as we already mentioned there are exactly $N - n$ such j's for every fixed k).
2) $r_1 = \cdots = r_n = 0$ and $p = 1$ and $k = 1, \dots, m_1$ and j is such that $\tilde{\lambda}_j^{(1,k)}$ equals the only negative eigenvalues of $aD^2 f(x^{(1,k)})$.

□

Remark 10.6. *Note that with the notation introduced in the proof above, in the nearest neighbour case* $a = \Lambda_\mu$, $E = \mathrm{Id}$ *and*

$$A^{p,k} \;=\; D^2 f(x^{(p,k)})\;\Lambda_\mu \;=\; a\;D^2 f(x^{(p,k)}) \quad .$$

The goal of the present section is to construct good quasimodes corresponding to the small eigenvalues of the semiclassical Witten Laplacian for $p = 1$. As emerged from the last section the main contribution to a given small eigenvalue comes either from a small neighbourhood of a saddle point[35] or of a minimum of f (but recall that the latter case is possible only if $N > n$).

Again we do not consider here explicitly the Witten laplacian for $p > 1$ for the only reason to simplify the presentation: there is no conceptual difficulty when passing from $p = 1$ to $p > 1$. The case $p = 0$ is special, due to the fact that we have at hand an explicit expression for the eigenfunction corresponding to the eigenvalue 0, namely $e^{-f/\varepsilon}$. This feature permits to construct very efficient quasimodes corresponding to the small eigenvalues of $\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$, defined not only locally around the minima of f. The details for this will be given in Section 14.

In the case $p = 1$ treated here, the quasimodes are constructed locally around the involved critical points through a WKB Ansatz. The main result is Theorem 11.1 below, which treats the case of a saddle point (for the case of a minimum see Remark 11.11). Given a saddle point $\bar{\zeta}$ of f, we use the following notation: $\mathscr{B}_{f,\mu} := (\mathfrak{e}_1, \dots, \mathfrak{e}_n)$ stands for a basis of V which simultaneously diagonalizes both μ and $\nabla^2 f(\bar{\zeta})$. To be precise, we assume that $(\mathfrak{e}_1, \dots, \mathfrak{e}_n)$ satisfies

$$\frac{1}{2}\int_V \mu(dw)\ \mathfrak{e}_i^*(w)\ \mathfrak{e}_j^*(w) = 1_{i,j} \quad \text{and} \quad \nabla^2_{\mathfrak{e}_i,\mathfrak{e}_j} f(\bar{\zeta}) = \kappa_j\ 1_{i,j} \quad , \tag{11.1}$$

where $(\mathfrak{e}_1^*, \dots, \mathfrak{e}_n^*)$ denotes the dual basis associated with $(\mathfrak{e}_1, \dots, \mathfrak{e}_n)$ and $\kappa_1, \dots, \kappa_n \in \mathbb{R}$ are the eigenvalues of the nondegenerate symmetric bilinear form $\nabla^2 f(\bar{\zeta})$ with respect to the scalar product induced by μ on V. Moreover we shall always assume that the basis is ordered in such a way that

$$\kappa_1 < 0 \quad \Big(\text{ and } \ \kappa_2, \dots, \kappa_n > 0 \Big) \quad .$$

Observe that in general, unlike the basis $\mathscr{B}_\Gamma := (b_1, \dots, b_n)$ introduced before (which does so by definition), $\mathscr{B}_{f,\mu}$ does not generate the lattice Γ. To avoid confusion we point also to the fact that while $\mathfrak{e}_i$ is a vector in $\mathscr{B}_{f,\mu}$ the symbol e_i stands for an element of E, the set of admissible jumps corresponding to μ.

[35]We use the expression saddle point as a shorthand for critical point of index 1.

Recall also the definition of $\tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\varepsilon,\mu}$ in (9.3) and that we work here under Assumptions II.1 and II.2 [36]. The meaning of the symbols used to denote asymptotic relations is standard and explained for completeness at the beginning of Section E in the appendix.

Theorem 11.1 (Local Existence of WKB-type Quasimodes)**.**

Fix a critical point $\bar\zeta$ of f having index 1. There exist an open neighbourhood Ω of $\bar\zeta$, a $\varphi \in C^\infty(M;\mathbb{R})$ and, for $\varepsilon > 0$, an $a_\varepsilon \in C^\infty(M;\mathbb{R}_a^{V^p,\mu})$ with the following properties:

(i)
$$e^{\frac{\varphi}{\varepsilon}} \quad \tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\varepsilon,\mu} \quad a_\varepsilon e^{-\frac{\varphi}{\varepsilon}} \,\Big|_{\Omega} \;\sim\; 0 \quad .$$

(ii)
$$\varphi(\bar\zeta) = 0 \quad , \quad \nabla\varphi(\bar\zeta) \equiv 0 \quad \textit{and} \quad \nabla^2_{\mathfrak{e}_i,\mathfrak{e}_j}\varphi(\bar\zeta) = |\kappa_j| \; 1_{i,j} \quad .$$

(iii) *there exists a sequence $\{\hat a_k\}_{k\in\mathbb{N}_0} \subset C^\infty(M;\mathbb{R}_a^{V^p,\mu})$ such that*
$$\hat a_0(\bar\zeta) \;=\; \mathfrak{e}_1 \qquad \textit{and} \qquad a_\varepsilon \;\sim\; \sum_{k=0}^{\infty} \varepsilon^k \;\; \hat a_k \quad .$$

Before giving the proof, which will occupy the rest of this section, we make the following remark on the phase function φ.

Remark 11.2.

It will follow from the proof below (in particular from Lemma 11.8) that the phase function φ appearing in Theorem 11.3 locally solves the eikonal equation given by the "reversed" hamiltonian
$$H^{\mathrm{rev}}_{f,\mu}(\zeta,\xi) \;:=\; -H_{f,\mu}(\zeta, i\xi) \;=\; \|2\sinh\frac{\xi}{2}|^2_\mu - \|2\sinh\frac{\nabla f(\zeta)}{2}|^2_\mu \quad .$$
To be specific, there exists an open neighbourhood Ω of $\bar\zeta$ such that
$$H^{\mathrm{rev}}_{f,\mu}(\zeta,\nabla\varphi(\zeta)) = 0 \quad \textit{for every } \zeta\in\Omega \quad . \tag{11.2}$$
As shown in [64]*, equation* (11.2) *together with the "boundary" conditions $\varphi(\bar\zeta) = 0$ and $\nabla^2\varphi(\bar\zeta) > 0$ permits to interpret $\varphi\Big|_\Omega$ as the restriction of a globally defined Finslerian distance $d_{Ag}(\bar\zeta,\cdot)$ from the point $\bar\zeta$. This distance*

[36] Indeed, as already mentioned, from Assumption II.2 only (i) is needed in this section, since our constructions are local.

plays for Hamilton operators on lattice graphs the analogous role of the Agmon distance in the theory of classical Schrödinger operators in continuous setting: it is in particular the basic geometric object which enters in the analysis of both the decay of eigenfunctions (Agmon estimates) and the splitting of eigenvalues in the semiclassical limit (see [64] *for Agmon estimates on the lattice and the Phd thesis* [87]*).*

In classical mechanics d_{Ag} is also known as the Jacobi distance associated with the Hamiltonian $H^{\mathrm{rev}}_{f,\mu}$, appearing in some formulation of Maupertius principle. A variational representation of d_{Ag} can be given as follows (see again [64] *for details).*

Let $E : M \times V \to \mathbb{R}$ be the energy function corresponding to the Hamiltonian $H^{\mathrm{rev}} := H^{\mathrm{rev}}_{f,\mu}$. Recall that the former is obtained from H^{rev} by a fiberwise Legendre transformation. More precisely, consider for every $\zeta \in M$ the map $\nabla H^{\mathrm{rev}}_{\zeta} : V^* \to V^{**} \simeq V^*$, where $H^{\mathrm{rev}}_{\zeta} : V^* \to \mathbb{R}$ is defined via $H^{\mathrm{rev}}_{\zeta}(\xi) := H^{\mathrm{rev}}(\zeta, \xi)$ (here ∇ denotes the differential with respect to the variable ξ). Then the energy E is given by

$$E(\zeta, v) \ := \ H^{\mathrm{rev}}(\zeta, [\nabla H^{\mathrm{rev}}_{\zeta}]^{-1}(v)) \quad ,$$

where $[\nabla H^{\mathrm{rev}}_{\zeta}]^{-1} : V \to V^*$ is the inverse of $\nabla H^{\mathrm{rev}}_{\zeta}$. Observe that for every $\xi, \xi' \in V^*$

$$\nabla_{\xi'} H^{\mathrm{rev}}_{\zeta} \ (\xi) \ = \ \langle 2 \sinh \xi, \xi' \rangle_{\mu} \quad .$$

In particular $\nabla H^{\mathrm{rev}}_{\zeta} \ (\xi)$ (and consequently also $[\nabla H^{\mathrm{rev}}_{\zeta}]^{-1} \ (v)$) is independent of ζ for every $\xi \in V^*$ (respectively for every $v \in V$). We shall write briefly $v(\xi) := \nabla \tilde{H}_{\zeta} \ (\xi)$ and $\xi(v) := [\nabla \tilde{H}_{\zeta}]^{-1} \ (v)$.

One can show that, given $(\zeta, v) \in M \times V \setminus \{0\}$, one can find a unique nonnegative scalar $r(\zeta, v)$ which by rescaling v projects (ζ, v) to the energy shell corresponding to energy zero:

$$E(\zeta, r(\zeta, v)v) = 0 \quad .$$

Next define for $(\zeta, v) \in M \times V$

$$L(\zeta, v) := \xi_v(r(\zeta, v)v) \quad .$$

This turns out to be an absolutely homogeneous Finsler function. The associated distance $d_{Ag} : M \times M \to \mathbb{R}_+$ is defined as

$$d_{Ag}(\zeta, \eta) = \inf \int_0^1 L(\gamma(t)), \gamma'(t)) \ dt \quad ,$$

where the infimum is taken over the set of piecewise C^1 paths such that $\gamma(0) = \zeta$ and $\gamma(1) = \eta$. As we already mentioned, one has locally around $\bar{\zeta}$

$$\varphi = d_{Ag}(\bar{\zeta}, \cdot)$$

Moreover $d_{Ag}(\bar{\zeta}, \cdot)$ is locally Lipshitz continuous and satisfies for almost every $\zeta \in M$ the eikonal inequality

$$H^{\text{rev}}_{f,\mu}(\zeta, \varphi(\zeta)) \leq 0 \quad .$$

Notice that in the case of the classical Witten Laplacian on a Riemannian manifold (M, g) (recall that in this case $H_{f,g}(\zeta, \xi) = \|\xi\|_g^2 + \|\nabla f(x)\|_g^2$, so $H^{\text{rev}}_{f,g}(\zeta, \xi) = \|\xi\|_g^2 - \|\nabla f(\zeta)\|^2$) the Legendre transformation and the scalar $r(\zeta, v)$ are explicitly computable and one gets $L(\zeta, v) = \|\nabla f(\zeta)\|_g \; \|v\|_g$. The associated distance is the usual Agmon distance

$$\inf \int_0^1 \|\nabla f(\gamma(t))\|_g \; \|\gamma'(t)\|_g \; dt \quad .$$

Observe also that (neglecting the critical points of f where in any case degeneracy occurs) this distance has the special property to be not only Finslerian but even Riemannian: it corresponds to the metric tensor $\|\nabla f\|_g \langle \cdot, \cdot \rangle_g$.

As a first step for the proof of Theorem 11.1 we shall first prove the following, slightly weaker statement.

Proposition 11.3 (Local existence of WKB-type Quasimodes. Weak version)**.**

Fix a critical point point $\bar{\zeta}$ of f having index 1. There exist an open neighbourhood Ω of $\bar{\zeta}$, a $\varphi \in C^\infty(M; \mathbb{R})$ and, for $\varepsilon > 0$, a $\nu_\varepsilon \in \mathbb{R}$ and an $a_\varepsilon \in C^\infty(M; \mathbb{R}^{V,\mu}_a)$ with the following properties:

(i)

$$e^{\frac{\varphi}{\varepsilon}} \left[\; \tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon, \varepsilon, \mu} - \nu_\varepsilon \; \right] a_\varepsilon e^{-\frac{\varphi}{\varepsilon}} \Big|_\Omega \; \sim \; 0 \quad .$$

(ii)

$$\varphi(\bar{\zeta}) = 0 \quad , \quad \nabla \varphi(\bar{\zeta}) \equiv 0 \quad \textit{and} \quad \nabla^2_{\mathfrak{e}_i, \mathfrak{e}_j} \varphi(\bar{\zeta}) = |\kappa_j| \; 1_{i,j} \quad .$$

(iii) *there exists a sequence* $\{\hat{\nu}_k\}_{k\in\mathbb{N}_0} \subset \mathbb{R}$ *such that*

$$\hat{\nu}_0 \;=\; \hat{\nu}_1 \;=\; 0 \qquad \textit{and} \qquad \nu_\varepsilon \sim \sum_{k=0}^{\infty} \varepsilon^k \; \hat{\nu}_k \quad .$$

(iv) *there exists a sequence* $\{\hat{a}_k\}_{k\in\mathbb{N}_0} \subset C^\infty(M; \mathbb{R}_a^{V^p,\mu})$ *such that*

$$\hat{a}_0(\bar{\zeta}) \;=\; \mathfrak{e}_1 \qquad \textit{and} \qquad a_\varepsilon \;\sim\; \sum_{k=0}^{\infty} \varepsilon^k \quad \hat{a}_k \quad .$$

Observe that in order to obtain Theorem 11.1 from this preliminary version one has just to show that $\hat{\nu}_k = 0$ for every $k \in \mathbb{N}_0$. This will be done at the end of the section exploiting the intertwining relations given by Proposition 8.2 (ii).

Remark 11.4. *Note that in Proposition* (11.3) *the set* Ω *can be shrinked to a smaller* $\tilde{\Omega} \subset \Omega$ *and that* a_ε *can be multiplied with a function* $\chi \in C^\infty(M; \mathbb{R})$ *having compact support and satisfying* $\chi \equiv 1$ *on* $\tilde{\Omega}$. *Thus, taking* Ω *and the support of* a_ε *sufficiently small one gets the following additional property:*

$$\varphi > 0 \quad \textit{on} \quad \textit{supp}\; a_\varepsilon \setminus \{0\} \quad \textit{for}\; \varepsilon > 0 \quad .$$

Remark 11.5. *With the requirement* $\hat{\nu}_1 = 0$ *we limit ourselves in Proposition 11.3 to the construction of a WKB-type quasimode associated with a low-lying eigenvalue of* $\tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\Lambda_{\varepsilon,\mu}}$ *(equivalently of* $\mathcal{H}^{(1)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$*). This is sufficient for the applications in Part III.*

Nevertheless, we remark that the WKB-methods for Schrödinger operators developed in [45] *can also be exploited in the asymptotic analysis of other eigenvalues* [37]*. This is also possible in the present setting: the paper* [66] *contains a general WKB-analysis of a class of discrete Hamilton Operators including* $\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$. *The consideration of generic eigenvalues involves some technical complications, due to the possible degeneracy of the associated eigenvalues in the harmonic approximation. Moreover the main statement has to be modified, since in general half-integer powers of* ε *appear in the expansion of* ν_ε.

The narrower scope we are interested in permits to simplify the arguments given in [66] *and to streamline the proof. On the other hand, we provide with Proposition 11.3 an extension of the results contained in* [66]*, which is crucial for the applications in Part III: we consider operators acting on*

[37] To be more precise: for *any* given integer N, one can have for ε small enough an asymptotic analysis of the first N eigenvalues.

1-functions and we add the properties of φ, a_ε and ν_ε which are specific to the particular Laplacian-structure of the Hamiltonian operator we are considering.

Remark 11.6. *Observe that the amplitude a_ε can be multiplied by $\sum_{j\geq 0}\varepsilon^j K_j$, with arbitrary $K_0 \in \mathbb{R}\setminus\{0\}$ and $K_j \in \mathbb{R}$ for $j \geq 1$, and an arbitrary constant $c \in \mathbb{R}$ can be added to the phase φ.*

With the choices $\varphi(\bar{\zeta}) = 0$ and $\|a_0(\bar{\zeta})\|_\mu = 1$ appearing in Proposition 11.3, the scaling properties of the norm $\|a_\varepsilon\ e^{-\varphi/\varepsilon}\|_{\Lambda_{\varepsilon,\mu}}$ are as follows: if we additionally assume that $\varphi > 0$ on $\operatorname{supp} a_\varepsilon \setminus \{0\}$ for $\varepsilon > 0$ (this is no loss of generality by Remark 11.4), it follows by repeatedly applying the Laplace asymptotics (see Corollary C.2) to every term of the Taylor expansion of $\|\tau_{\varepsilon *}\ \hat{a}_k\ e^{-\varphi/\varepsilon}\|_\mu$ for every $k \in \mathbb{N}_0$, that

$$\varepsilon^{n/4}\ \|a_\varepsilon\ e^{-\varphi/\varepsilon}\|_{\Lambda_{\varepsilon,\mu}} \ \sim\ \sum_{k=0}^{\infty} \varepsilon^k\ I_k \quad ,$$

where $(I_k)_{k\in\mathbb{N}_0}$ is a sequence in $\mathbb{R}$, with

$$I_0 \ =\ \frac{\pi^{n/4}}{(\det \operatorname{Hess}\varphi(0))^{1/4}} \quad .$$

Remark 11.7. *The pointwise estimate (i) in Proposition 11.3 leads easily to the following norm estimate, which will be exploited in the sequel:*

Let $\Omega \subset M$, $\varphi \in C^\infty(M;\mathbb{R})$ and, for $\varepsilon > 0$, $\nu_\varepsilon \in \mathbb{R}$ and $a_\varepsilon \in C^\infty(M;\mathbb{R}_a^{Vp,\mu})$ as in Proposition 11.3. Assume furthermore that $\varphi > 0$ on $\operatorname{supp} a_\varepsilon \setminus \{0\}$ for $\varepsilon > 0$ (this is no loss of generality by Remark 11.4). Then

$$\|(\tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\varepsilon,\mu} - \nu_\varepsilon)\ a_\varepsilon e^{-\varphi/\varepsilon}\|_{\Lambda_{\varepsilon,\mu}} \ =\ \mathcal{O}(\varepsilon^\infty) \quad . \tag{11.3}$$

In fact, taking a compact $K \subset \Omega$ containing an open neighbourhood of $\bar{\zeta}$, we have

$$\|(\tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\varepsilon,\mu} - \nu_\varepsilon)\ a_\varepsilon e^{-\varphi/\varepsilon}\|^2_{\Lambda_{\varepsilon,\mu}} \ = \tag{11.4}$$

$$= \int_K \|\tau_{\varepsilon *}\ (\tilde{\mathcal{H}}_{\rho_\varepsilon,\varepsilon,\mu} - \nu_\varepsilon)\ a_\varepsilon e^{-\varphi/\varepsilon}\ (\zeta)\|_\mu\ \Lambda_\varepsilon(d\zeta)\ +$$
$$+ \int_{K^c} \|\tau_{\varepsilon *}\ (\tilde{\mathcal{H}}_{\rho_\varepsilon,\varepsilon,\mu} - \nu_\varepsilon)\ a_\varepsilon e^{-\varphi/\varepsilon}\ (\zeta)\|_\mu\ \Lambda_\varepsilon(d\zeta) \quad .$$

For the first term in the right hand side of (11.4) *we use (i) of Proposition 11.3, giving for every* $\zeta \in K$, $N \in \mathbb{N}_0$ *and* ε *sufficiently small (see also Remark E.1 in the appendix)*

$$\|\tau_{\varepsilon *}\ (\tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\varepsilon,\mu} - \nu_\varepsilon)\ a_\varepsilon e^{-\varphi/\varepsilon}\ (\zeta)\|_\mu \leq \mathrm{Const}\,\varepsilon^N\ e^{-\varphi(\zeta)/\varepsilon}$$

with ε*-independent constant. It follows (by using for example Corollary C.2) that*

$$\int_K \|\tau_{\varepsilon *}\ (\tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\varepsilon,\mu} - \nu_\varepsilon)\ a_\varepsilon e^{-\varphi/\varepsilon}\ (\zeta)\|_\mu\ \Lambda_\varepsilon(d\zeta)\ =\ \mathcal{O}(\varepsilon^\infty)\quad .$$

For the second term in the right hand side of (11.4) *we use that away from a fixed neighbourhood of* $\bar{\zeta}$ *the bound* $\varphi \geq \mathrm{Const} > 0$ *holds on* $\operatorname{supp} a_\varepsilon$*. Exploiting that* $\operatorname{supp} a_\varepsilon$ *has* ε*-independent compact support and Remark 9.4 one gets*

$$\int_{K^c} \|\tau_{\varepsilon *}\ (\tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\varepsilon,\mu} - \nu_\varepsilon)\ a_\varepsilon e^{-\varphi/\varepsilon}\ (\zeta)\|_\mu\ \Lambda_\varepsilon(d\zeta)\ \leq\ e^{-\gamma/\varepsilon}$$

for some $\gamma > 0$*.*

Notice also that, due to the intertwining relations (Proposition 8.2 (ii)), both the pointwise estimate (i) in Proposition 11.3 and the norm estimate (11.3) *still hold true when substituting* $a_\varepsilon e^{-\varphi/\varepsilon}$ *with* $\tilde{\delta}_{\rho_\varepsilon,\varepsilon}\ a_\varepsilon e^{-\varphi/\varepsilon}$ *or with* $\tilde{\delta}^{*\mu}_{\rho_\varepsilon,\varepsilon}\ a_\varepsilon e^{-\varphi/\varepsilon}$*, where*

$$\tilde{\delta}_{\rho_\varepsilon,\varepsilon}\ := \Psi_\varepsilon\ \delta_{\rho_\varepsilon}\ \Psi_\varepsilon^{-1}\qquad \text{and}\qquad \tilde{\delta}^{*\mu}_{\rho_\varepsilon,\varepsilon}\ :=\ \Psi_\varepsilon\ \delta^{*\mu_\varepsilon}_{\rho_\varepsilon}\ \Psi_\varepsilon^{-1}\quad . \tag{11.5}$$

More explicilty, we shall use in the sequel that

$$\|(\tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\varepsilon,\mu} - \nu_\varepsilon)\ \tilde{\delta}_{\rho_\varepsilon,\varepsilon}\ a_\varepsilon e^{-\varphi/\varepsilon}\|_{\Lambda_{\varepsilon,\mu}}\ =\ \mathcal{O}(\varepsilon^\infty) \tag{11.6}$$

and

$$\|(\tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\varepsilon,\mu} - \nu_\varepsilon)\ \tilde{\delta}^{*\mu}_{\rho_\varepsilon,\varepsilon}\ a_\varepsilon e^{-\varphi/\varepsilon}\|_{\Lambda_{\varepsilon,\mu}}\ =\ \mathcal{O}(\varepsilon^\infty)\quad .$$

Proof of Proposition 11.3. We essentially follow the standard strategy for establishing WKB-type results for the ground state of a classical Schrödinger operator in $\mathbb{R}^n$ with a nondegenerate potential minimum (see for example [40],[27]).

Step 1:

Let $\varphi \in C^\infty(M;\mathbb{R})$ and let , for $\varepsilon > 0$, $\nu_\varepsilon \in \mathbb{R}$ and $a_\varepsilon \in C^\infty(M;\mathbb{R}_a^{V,\mu})$. If ν_ε and a_ε admit expansions

$$\nu_\varepsilon \sim \sum_{k=0}^{\infty} \varepsilon^k \ \hat{\nu}_k \quad \text{and} \quad a_\varepsilon \Big|_\Omega \sim \sum_{k=0}^{\infty} \varepsilon^k \ \ \hat{a}_k$$

for some open neighbourhood Ω of $\bar{\zeta}$, then the left hand side appearing in (i) admits an expansion in powers of ε:

$$e^{\frac{\varphi}{\varepsilon}} \left[\ \tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\varepsilon,\mu} - \nu_\varepsilon \ \right] a_\varepsilon e^{-\frac{\varphi}{\varepsilon}} \Big|_\Omega \ \sim \ \sum_{k=0}^{\infty} \varepsilon^k \ \ \gamma_k \ \ , \tag{11.7}$$

with $\gamma_k \in C^\infty(\Omega;\mathbb{R}_a^{Vp,\mu})$ for every $k \in \mathbb{N}_0$. Statement (11.7) is obtained by direct computation using Taylor expansions. The details, together with explicit expressions for the γ_k's in terms of φ, $(\hat{a}_k)_{k\in\mathbb{N}_0}$ and $(\nu_k)_{k\in\mathbb{N}_0)}$ are given in Lemma 11.8 below.

Step 2:

We show that one can find an open neighbourhood Ω of $\bar{\zeta}$, $\varphi \in C^\infty(\Omega;\mathbb{R})$, a sequence $(\hat{a}_k)_{k\in\mathbb{N}_0}$ in $C^\infty(\Omega;\mathbb{R}_a^{Vp,\mu})$ and a sequence $(\nu_k)_{k\in\mathbb{N}_0}$ in $\mathbb{R}$ such that

- the γ_k's appearing in (11.7) do identically vanish
- φ satisfies (ii) and $\hat{\nu}_0$, $\hat{\nu}_1$, $\hat{a}_0(\bar{\zeta})$ are given as in (iii) and (iv).

This amounts to show local solvability of singular partial (eiconal and transport type equations). The details are given in Lemma 11.10 below.

Step 3

Let Ω, φ,$(\hat{a}_k)_{k\in\mathbb{N}_0}$ and $(\nu_k)_{k\in\mathbb{N}_0}$ be as in Step 2. A standard Borel summation in ε gives the existence of ν_ε and a_ε such that

$$\nu_\varepsilon \sim \sum_{k=0}^{\infty} \varepsilon^k \ \hat{\nu}_k \quad \text{and} \quad a_\varepsilon \sim \sum_{k=0}^{\infty} \varepsilon^k \ \ \hat{a}_k \ \ .$$

Finally, multiplying both a_ε and φ with a function $\chi \in C^\infty(M;\mathbb{R})$ having compact support and satisfying $\chi = 1$ on an open neighbourhood of $\bar{\zeta}$ finishes the proof. $\square$

For the next lemma recall the definition of the Hamiltonian $H_{f,\mu}$ and of the subleading symbol $M_{f,\mu}$ given in (9.8) and (9.9).

Lemma 11.8 (Expansion of the WKB Ansatz)**.**

Let $\varphi \in C^\infty(M;\mathbb{R})$ and for $\varepsilon > 0$ let $\nu_\varepsilon \in \mathbb{R}$ and $a_\varepsilon \in C^\infty(M;\mathbb{R}_a^{V^p,\mu})$. Assume that

(i) *there exists a sequence $\{\hat\nu_k\}_{k\in\mathbb{N}_0} \subset \mathbb{R}$ such that*

$$\nu_\varepsilon \sim \sum_{k=0}^{\infty} \varepsilon^k \ \hat\nu_k \quad .$$

(ii) *there exist an open $\Omega \subset M$ and a sequence $\{\hat a_k\}_{k\in\mathbb{N}_0} \subset C^\infty(\Omega;\mathbb{R}_a^{V,\mu})$ such that*

$$a_\varepsilon \Big|_\Omega \sim \sum_{k=0}^{\infty} \varepsilon^k \quad \hat a_k \quad . \tag{11.8}$$

Then

$$e^{\varphi/\varepsilon} \ \Big[\ \tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\varepsilon,\mu} - \nu_\varepsilon \ \Big] \ e^{-\varphi/\varepsilon} a_\varepsilon \ \Big|_\Omega \quad \sim$$

$$\sim \quad \sum_{k=0}^{\infty} \ \varepsilon^k \quad \Big[\ H_{f,\mu}(\cdot, i\nabla\varphi) - \hat\nu_0 \ \Big] \ \hat a_k \ + \ \sum_{k=1}^{\infty} \ \varepsilon^k \quad \Big[\ T - (Q_k + \hat\nu_1) \ \Big] \ \hat a_{k-1} \quad ,$$

where $T : C^\infty(\Omega;\mathbb{R}_a^{V^p,\mu}) \to C^\infty(\Omega;\mathbb{R}_a^{V^p,\mu})$ is a smooth first order differential operator given by

$$T := \mathrm{Tr}_\mu \Big[\ 2\sinh(\nabla\varphi) \ \nabla \ + \ \nabla(\sinh\nabla\varphi) \ \Big] \ + \ M_{f,\mu}(\cdot, -i\nabla\varphi)$$

and, for every $k \in \mathbb{N}_*$, Q_k is in $C^\infty(\Omega;\mathbb{R}_a^{V^p,\mu})$ and has the form

$$Q_k := \sum_{l=0}^{k-2} \ \Big\{ \ D_{k,l} \ \hat a_l \ + \ \hat\nu_{l+2} \ \hat a_{k-l-2} \ \Big\} \quad ,$$

with $D_{k,l} : C^\infty(\Omega;\mathbb{R}_a^{V^p,\mu}) \to C^\infty(\Omega;\mathbb{R}_a^{V^p,\mu})$ for $k \in \mathbb{N}_*, l \in \{0,\dots,k-2\}$.

Remark 11.9. *Observe that $Q_1 \equiv 0$. Moreover it will follow from the proof of Lemma 11.8 that $D_{k,l}$ is a smooth linear differential operator of order $k-l$ given by*

$$D_{k,l} \ =$$

$$= \sum_{m=0}^{k-l} \sum_{\mathbf{s}\in\{-1,1\}^2} \mathrm{sign}(\mathbf{s}) \ \Big\{ \ \mathrm{Tr}_\mu \ \big(\frac{\hat{\mathfrak{c}}_{k-l-m}}{m!} \ \bar\nabla^m\big)_{\mathbf{s}} \ - \ \big(\frac{\hat{\bar{\mathfrak{c}}}_{k-l-m}}{m!} \ \bar\nabla^m\big)_{\mathbf{s}}^{\sharp\mu} \ \Big\} \quad ,$$

where $(\bar\nabla_{v_1,v_2})_{v_1,v_2\in V}$ is defined via

$$\bar\nabla_{v_1,v_2} \ := \ \frac{1}{2} \ (\ \nabla_{v_1} \ + \ \nabla_{v_2} \ ) \tag{11.9}$$

and $\hat{\mathfrak{c}}_k := \{\hat{\mathfrak{c}}_{k;v_1,v_2}\}_{v_1,v_2\in V^2}$, $\hat{\bar{\mathfrak{c}}}_k := \{\hat{\bar{\mathfrak{c}}}_{k;v_1,v_2}\}_{v_1,v_2\in V^2}$ *with* $\hat{\mathfrak{c}}_{k;v_1,v_2}, \hat{\bar{\mathfrak{c}}}_{k;v_1,v_2} \in C^\infty(M;\mathbb{R})$. *(For more explicit expressions of the latter see Lemma E.8 in the appendix)*

Proof of Lemma 11.8. First observe that by Remark 8.8 the operator obtained by conjugating $\tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\varepsilon,\mu}$ with $e^{-\varphi/\varepsilon}$ is given by

$$e^{\varphi/\varepsilon}\ \tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\varepsilon,\mu}\ e^{-\varphi/\varepsilon} \ = \tag{11.10}$$
$$\sum_{\mathbf{s}\in\{-1,1\}^2} \operatorname{sign}(\mathbf{s}) \Big\{ \ - \operatorname{Tr}_\mu \ \big(\mathfrak{c}_\varepsilon \ \mathcal{T}^2_\varepsilon\big)_{\mathbf{s}} \ + \ \big(\bar{\mathfrak{c}}_\varepsilon \ \mathcal{T}^2_\varepsilon\big)_{\mathbf{s}}^{\sharp\mu} \Big\} \ ,$$

where, with $\tilde{\rho}_\varepsilon := e^{-2\varphi/\varepsilon}$, for $w_1, w_2 \in V$

$$\mathfrak{c}_{\varepsilon;w_1,w_2} := \mathfrak{c}_{f,\varepsilon;w_1,w_2} := \frac{1}{\sqrt{\rho_\varepsilon\tilde{\rho}_\varepsilon}}\ \mathcal{T}_{\varepsilon w_1}\ \rho_\varepsilon\ \mathcal{T}_{\varepsilon w_2}\ \sqrt{\frac{\tilde{\rho}_\varepsilon}{\rho_\varepsilon}}$$

and

$$-\bar{\mathfrak{c}}_{\varepsilon;w_1,w_2} := \mathfrak{c}_{-f,\varepsilon;w_1,w_2} - \mathfrak{c}_{f,\varepsilon;w_2,w_1} \quad .$$

The statement of Lemma 11.8 follows now in a straightforward manner by Taylor expansions of arbitrary order of the coefficients $\mathfrak{c}_\varepsilon$, $\bar{\mathfrak{c}}_\varepsilon$ and of $\mathcal{T}^2_\varepsilon$. All the computations are reported hereafter for completeness. We shall use that for every $N \in \mathbb{N}_0$ (with $\bar{\nabla}$ as in (11.9))

$$\mathcal{T}^2_\varepsilon = \sum_{k=0}^{N} \ \varepsilon^k \ \ \frac{1}{k!}\bar{\nabla}^k \ + \ \varepsilon^{N+1} \quad \int_0^1 dt\ \frac{(1-t)^N}{N!}\ \mathcal{T}^2_{\varepsilon t}\ \bar{\nabla}^{N+1} \tag{11.11}$$

and (see Lemma E.8 in the appendix) that

$$\mathfrak{c}_\varepsilon \ = \ \sum_{k=0}^{N} \ \varepsilon^k \ \ \hat{\mathfrak{c}}_k \ + \ \varepsilon^{N+1} \ \ r^{(N+1)}_{\mathfrak{c},\varepsilon} \tag{11.12}$$

and

$$\bar{\mathfrak{c}}_\varepsilon \ = \ \sum_{k=0}^{N} \ \varepsilon^k \ \ \hat{\bar{\mathfrak{c}}}_k \ + \ \varepsilon^{N+1} \ \ r^{(N+1)}_{\bar{\mathfrak{c}},\varepsilon} \tag{11.13}$$

with for every $k, N \in \mathbb{N}_0$, $w_1, w_2 \in V$, $\varepsilon > 0$ the functions $\hat{\mathfrak{c}}_{k;w_1,w_2}$, $\hat{\bar{\mathfrak{c}}}_{k;w_1,w_2}$, $r^{(N+1)}_{\mathfrak{c},\varepsilon;w_1,w_2}$, $r^{(N+1)}_{\bar{\mathfrak{c}},\varepsilon;w_1,w_2}$ in $C^\infty(M;\mathbb{R})$ and

$$r^{(N+1)}_{\mathfrak{c},\varepsilon;w_1,w_2} \quad , r^{(N+1)}_{\bar{\mathfrak{c}},\varepsilon;w_1,w_2} = \mathcal{O}(1) \quad .$$

Step 1:

We show that in Ω for every $N \in \mathbb{N}_0$

$$e^{\varphi/\varepsilon} \ \tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\varepsilon,\mu} \ \ e^{-\varphi/\varepsilon} a_\varepsilon \ = \ \sum_{k=0}^{N} \varepsilon^k \ \ P_k \ \ + \varepsilon^{N+1} \ \ R^{(N+1)}_\varepsilon \ \ , \tag{11.14}$$

where for $k \in \mathbb{N}_0$

$$P_k \ := \sum_{k_1=0}^{k} \sum_{k_2=0}^{k-k_1} \sum_{\mathbf{s}\in\{-1,1\}^2} \operatorname{sign}(\mathbf{s}) \Big\{ - \operatorname{Tr}_\mu \ \big(\frac{\hat{\mathfrak{c}}_{k-k_1-k_2}}{k_2!} \ \bar{\nabla}^{k_2}\big)_{\mathbf{s}} + \tag{11.15}$$

$$+ \ \big(\frac{\hat{\bar{\mathfrak{c}}}_{k-k_1-k_2}}{k_2!} \ \bar{\nabla}^{k_2}\big)_{\mathbf{s}}^{\sharp\mu} \Big\} \, \hat{a}_{k_1}$$

and, for every $N \in \mathbb{N}_0$, $R^{(N+1)}_\varepsilon$ is in $C^\infty(\Omega;\mathbb{R}^{V,\mu})$ and satisfies $R^{(N+1)}_\varepsilon = \mathcal{O}(1)$.

Indeed, combining (11.11) with (11.12) yields for every $N \in \mathbb{N}_0$

$$\mathfrak{c}_\varepsilon \ \mathcal{T}^2_\varepsilon = \sum_{k_1=0}^{N} \sum_{k_2=0}^{N-k_1} \varepsilon^{k_1+k_2} \ \ \hat{\mathfrak{c}}_{k_1} \ \frac{1}{k_2!} \bar{\nabla}^{k_2} \ \ + \ \ \varepsilon^{N+1} \ \ \mathcal{R}^{(N+1)}_{\mathfrak{c},\varepsilon} \ \ , \tag{11.16}$$

with

$$\mathcal{R}^{(N+1)}_{\mathfrak{c},\varepsilon} \ := \tag{11.17}$$

$$= \sum_{k_1=0}^{N} \varepsilon^{k_1} \ \ \hat{\mathfrak{c}}_{k_1} \ \varepsilon^{-k_1} \ \ \int_0^1 dt \ \frac{(1-t)^{N-k_1}}{(N-k_1)!} \ \mathcal{T}^2_{\varepsilon t} \ \bar{\nabla}^{N-k_1+1} \ \ + \ \ r^{(N+1)}_{\mathfrak{c},\varepsilon} \ \mathcal{T}^2_\varepsilon \ \ .$$

Rearranging terms in (11.16) and (11.17) we get

$$\mathfrak{c}_\varepsilon \ \mathcal{T}^2_\varepsilon = \sum_{k=0}^{N} \varepsilon^k \ \ \sum_{k'=0}^{k} \hat{\mathfrak{c}}_{k-k'} \ \frac{1}{k'!} \bar{\nabla}^{k'} \ \ + \ \ \varepsilon^{N+1} \ \mathcal{R}^{(N+1)}_{\mathfrak{c},\varepsilon} \tag{11.18}$$

and

$$\mathcal{R}^{(N+1)}_{\mathfrak{c},\varepsilon} \ := \tag{11.19}$$

$$= \sum_{k_1=0}^{N} \ \ \hat{\mathfrak{c}}_{k_1} \ \ \int_0^1 dt \ \frac{(1-t)^{N-k_1}}{(N-k_1)!} \ \mathcal{T}^2_{\varepsilon t} \ \bar{\nabla}^{N-k_1+1} \ \ + \ \ r^{(N+1)}_{\mathfrak{c},\varepsilon} \ \mathcal{T}^2_\varepsilon \ \ .$$

Putting together (11.18) and (11.19), the analogous formulas with $\bar{\mathfrak{c}}_\varepsilon$, $\mathcal{R}^{(N+1)}_{\bar{\mathfrak{c}},\varepsilon}$ instead of $\mathfrak{c}_\varepsilon$, $\mathcal{R}^{(N+1)}_{\mathfrak{c},\varepsilon}$ the expression (11.10) and assumption (11.8) we get in Ω for every $N \in \mathbb{N}_0$

$$e^{\varphi/\varepsilon} \ \tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\varepsilon,\mu} \ \ e^{-\varphi/\varepsilon} a_\varepsilon \ =$$

$$\sum_{k_1=0}^{N} \sum_{k_2=0}^{N-k_1} \varepsilon^{k_1+k_2} \ \ \sum_{k'=0}^{k_1} \sum_{\mathbf{s}\in\{-1,1\}^2} \mathrm{sign}(\mathbf{s}) \Big\{ \ - \mathrm{Tr}_\mu \ \big(\frac{\hat{\mathfrak{c}}_{k_1-k'}}{k'!} \ \bar{\nabla}^{k'}\big)_{\mathbf{s}} \ + \quad (11.20)$$

$$+ \ \ \big(\frac{\hat{\bar{\mathfrak{c}}}_{k_1-k'}}{k'!} \ \bar{\nabla}^{k'}\big)_{\mathbf{s}}^{\sharp\mu} \ \Big\} \ \hat{a}_{k_2} \ \ + \ \ \varepsilon^{N+1} \ \ R^{(N+1)}_\varepsilon \quad ,$$

with $R^{(N+1)}_\varepsilon \in C^\infty(\Omega;\mathbb{R}^{V,\mu})$ given by

$$R^{(N+1)}_\varepsilon \ := \ \sum_{k_1=0}^{N} \varepsilon^{k_1} \ \sum_{k'=0}^{k_1} \sum_{\mathbf{s}\in\{-1,1\}^2} \mathrm{sign}(\mathbf{s}) \Big\{ \ - \mathrm{Tr}_\mu \ \big(\frac{\hat{\mathfrak{c}}_{k_1-k'}}{k'!} \ \bar{\nabla}^{k'}\big)_{\mathbf{s}} \ +$$

$$+ \ \ \big(\frac{\hat{\bar{\mathfrak{c}}}_{k_1-k'}}{k'!} \bar{\nabla}^{k'}\big)_{\mathbf{s}}^{\sharp\mu} \ \Big\} \ \varepsilon^{-k_1} \ \ r^{(N-k_1+1)}_{b,\varepsilon} \ \ +$$

$$+ \ \ \sum_{\mathbf{s}\in\{-1,1\}^2} \mathrm{sign}(\mathbf{s}) \Big\{ \ - \mathrm{Tr}_\mu \ \mathcal{R}^{(N+1)}_{\mathfrak{c},\varepsilon;\mathbf{s}} \ + \ \ \mathcal{R}^{(N+1)\sharp\mu}_{\bar{\mathfrak{c}},\varepsilon;\mathbf{s}} \ \Big\} \ a_\varepsilon$$

and

$$r^{(N+1)}_{a,\varepsilon} := \varepsilon^{-N-1} \ \big(\ a_\varepsilon - \sum_{k=0}^{N} \varepsilon^k \ \ \hat{a}_k \ \big) = \mathcal{O}(1) \quad .$$

Since also $a_\varepsilon = \mathcal{O}(1)$, we can conclude using (11.19) (and the analogous expression for $\mathcal{R}^{(N+1)}_{\bar{\mathfrak{c}},\varepsilon}$) that $R^{(N+1)}_\varepsilon = \mathcal{O}(1)$. Moreover, rearranging terms in (11.20), gives (11.14) as claimed.

Step 2:

We compute in four steps the term P_k appearing in (11.14) and defined in (11.15).

1) Taking in (11.15) the summands corresponding to $k_1 = k$ and $k_2 = 0$ we remain with

$$\sum_{\mathbf{s}\in\{-1,1\}^2} \mathrm{sign}(\mathbf{s}) \Big\{ \ - \mathrm{Tr}_\mu \ \hat{\mathfrak{c}}_{0;\mathbf{s}} \ + \ \ \hat{\bar{\mathfrak{c}}}_{0;\mathbf{s}}^{\ \sharp\mu} \ \Big\} \ \hat{a}_k \quad . \qquad (11.21)$$

Since (see Remark E.9, in particular (E.13) and (E.15) for details)

$$\sum_{\mathbf{s}\in\{-1,1\}^2} \mathrm{sign}(\mathbf{s}) \ \hat{\mathfrak{c}}_{0;s_1 v, s_2 v} = 2\cosh\nabla_v\varphi - 2\cosh\nabla_v f$$

and $\hat{\hat{\mathfrak{c}}}_0 \equiv 0$, we get for (11.21) the expression

$$-\frac{1}{2}\int_V \mu(dv)\ \big[\ 2\cosh\nabla_v\varphi - 2\cosh\nabla_v f\ \big]\ \hat{a}_k = H_{f,\mu}(\cdot, \mathrm{i}\nabla\varphi)\ \ \hat{a}_k \quad ,$$

the last equality being due to Remark 9.5.

2) If $k \geq 1$, taking in (11.15) the summands corresponding to $k_1 = k-1$ and $k_2 = 0$, we get

$$\sum_{\mathbf{s}\in\{-1,1\}^2} \mathrm{sign}(\mathbf{s})\ \Big\{\ -\mathrm{Tr}_\mu\ \hat{\mathfrak{c}}_{1;\mathbf{s}}\ +\ \hat{\hat{\mathfrak{c}}}_{1;\mathbf{s}}{}^{\sharp\mu}\ \Big\}\ \hat{a}_{k-1} \quad . \tag{11.22}$$

Since (see Remark E.10, in particular (E.17) and (E.19) for details and recall Remark 9.5)

$$\sum_{\mathbf{s}\in\{-1,1\}^2} \mathrm{sign}(\mathbf{s})\ \hat{\mathfrak{c}}_{1;s_1w,s_2w}\ =$$

$$=\ -\nabla_w^2\varphi\ \cosh\nabla_w\varphi\ +\ \nabla_w^2 f\ \Big(\ \sinh^2\frac{\nabla_w\varphi}{2} + \cosh^2\frac{\nabla_w f}{2}\ \Big)$$

and

$$\sum_{\mathbf{s}\in\{-1,1\}^2} \mathrm{sign}(\mathbf{s})\ \hat{\hat{\mathfrak{c}}}_{1;s_1w_1,s_2w_2}\ =$$

$$=\ 2\nabla_{w_1}\nabla_{w_2} f\ \ \cosh\frac{\nabla_{w_1}(f-\varphi)}{2}\cosh\frac{\nabla_{w_2}(f+\varphi)}{2} \quad ,$$

we get for (11.22) the expression

$$\big[\ \mathrm{Tr}_\mu\ \ \nabla(\sinh\nabla\varphi)\ +\ M_{f,\mu}(\cdot, -\mathrm{i}\nabla\varphi)\ \big]\ \hat{a}_{k-1} \quad .$$

3) If $k \geq 1$, taking in (11.15) the summands corresponding to $k_1 = k-1$ and $k_2 = 1$ we get

$$\sum_{\mathbf{s}\in\{-1,1\}^2} \mathrm{sign}(\mathbf{s})\ \Big\{\ -\mathrm{Tr}_\mu\ \big(\hat{\mathfrak{c}}_0\ \bar{\nabla}\big)_{\mathbf{s}}\ +\ \big(\hat{\hat{\mathfrak{c}}}_0\ \bar{\nabla}\big)_{\mathbf{s}}^{\sharp\mu}\ \Big\}\ \hat{a}_{k-1} \quad . \tag{11.23}$$

Since (see again Remark E.9, in particular (E.12) and (E.15), for details)

$$\hat{\mathfrak{c}}_{0;w,w}\ =\ e^{-\nabla_w\varphi}\quad ,\quad \hat{\mathfrak{c}}_{0;-w,-w}\ =\ e^{\nabla_w\varphi}\ \ \text{and}\ \hat{\hat{\mathfrak{c}}}_{0;w_1,w_2} = 0 \quad ,$$

we get for (11.23) the expression

$$\langle 2\sinh \nabla\varphi, \nabla \hat{a}_{k-1}\rangle_\mu \quad .$$

4) If $k = 0, 1$ we computed all the summands in (11.15) in the preceeding steps. If $k \geq 2$ the summands not considered until now correspond to the indexes k_1, k_2 such that $0 \leq k_1 \leq k-2$ and $0 \leq k_2 \leq k - k_1$:

$$\sum_{k_1=0}^{k-2}\sum_{k_2=0}^{k-k_1}\sum_{\mathbf{s}\in\{-1,1\}^2} \operatorname{sign}(\mathbf{s})\Big\{ -\mathrm{Tr}_\mu \ \big(\frac{\hat{\mathfrak{c}}_{k-k_1-k_2}}{k_2!}\ \bar{\nabla}^{k_2}\big)_{\mathbf{s}} + \frac{\hat{\hat{\mathfrak{c}}}_{k-k_1-k_2}}{k_2!}\ \bar{\nabla}^{k_2}\big)_{\mathbf{s}}^{\sharp\mu} \Big\}\ \hat{a}_{k_1} \quad . \tag{11.24}$$

The proof of the lemma is thus completed by defining for $k \in \mathbb{N}_*$ and $k_1 \in \{0, \ldots, k-2\}$ the operator $D_{k,k_1} : C^\infty(\Omega; \mathbb{R}_a^{V^p,\mu}) \to C^\infty(\Omega; \mathbb{R}_a^{V^p,\mu})$ as the operator given by the two internal sums in (11.24), i.e. via

$$D_{k,k_1} \ :=$$

$$= \sum_{k_2=0}^{k-k_1}\sum_{\mathbf{s}\in\{-1,1\}^2} \operatorname{sign}(\mathbf{s})\ \Big\{ \ -\ \mathrm{Tr}_\mu \ \big(\frac{\hat{\mathfrak{c}}_{k-k_1-k_2}}{k_2!}\ \bar{\nabla}^{k_2}\big)_{\mathbf{s}} \ + \ \big(\frac{\hat{\hat{\mathfrak{c}}}_{k-k_1-k_2;\mathbf{s}}}{k_2!}\ \bar{\nabla}^{k_2}\big)_{\mathbf{s}}^{\sharp\mu} \ \Big\}$$

and observing that

$$-\nu_\varepsilon\ a_\varepsilon\Big|_\Omega \ \sim\ -\sum_{k=0}^{\infty} \varepsilon^k \quad \sum_{k_1=0}^{k} \hat{\nu}_{k_1}\ \hat{a}_{k-k_1} \ =$$

$$= \ -\sum_{k=0}^{\infty} \varepsilon^k \ \ \hat{\nu}_0\ \hat{a}_k \ \ -\ \sum_{k=1}^{\infty} \varepsilon^k \ \ \Big[\ \hat{\nu}_1\ \hat{a}_{k-1} \ +\ \sum_{k_1=2}^{k} \hat{\nu}_{k_1}\ \hat{a}_{k-k_1}\ \Big] \quad .$$

□

Lemma 11.10.

Fix a critical point $\bar{\zeta}$ of f having index 1. There exist a sequence $\{\nu_k\}_{k=2,\ldots} \subset \mathbb{R}$, an open neighbourhood Ω of $\bar{\zeta}$, a $\varphi \in C^\infty(\Omega;\mathbb{R})$ and a sequence $\{a_k\}_{k\in\mathbb{N}_0} \subset C^\infty(\Omega; \mathbb{R}_a^{V^p,\mu})$ such that

(i) $\varphi(\bar{\zeta}) = 0$, $\nabla\varphi(\bar{\zeta}) \equiv 0$, $\nabla^2_{\mathfrak{e}_i,\mathfrak{e}_j}\varphi(\bar{\zeta}) = |\kappa_j|\ 1_{i,j}$ *and*

$$H_{f,\mu}(\zeta, i\nabla\varphi(\zeta)) \ = \ 0 \qquad \textit{for every } \zeta \in \Omega \quad .$$

(ii) $a_0(\bar{\zeta}) = \mathfrak{e}_1$ *and for every* $k \in \mathbb{N}_*$

$$T\ a_{k-1}\ (\zeta) = Q_k(\zeta) \qquad \textit{for every } \zeta \in \Omega \quad , \tag{11.25}$$

where $T : C^\infty(\Omega; \mathbb{R}_a^{V^p,\mu}) \to C^\infty(\Omega; \mathbb{R}_a^{V^p,\mu})$ *is the first order differential operator*

$$T := \mathrm{Tr}_\mu \left[\ 2\sinh(\nabla\varphi)\ \nabla\ +\ \nabla(\sinh \nabla\varphi)\ \right]\ +\ M_{f,\mu}(\cdot, -i\nabla\varphi)$$

and, for every $k \in \mathbb{N}_*$, Q_k *is in* $C^\infty(\Omega; \mathbb{R}_a^{V^p,\mu})$ *and has the form*

$$Q_k := \sum_{l=0}^{k-2} \left\{\ D_{k,l}\ a_l\ +\ \nu_{l+2}\ a_{k-l-2}\ \right\}$$

with $D_{k,l} : C^\infty(\Omega; \mathbb{R}_a^{V^p,\mu}) \to C^\infty(\Omega; \mathbb{R}_a^{V^p,\mu})$ *for* $k \in \mathbb{N}_*, l \in \{0, \ldots, k-2\}$.

Proof. (i) follows immediately from general results on the existence of solutions of singular eikonal equations, which can be proven by an application of the local stable manifold theorem for hyperbolic dynamical systems. We refer to Lemma 3.1 in [66] for a detailed proof.

To prove (ii) we proceed in the standard way by iteration and exploiting a general result for the existence of solutions of singular transport equations (see Appendix A, in particular Theorem A.1).

To check that we are in the situation of Theorem A.1, observe that for every $a \in C^\infty(\Omega; \mathbb{R}_a^{V^p,\mu})$

$$T\ a(\zeta) = \sum_{j=1}^{n} \mathcal{V}_j(\zeta)\ \nabla_{\mathfrak{e}_j}\ a\ (\zeta)\ +\ W(\zeta)\ a\ (\zeta)$$

with

$$\mathcal{V}_j = \frac{1}{2} \int_V \mu(dw)\ \mathfrak{e}_j^*(w)\ 2\sinh \nabla_w\varphi$$

and

$$W := \mathrm{Tr}_\mu\ \nabla(\sinh \nabla\varphi)\ +\ M_{f,\mu}(\cdot, -\mathrm{i}\nabla\varphi) \quad .$$

Note that

(1) $\mathcal{V}_j(\bar{\zeta}) = 0$ for every $j = 1, \ldots, n$ and the matrix

$$\left(\nabla_{\mathfrak{e}_l} \mathcal{V}_j(\bar{\zeta}) \right)_{l,j} = \left(\nabla^2_{\mathfrak{e}_j, \mathfrak{e}_l} \varphi(\bar{\zeta}) \right)_{l,j} = |\kappa_j| \; 1_{j,l}$$

is diagonal with strictly positive eigenvalues.

(2) The operator

$$W(\bar{\zeta}) \;=\; \mathrm{Tr}_\mu \, \nabla^2(\varphi - f)(\bar{\zeta}) \;+\; \nabla^2 f(\bar{\zeta})^{\;\sharp\mu}$$

is selfadjoint on the Hilbert space $\mathbb{R}_a^{V^p,\mu}$. Moreover one can check as follows that it is also nonnegative and has a 1-dim kernel generated by $\mathfrak{e}_1$.

Indeed, by definition for every $\phi \in \mathbb{R}_a^{V,\mu}$ with $\|\phi\|_\mu = 1$

$$\langle W(\bar{\zeta})\phi, \phi\rangle_\mu \;=\; \\ =\; 2|\kappa_1| \;+\; \frac{1}{4}\int_{V^2} \mu(dv)\mu(dw)\; 2\nabla_{v,w} f(\bar{\zeta}) \; \phi_w \; \phi_v \quad . \tag{11.26}$$

The second summand in (11.26) equals

$$2\sum_{j=1}^{n} \kappa_j \;\; \frac{1}{4}\int_{V^2} \mu(dv)\mu(dw)\; \mathfrak{e}_j^*(v)\; \mathfrak{e}_j^*(w)\; \phi_w \; \phi_v \;= \\ =\; 2\sum_{j=1}^{n} \kappa_j \; \left(\frac{1}{2}\int_V \mu(dw)\; \mathfrak{e}_j^*(w)\; \phi_w \right)^2 \quad .$$

Since $\kappa_j > 0$ for $j > 1$ we get

$$\langle W(\bar{\zeta})\phi, \phi\rangle_\mu \;\geq \\ \geq\; 2|\kappa_1| \;+\; 2\kappa_1 \left(\frac{1}{2}\int_V \mu(dw)\; \mathfrak{e}_1^*(w)\; \phi_w \right)^2 \quad . \tag{11.27}$$

Cauchy-Schwarz gives

$$\left(\frac{1}{2}\int_V \mu(dw)\; \mathfrak{e}_1^*(w)\; \phi_w \right)^2 \;\leq \\ \leq \frac{1}{2}\int_V \mu(dw)\; (\mathfrak{e}_1^*(w))^2 \; \frac{1}{2}\int_V \mu(dw)\; \phi_w^2 = \|\phi\|^2 = 1 \quad ,$$

with equality holding if and only if φ is μ-almost everywhere a scalar multiple of $\mathfrak{e}_1^*$. Inserting into (11.27) leads to

$$\langle W(\bar{\zeta})\phi, \phi\rangle_\mu \;\geq\; 2|\kappa_1| \;+\; 2\kappa_1 \;= 0 \quad ,$$

with equality only in the mentioned case. Moreover

$$W(\bar{\zeta})\ \mathfrak{e}_1^*(v) = 2|\kappa_1|\ \mathfrak{e}_1^*(v)\ +\ \frac{1}{2}\int_V \mu(dw)\ 2\nabla^2_{w,v} f(\bar{\zeta})\ \mathfrak{e}_1^*(w)\ =$$

$$=\ 2|\kappa_1|\ \mathfrak{e}_1^*(v)\ +\ 2\sum_{j,l=1}^{n} \kappa_j\ \frac{1}{2}\int_V \mu(dw)\ 1_{j,l}\ \mathfrak{e}_j^*(w)\ \mathfrak{e}_l^*(v)\ \mathfrak{e}_1^*(w)\ =$$

$$=\ 2(|\kappa_1| + \kappa_1)\ \mathfrak{e}_1^*(v) = 0\ \ .$$

Now consider the equation (11.25) for $k = 1$ (note that $Q_1 \equiv 0$). By Theorem A.1 there exists an open neighbourhood Ω of $\bar{\zeta}$ and $a_0 \in C^\infty(\Omega; \mathbb{R}_a^{V,\mu})$ satisfying

$$\begin{cases} T\ a_0\ (\zeta) = 0 \ \text{ for every } \zeta \in \Omega \\ a_0(\bar{\zeta}) = \mathfrak{e}_1^* \end{cases} .$$

For $k = 2$ we have

$$Q_2 :=\ D_{2,0}\ a_0\ -\ \nu_2\ a_0$$

and we fix ν_2 such that $Q_2(\bar{\zeta})$ is orthogonal to a_0, i.e. such that $Q_2(\bar{\zeta})$ is in the range of $W(\bar{\zeta})$. To be specific we let

$$\nu_2 := \frac{\langle D_{2,0}\ a_0(\bar{\zeta}), a_0(\bar{\zeta})\rangle_\mu}{\|a_0(\bar{\zeta})\|_\mu^2}\ \ .$$

Again by Theorem A.1 there exists an a_1 satisfying

$$T\ a_1\ (\zeta) = Q_2(\zeta) \ \text{ for every } \ \zeta \in \Omega\ \ .$$

Iterating, once $\nu_2, \ldots, \nu_k \in \mathbb{R}$ and $a_0, \ldots, a_{k-1} \in C^\infty(\Omega; \mathbb{R}^{V,\mu})$ are constructed, we let

$$\nu_{k+2} := \frac{\langle \sum_{l=0}^{k-1}\ D_{k+1,l+2}\ a_l(\bar{\zeta}), a_0(\bar{\zeta})\rangle_\mu\ -\ \langle \sum_{l=0}^{k-2} \nu_{l+2}\ a_{k-l-1}(\bar{\zeta}), a_0(\bar{\zeta})\rangle_\mu}{\|a_0(\bar{\zeta})\|_\mu^2}$$

and define a_k as a solution of (11.25) in Ω whose existence is again guaranteed by Theorem A.1. □

Having established Proposition 11.3 we can now complete the proof of Theorem 11.1. We follow here ideas taken from Proposition 5.2.6 in [40].

Proof of Theorem 11.1. Take $\Omega \subset M$, $\varphi \in C^\infty(M; \mathbb{R})$ and, for $\varepsilon > 0$, $\nu_\varepsilon \in \mathbb{R}$ and $a_\varepsilon \in C^\infty(M; \mathbb{R}_a^{V^p,\mu})$ as in Proposition 11.3. Assume furthermore that $\varphi > 0$ on supp $a_\varepsilon \backslash \{0\}$ for $\varepsilon > 0$ (this is no loss of generality by Remark 11.4).

We have to show that $\nu_\varepsilon \sim 0$. To this end, observe that it is sufficient to show that

$$\|\tilde{\delta}_{\rho_\varepsilon,\varepsilon}\, a_\varepsilon e^{-\varphi/\varepsilon}\|^2_{\Lambda_{\varepsilon,\mu}} \;=\; \mathcal{O}(\varepsilon^\infty) \;\text{ and }\; \|\tilde{\delta}^{*\mu}_{\rho_\varepsilon,\varepsilon}\, a_\varepsilon e^{-\varphi/\varepsilon}\|^2_{\Lambda_{\varepsilon,\mu}} \;=\; \mathcal{O}(\varepsilon^\infty)\;, \tag{11.28}$$

with $\tilde{\delta}_{\rho_\varepsilon,\varepsilon}$ and $\tilde{\delta}^{*\mu}_{\rho_\varepsilon,\varepsilon}$ as in (11.5). In fact, on one hand, from the very definition of $\tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\varepsilon,\mu}$ and Proposition 8.2 (iii), the property in (11.28) is equivalent to

$$\langle a_\varepsilon\; e^{-\varphi/\varepsilon}, \tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\varepsilon,\mu}\; a_\varepsilon\; e^{-\varphi/\varepsilon}\rangle_{\Lambda_{\varepsilon,\mu}} \;=\; \mathcal{O}(\varepsilon^\infty)\;\;. \tag{11.29}$$

On the other hand we have by the Cauchy-Schwarz inequality and (11.3) (we also use that by Remark 11.6 the norm of $a_\varepsilon\; e^{-\varphi/\varepsilon}$ does not grow more than polynomially in ε) that

$$\langle a_\varepsilon\; e^{-\varphi/\varepsilon}, (\tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\varepsilon,\mu} - \nu_\varepsilon)\; a_\varepsilon\; e^{-\varphi/\varepsilon}\rangle_{\Lambda_{\varepsilon,\mu}} \;=\; \mathcal{O}(\varepsilon^\infty)\;\;,$$

i.e.

$$\langle a_\varepsilon\; e^{-\varphi/\varepsilon}, \tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\varepsilon,\mu}\; a_\varepsilon\; e^{-\varphi/\varepsilon}\rangle_{\Lambda_{\varepsilon,\mu}} \;=\; \nu_\varepsilon\; \|a_\varepsilon\; e^{-\varphi/\varepsilon}\|^2_{\Lambda_{\varepsilon,\mu}} \;+\; \mathcal{O}(\varepsilon^\infty)\;\;. \tag{11.30}$$

From (11.29) and (11.30) (and using again the control on $\|a_\varepsilon\; e^{-\varphi/\varepsilon}\|_{\Lambda_{\varepsilon,\mu}}$ given in Remark 11.6) it would follow that $\nu_\varepsilon = \mathcal{O}(\varepsilon^\infty)$ as claimed.

To prove the estimate on $\tilde{\delta}_{\rho_\varepsilon,\varepsilon}\;\; a_\varepsilon e^{-\varphi/\varepsilon}$ in (11.28) one can proceed as follows (the estimates on $\delta^{*\mu_\varepsilon}_{\rho_\varepsilon}\;\; a_\varepsilon\; e^{-\varphi/\varepsilon}$ can be made in analogous way).

By possibly multiplying a_ε with a suitable cut-off function we shall assume henceforth that $B_2(\operatorname{supp} a_\varepsilon)$ (the ball of radius 2 around $\operatorname{supp} a_\varepsilon$) contains no critical points of f except $\bar{\zeta}$. Moreover we switch to a 1-well situation by modifying the function f outside $\operatorname{supp} a_\varepsilon$. To be specific, we consider $\tilde{f} \in C^\infty(M)$ having the property that

$$\tilde{f}(\zeta) = f(\zeta) \quad \text{for every} \;\; \zeta \in B_1(\operatorname{supp} a_\varepsilon)$$

and

$$\nabla \tilde{f}(\zeta) \neq 0 \;\; \text{for every} \;\; \zeta \in B_1^c(\operatorname{supp} a_\varepsilon)\;\;.$$

Now set $\tilde{\rho}_\varepsilon := e^{-2\tilde{f}/\varepsilon}$ and observe that for ε sufficiently small

$$\tilde{\mathcal{H}}^{(1)}_{\tilde{\rho}_\varepsilon,\varepsilon,\mu}\; \tilde{\delta}_{\tilde{\rho}_\varepsilon,\varepsilon}\; a_\varepsilon\; e^{-\varphi/\varepsilon} \;=\; \tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\varepsilon,\mu}\; \tilde{\delta}_{\rho_\varepsilon,\varepsilon}\; a_\varepsilon\; e^{-\varphi/\varepsilon}\;\;.$$

It follows by using Remark 11.3 (in particular (11.6)) that

$$\|(\tilde{\mathcal{H}}^{(1)}_{\tilde{\rho}_\varepsilon,\varepsilon,\mu} - \nu_\varepsilon)\; \tilde{\delta}_{\tilde{\rho}_\varepsilon,\varepsilon}\; a_\varepsilon\; e^{-\varphi/\varepsilon}\|_{\Lambda_{\varepsilon,\mu}} \;=\; \mathcal{O}(\varepsilon^\infty)\;\;. \tag{11.31}$$

As a consequence of the spectral theorem we get from (11.31)

$$\operatorname{dist}\big(\;\nu_\varepsilon\;,\;\operatorname{Spec}(\tilde{\mathcal{H}}^{(1)}_{\tilde{\rho}_\varepsilon,\Lambda_{\varepsilon,\mu}})\;\big)\;\; \|\tilde{\delta}_{\tilde{\rho}_\varepsilon,\varepsilon}\; a_\varepsilon\; e^{-\varphi/\varepsilon}\|_{\Lambda_{\varepsilon,\mu}} \;=\; \mathcal{O}(\varepsilon^\infty)\;\;. \tag{11.32}$$

Moreover, by invoking Theorem B.5, there exists a strictly positive constant C such that

$$\operatorname{dist}\big(\, \nu_\varepsilon \ , \ \operatorname{Spec}(\tilde{\mathcal{H}}^{(1)}_{\tilde{\rho}_\varepsilon,\Lambda_{\varepsilon,\mu}})\ \big) \ \geq \ C\ \varepsilon^2 \quad ,$$

which together with (11.32) yields $\|\delta_{\tilde{\rho}_\varepsilon}\ a_\varepsilon\ e^{-\varphi/\varepsilon}\|_{\Lambda_{\varepsilon,\mu}} \ = \ \mathcal{O}(\varepsilon^\infty)$. Finally observe that for ε sufficiently small $\|\tilde{\delta}_{\rho_\varepsilon,\varepsilon}\ a_\varepsilon\ e^{-\varphi/\varepsilon}\|_{\Lambda_{\varepsilon,\mu}} \ = \ \|\delta_{\tilde{\rho}_\varepsilon}\ a_\varepsilon\ e^{-\varphi/\varepsilon}\|_{\Lambda_{\varepsilon,\mu}}$.
□

Remark 11.11. *Note that if $N > n$ Theorem 11.1 provided quasimodes for only a part of the low-lying spectrum of $\mathcal{H}^{(1)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$, namely the part associated with the critical points of f having index 1. We know from Theorem 10.1 that there are further $m_0(N-n)$ small eigenvalues related to the local minima of f. Local WKB-type quasimodes corresponding to these additional small eigenvalues can be constructed along the same lines. We will not need this, since for simplicity we will restrict in Part III to the case $N = n$.*

Part III. Asymptotics of small eigenvalues of $\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$

In this part we will give a refined analysis in the limit $\varepsilon \to 0$ of the low-lying spectrum of $\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$, the rescaled Witten Laplacian acting on functions as introduced in Part II. The main theorem (see Section 17) shows for each small eigenvalue the existence of a complete expansion in ε and provides explicit expressions for the leading term in the expansion. The proof heavily exploits the results of the previous Part II concerning $\mathcal{H}^{(1)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$, the rescaled Witten Laplacian on 1-functions (see in particular Theorem 10.1 and 11.1).

12. Assumptions

The setup of this part is, besides the addition of Assumption III.2 below, the same as the one of Part II, as described in Section 9. For convenience of the reader we recall here briefly some crucial definitions and gather all the assumptions made throughout this part.

We consider throughout an n-dimensional affine space M with underlying vector space V and assume given an inhomogeneous discrete geometry $\rho\mu$ on M. Recall from Section 5 in Part I, that $\rho\mu$ consists of a function $\rho : M \to (0,\infty)$ and a symmetric measure μ on V with a finite support which generates a lattice Γ in V. Recall also that $E = \operatorname{supp}\mu \setminus \{0\}$ is referred to as the set of admissible jumps. For $\varepsilon > 0$ the rescaled inhomogeneous geometry $\rho_\varepsilon\mu_\varepsilon := (\rho_\varepsilon, \mu_\varepsilon)$ is defined by setting for every $\zeta \in M$

$$\rho_\varepsilon(\zeta) \; := \; e^{-2f(\zeta)/\varepsilon} \quad ,$$

where $f := -\frac{1}{2}\log\rho$, and by setting for every measurable set S in V

$$\mu_\varepsilon(S) \; := \; \mu(\varepsilon^{-1}S) \quad .$$

Moreover we fix for $\varepsilon > 0$ an equivalence class in M under $\sim_{\varepsilon\Gamma}$ and denote by Λ_ε the elements of the chosen equivalence class. The weighted graph with vertices Λ_ε, edges determined by εE and weight μ_ε on the edges will be denoted by $\Lambda_{\mu_\varepsilon}$.

The rescaled formal Witten Laplacian $\mathcal{H}_{\rho_\varepsilon,\mu_\varepsilon} = \oplus_{p=0}^{\infty}\mathcal{H}^{(p)}_{\rho_\varepsilon,\mu_\varepsilon}$ is defined via

$$\mathcal{H}_{\rho_\varepsilon,\mu_\varepsilon} \; := \; \delta^{*\mu_\varepsilon}_{\rho_\varepsilon}\delta_{\rho_\varepsilon} \; + \; \delta_{\rho_\varepsilon}\delta^{*\mu_\varepsilon}_{\rho_\varepsilon} \quad ,$$

where

$$\delta_{\rho_\varepsilon} \ := \ \sqrt{\rho_\varepsilon}\ \delta\ \frac{1}{\sqrt{\rho}_\varepsilon} \qquad \text{and} \qquad \delta^{*\mu_\varepsilon}_{\rho_\varepsilon} \ := \ \frac{1}{\sqrt{\rho}_\varepsilon}\ \delta^{*\mu_\varepsilon}\ \sqrt{\rho_\varepsilon}$$

and δ and $\delta^{*\mu_\varepsilon}$.

The Friedrichs extension in $L^2_a(M \times V^p, \Lambda_{\mu_\varepsilon})$ of the restriction of $\mathcal{H}^{(p)}_{\rho_\varepsilon,\mu_\varepsilon}$ to p-functions with compact support is denoted by $\mathcal{H}^{(p)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$.

As in Part II we assume

Assumption III.1.

(i) *$f \in C^\infty(M;\mathbb{R})$ and is a Morse function.*
(ii) *There exists a point $O \in M$ such that $O \in \Lambda_\varepsilon$ for $\varepsilon > 0$.*
(iii) *There exists a compact $K \subset \mathbb{R}^n$ and coordinates $z = (z_1, \dots, z_n)$ on M such that for $z \in \mathbb{R}^n \setminus K$*

$$f(z) \ = \ \sum_i z_i^2 \quad .$$

The Morse property and (iii) imply in particular that f has only a finite number of critical points. We shall denote for $p = 0, \dots, n$ by $\mathcal{C}_p$ the set of critical points of f having index p and by $\mathcal{C} := \cup_p \mathcal{C}_p$, the set of all critical points of f. Moreover we let m_p (resp. m) the cardinality of $\mathcal{C}_p$ (resp. $\mathcal{C}$). In accordance with $\lim_{|\zeta|\to\infty} f(\zeta) = +\infty$ we also set for convenience $f(\infty) := +\infty$.

Our main concern is to get asymptotic results as accurate as possible on the first m_0 eigenvalues $\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$, whose existence under Assumption III.1 is guaranteed (for sufficiently small ε) by Theorem 10.1. We shall denote these small eigenvalues of $\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$ by

$$\nu_{1,\varepsilon} \leq \ \cdots \leq \ \nu_{m_0,\varepsilon} \quad .$$

Note that by Remark 10.4 we have $\nu_{1,\varepsilon} = 0$ and $e^{-f/\varepsilon}$ as an associated eigenfunction.

Throughout this part we make for simplicity the additional

Assumption III.2.

(i) *The critical values $\{f(\zeta) : \zeta \in \mathcal{C}\}$ are distinct.*
(ii) *The quantities $\{f(\zeta^{(1)}) - f(\zeta^{(0)}) : \zeta^{(1)} \in \mathcal{C}^{(1)}, \zeta^{(0)} \in \mathcal{C}^{(0)}\}$ are distinct.*
(iii) *μ is a nearest neighbour discrete geometry .*

Recall that (iii) means that the set E of admissible jumps has cardinality $2n$. In other terms the size of μ equals the dimension of the affine space M. This hypothesis is chosen just to simplify the presentation. Requirement (i) could be relaxed without alterating the final results, by assuming uniqueness of the relevant saddle point attached to a minimum as done in [42]. Finally (i) is chosen to avoid the problem of possible degeneracy of the small eigenvalues.

13. Labelling of local minima and relevant saddle points

The aim of this section is to introduce a convenient labelling of the local minima of f, to attach to each of them a so-called relevant saddle point at which exit from the metastable basin of attraction of the considered minimum occurs. There are several equivalent ways to do this (see for example [13] and [42]), we follow here in particular [70]. We stress that the discussion below concerns only the geometry of f: the Witten Laplacian, in particular the discrete nature of the one we are considering in this work, plays no role here.

For $z \in \mathbb{R}$ let $\mathcal{N}_f(z)$ be the number of connected components of the sublevel set $f^{-1}((-\infty, z))$.

Observe that the function $\mathcal{N}_f : z \to \mathcal{N}_f(z)$ satisfies the following properties:

(a) it is locally constant around every $z \notin f(\mathcal{C}_0 \cup \mathcal{C}_1)$.

(b) it increases by 1 at critical values of f corresponding to minima. More precisely, if $z_0 \in f(\mathcal{C}_0)$,

$$\lim_{z \downarrow z_0} N_f(z) = \lim_{z \uparrow z_0} N_f(z) + 1 = N_f(z_0) + 1 \quad .$$

(c) it can decrease by 1 at critical values of f corresponding to saddle points. More precisely, if $z_1 \in f(\mathcal{C}_1)$ either N_f remains constant around z_1 or

$$\lim_{z \downarrow z_1} N_f(z) = \lim_{z \uparrow z_1} N_f(z) - 1 = N_f(z_1) - 1 \quad .$$

(d) $N_f \equiv 0$ for z small enough and $N_f \equiv 1$ for z big enough.

Indeed, recalling that by Assumptions III.1.(i) and III.2.(i) f is a Morse function with distinct critical values, properties (a) to (c) are a consequence of the local structure of Morse functions. Property (d) is due to the fact that by Assumption III.1(iii) f admits a global minimum and the set of its critical points is contained in a compact set.

Remark 13.1. *From the above properties of N_f one can easily deduce the following relation*

$$m_1 + 1 \geq m_0 \quad .$$

Definition 13.2 (Labelling of local minima and saddle points)**.**

A labelling $\{\zeta_1^{(0)}, \dots, \zeta_{m_0}^{(1)}\}$ *(resp.* $\{\zeta_1^{(1)}, \dots, \zeta_{m_1+1}^{(1)}\}$*) for the elements of* $\mathcal{C}_0$ *(resp.* $\mathcal{C}_1 \cup \{\infty\}$*) is defined according to the following inductive recipe:*

(1) *Set* $\zeta_1^{(1)} := \infty$ *and denote by* $\zeta_1^{(0)}$ *the global minimum of* f*, which exists thanks to Assumption III.1(iii).*

(2) *Once* $\zeta_i^{(0)}$ *and* $\zeta_i^{(1)}$ *are chosen for some* $i < m_0$*, consider the value*

$$\bar{z} = \max\{z \in \mathbb{R} : z < f(\zeta_i^{(1)}) \text{ and } N_f(z) = N_f(\zeta_i^{(1)}) + 1\} \quad .$$

Denote by $\zeta_{i+1}^{(1)}$ *the unique element* $\zeta^{(1)}$ *of* $\mathcal{C}_1$ *satisfying* $f(\zeta^{(1)}) = \bar{z}$ *and by* $\zeta_{i+1}^{(0)}$ *the unique global minimum of the set obtained by subtracting from* $f^{-1}((-\infty, \zeta_{i+1}^{(1)}))$ *its connected components containing at least one element of* $\{\zeta_1^{(0)}, \dots, \zeta_i^{(0)}\}$*.*

(3) *Once* $\zeta_{m_0}^{(1)}$ *is chosen, fix an arbitrary labelling* $\zeta_{m_0+1}^{(1)}, \dots, \zeta_{m_1+1}^{(1)}$ *for the remaining elements of* $\mathcal{C}_1$*.*

(4) *Permute the i's in order to make the sequence*

$$\{f(\zeta_i^{(1)}) - f(\zeta_i^{(0)})\}_{i=2,\dots,m_0}$$

strictly decreasing, which is possible thanks to Assumption III.2.(ii).

Observe that these labellings provide in particular a one to one correspondance between $\mathcal{C}_0$ and a subset of $\mathcal{C}_1 \cup \{\infty\}$:

Definition 13.3 (Relevant saddle points)**.**

For $i = 1, \dots, m_0$ *the point* $\zeta_i^{(1)}$ *is called the relevant saddle point attached to the local minimum* $\zeta_i^{(0)}$*.*

Definition 13.4 (Basins of attraction)**.**

For $i = 1, \dots, m_0$ *we define the basin of attraction* $\mathcal{B}_i$ *of the local minimum* $\zeta_i^{(0)}$ *as the closure of the connected component of the set*

$$f^{-1}\big(\,(-\infty, f(\zeta_i^{(1)}))\,\big)$$

containing $\zeta_i^{(0)}$*.*

Observe that from our conventions it follows that $\mathcal{B}_1 = M$. Moreover, for $i = 2, \dots, m_0$ the basin $\mathcal{B}_i$ is compact and contains $\zeta_i^{(1)}$ in its boundary.

Proposition 13.5. *The following statements hold true:*

(i) $\zeta_i^{(0)}$ *is a strict global minimum of* f *in* $\mathcal{B}_i$*.*

(ii) *Let* $i, j = 1, \ldots, m_0$. *Then either* $\mathcal{B}_i \cap \mathcal{B}_j = \emptyset$ *or* $\mathcal{B}_j \subset \mathring{\mathcal{B}}_i$ *or* $\mathcal{B}_i \subset \mathring{\mathcal{B}}_j$.

Proof. Statement (i) holds by definition of the $\zeta_i^{(0)}$'s and $\mathcal{B}_i$'s (recall also Assumption III.2.(i)).

To prove (ii) observe first that by Assumption III.2.(i) we have

$$\partial\mathcal{B}_i \cap \partial\mathcal{B}_j = \emptyset \quad . \tag{13.1}$$

Assume now $f(\zeta_i^{(1)}) < f(\zeta_j^{(1)})$. Then every connected component of the set $f^{-1}\big(\,(-\infty, f(\zeta_i^{(1)}))\,\big)$ is contained in a connected component of the set $f^{-1}\big(\,(-\infty, f(\zeta_j^{(1)}))\,\big)$, so that either $\mathring{\mathcal{B}}_i \subset \mathring{\mathcal{B}}_j$ or $\mathring{\mathcal{B}}_i \cap \mathring{\mathcal{B}}_j = \emptyset$. The first case together with (13.1) gives $\mathcal{B}_i \subset \mathring{\mathcal{B}}_j$. The second case implies also $\mathring{\mathcal{B}}_i \cap \partial\mathcal{B}_j = \emptyset$ and $\partial\mathcal{B}_i \cap \mathring{\mathcal{B}}_j = \emptyset$, so that using again (13.1) we get $\mathcal{B}_i \cap \mathcal{B}_j = \emptyset$. Analogous considerations with the Assumption $f(\zeta_i^{(1)}) > f(\zeta_j^{(1)})$ complete the proof of (ii). □

Note that for $i = 2, \ldots, m_0$ the basin $\mathcal{B}_i$ has a corner at $\zeta_i^{(1)}$. To facilitate the construction of suitable smooth cut-off functions it is convenient to slightly modify the basins of attraction around the corresponding relevant saddle points, introducing smooth versions of them. In order to describe this small surgery we consider the following coordinate systems on M, each one centered at a relevant saddle point and adapted to the corresponding quadratic part of f. We shall denote henceforth by κ_1 the negative and by $\kappa_2 \ldots, \kappa_n$ the positive eigenvalues of the nondegenerate symmetric bilinear form $\nabla^2 f(\zeta_i^{(1)})$ with respect to the scalar product induced by μ on V. We also write $\kappa_j^{(i)}$ for $j = 1, \ldots, n$ to stress the dependence on $i = 2, \ldots, m_0$, and $\kappa_{f,\mu,j}^{(i)}$ to highlight the dependence on f and μ.

Definition 13.6 (Adapted Coordinates)**.**

Let $i = 2, \ldots, m_0$. *We fix a basis* $\mathscr{B}_{f,\mu}^{\text{inw}} := (\mathfrak{e}_1, \ldots, \mathfrak{e}_n)$ *of* V *such that, denoting by* $(\mathfrak{e}_1^*, \ldots, \mathfrak{e}_n^*)$ *its associated dual basis,*

$$\frac{1}{2}\int_V \mu(dw)\ \mathfrak{e}_l^*(w)\ \mathfrak{e}_j^*(w) \;=\; 1_{l,j} \quad \textit{and} \quad \nabla^2_{\mathfrak{e}_l,\mathfrak{e}_j} f(\bar{\zeta}) \;=\; \kappa_j\ 1_{l,j}$$

and such that for sufficiently small $t > 0$

$$\zeta_i^{(1)} + t\mathfrak{e}_1 \in \mathcal{B}_i \quad . \tag{13.2}$$

Moreover we shall denote by $(y, z) \in \mathbb{R}^n$, *with* $y \in \mathbb{R}$ *and* $z = (z_2, \ldots, z_n) \in \mathbb{R}^{n-1}$ *a coordinate system in* M, *centered at* $\zeta_i^{(1)}$ *and induced by the basis*

$(\mathfrak{e}_1, \ldots, \mathfrak{e}_n)$. *We write also* $y^{(i)}$, $z^{(i)}$ *and* $\mathfrak{e}_j^{(i)}$ *for every* $j = 1, \ldots, n$ *to highlight the dependence on the index* i.

Remark 13.7. *Note that a basis* $\mathscr{B}_{f,\mu}^{\mathrm{inw}}$ *has the same properties of a basis* $\mathscr{B}_{f,\mu}$ *as chosen in Section 11 (see* (11.1)*), apart that here we add condition* (13.2) *expressing the fact that* $\mathfrak{e}_1$ *is pointing inwards the corresponding basin of attraction. This is only a convention and also the outward vector* $-\mathfrak{e}_1$ *could have been chosen at this point: signs had to be changed accordingly in the sequel. The final result (Theorem 17.1) is of course independent of this convention.*

We stress that in general $\mathscr{B}_{f,\mu}^{\mathrm{inw}}$ *is not adapted to (i.e. does not generate) the lattice* Γ. *To avoid confusion we point also to the fact that while* $\mathfrak{e}_i$ *denotes in the sequel a vector in* $\mathscr{B}_{f,\mu}^{\mathrm{inw}}$ *the symbol* e_i *stands for an element of* E*, the set of admissible jumps corresponding to* μ.

Observe that with respect to the coordinates (y, z) adapted to $\zeta_i^{(1)}$ we have[38]

$$f(y,z) \;=\; f(\zeta_i^{(1)}) \;-\frac{1}{2}|\kappa_1|\;y^2 + \frac{1}{2}\sum_j \;\kappa_j\;z_j^2 \;+\; R_f(y,z) \quad , \qquad (13.3)$$

with

$$|R_f(y,z)| \;\le\; \text{Const}\;(|y|^3 + |y|^2\|z\| + |y|\|z\|^2 + \|z\|^3)$$

for every (y, z) contained in a fixed compact subset of $\mathbb{R}^n$. Here $\|\cdot\|$ denotes a generic norm in $\mathbb{R}^{n-1}$. We shall consider in the sequel in particular the norm $\|z\|_{\kappa^{(i)}}$, defined for $z = (z_2, \ldots, z_n)$ as

$$\|z\|_{\kappa^{(i)}} \;:=\; \sqrt{\sum_{j=2}^n \frac{\kappa_j^{(i)}}{|\kappa_1^{(i)}|}\;z_j^2} \quad .$$

We shall use the following short notations: for each $i = 2, \cdots, m_0$ and $r > 0$ we define the strips

$$S_{i,r}^- \;:=\; \{\;\zeta \in M:\;|y^{(i)}(\zeta)| \le r\;\}$$

and

$$S_{i,r}^+ \;:=\; \{\;\zeta \in M:\;\|z^{(i)}(\zeta)\|_{\kappa^{(i)}} \le r\;\} \quad .$$

Moreover, for $R, r > 0$, we define

$$Q_{i,r,R} \;:=\; S_{i,r}^- \;\cap\; S_{i,R}^+ \quad \text{and} \quad Q_{i,R} := Q_{i,R,R} \quad . \qquad (13.4)$$

[38]With usual abuse of notation we do not distinguish here and in the sequel between a function on M and the corresponding function on coordinate space.

Finally, given $S \subset M$ and $R > 0$ we denote by $B_R(S)$ the ball of radius R around S, i.e.

$$B_R(S) \; := \; \Big\{ \; \zeta \in M : \; \mathrm{dist}_\mu(\zeta, S) \leq R \; \Big\} \; .$$

Definition 13.8 (Modified basins of attraction)**.**

Let $i = 2, \cdots, m_0$. We denote by $\tilde{\mathcal{B}}_i$ a compact n-dimensional smooth submanifold of M containing $\mathcal{B}_i$ and having the following properties:

(i) *there exists an $R := R_i > 0$ such that*
  a) $\partial\tilde{\mathcal{B}}_i \cap Q_{i,2R} \; = \; \Big\{ \zeta \in M : \; y^{(i)}(\zeta) = 0 \;$ *and* $\; \|z(\zeta)\|_{\kappa^{(i)}} \leq 2R \; \Big\}$
  b) *if $r > 0$ is sufficiently small, then $f(\zeta) \; > \; f(\zeta_i^{(1)})$ for every $\zeta \in B_r(\partial\tilde{\mathcal{B}}_i) \; \setminus \; Q_{i,R}$*

(ii) *if $\mathcal{B}_i \cap \mathcal{B}_j = \emptyset$ then also $\tilde{\mathcal{B}}_i \cap \tilde{\mathcal{B}}_j = \emptyset$ and if $\mathcal{B}_i \subset \mathring{\mathcal{B}}_j$ then also $\tilde{\mathcal{B}}_i \subset \mathring{\tilde{\mathcal{B}}}_j$*

(iii) *For $r > 0$ sufficiently small the only critical point contained in $B_r(\partial\tilde{\mathcal{B}}_i)$ is $\zeta_i^{(1)}$.*

The existence of modified basins of attractions can be shown by means of the following discussion on the local structure of f around saddle points and using Assumption III.2 (i).

To start with, note that, in the special case in which for some $R > 0$ the energy f happens to be exactly quadratic in each $Q_{i,R}$, we have for every $i = 2, \cdots, m_0$

$$f^{-1}(\zeta_i^{(1)}) \; \cap \; Q_{i,R} \; = \; \Big\{ \; \zeta \in M : \; y^{(i)}(\zeta) = \pm \|z^{(i)}(\zeta)\|_{\kappa^{(i)}} \; \Big\} \; \cap \; Q_{i,R}$$

and in particular

$$\partial\mathcal{B}_i \; \cap \; Q_{i,R} \; = \; \Big\{ \; \zeta \in M : \; y^{(i)}(\zeta) = \|z^{(i)}(\zeta)\|_{\kappa^{(i)}} \; \Big\} \; \cap \; Q_{i,R} \; .$$

In the general situation we shall use the following rough estimate on the behaviour $f^{-1}(\zeta_i^{(1)})$ near the relevant saddle point (see Fig. 5).

Lemma 13.9.

There exists an $\tilde{R} > 0$ such that for every $i = 2, \cdots, m_0$,

$$f^{-1}(\zeta_i^{(1)}) \cap Q_{i,\tilde{R}} \; \subset \; \Big\{ \; \zeta \in M : \; \Big| \pm y^{(i)}(\zeta) - \|z^{(i)}(\zeta)\|_{\kappa^{(i)}} \Big| \leq \frac{1}{4}\|z^{(i)}(\zeta)\|_{\kappa^{(i)}} \Big\} \cap Q_{i,\tilde{R}} \tag{13.5}$$

and

$$\partial\mathcal{B}_i \cap Q_{i,\tilde{R}} \subset \left\{ \zeta \in M : \left| y^{(i)}(\zeta) - \|z^{(i)}(\zeta)\|_{\kappa^{(i)}} \right| \le \frac{1}{4}\|z^{(i)}(\zeta)\|_{\kappa^{(i)}} \right\} \cap Q_{i,\tilde{R}} \ . \tag{13.6}$$

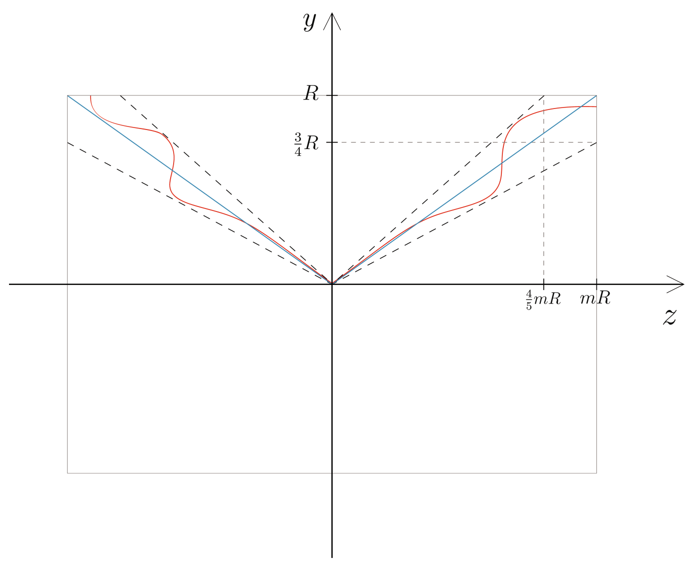

Figure 5. Picture of Lemma 13.9 in dimension $n = 1$ with $m := (\ |\kappa_1^{(i)}|/\kappa_2^{(i)}\ )^{\frac{1}{2}}$. In blue the set $\{\ \zeta \in M :\ y^{(i)}(\zeta) = \|z^{(i)}(\zeta)\|_{\kappa^{(i)}}\ \}$ and in red the set $\partial\mathcal{B}_i$.

Proof. We only show (13.6). Equation (13.5) can be shown analogously. First take $R > 0$ sufficiently small such that for every $i = 2, \dots, m_0$

$$\{\ \zeta \in M :\ y^{(i)}(\zeta) \in (-R, 0)\ \} \ \cap\ \mathcal{B}_i \ =\ \emptyset \ . \tag{13.7}$$

Let now $i = 2, \dots, m_0$ and $\zeta \in \partial\mathcal{B}_i \setminus \{z_i^{(1)}\} \ \cap\ Q_{i,R}$. Note that $y^{(i)}(\zeta) \ge 0$ due to (13.7). Moreover, by (13.3), we can find a constant K independent of i and ζ such that with $x^{(i)}(\zeta) := (y^{(i)}(\zeta), z^{(i)}(\zeta))$

$$\left|\ |y^{(i)}(\zeta)|^2 - \|z^{(i)}(\zeta)\|^2_{\kappa^{(i)}}\ \right| \ \le K\ \|x^{(i)}(\zeta)\|^3 \ \ ,$$

i.e.

$$\left|\ y^{(i)}(\zeta) - \|z^{(i)}(\zeta)\|_{\kappa^{(i)}}\ \right| \ \le K\ \frac{\|x^{(i)}(\zeta)\|^3}{y^{(i)}(\zeta) + \|z^{(i)}(\zeta)\|_{\kappa^{(i)}}} \ \ . \tag{13.8}$$

In the case $y^{(i)}(\zeta) \ge \|z^{(i)}(\zeta)\|_{\kappa^{(i)}}$ (implying $y^{(i)}(\zeta) \neq 0$) we get from (13.8) by possibly taking a smaller $R > 0$

$$y^{(i)}(\zeta) - \|z^{(i)}(\zeta)\|_{\kappa^{(i)}} \ \le K'\ \frac{|y^{(i)}(\zeta)|^3}{y^{(i)}(\zeta)} \ \le\ \frac{1}{5}y^{(i)}(\zeta) \ \ ,$$

i.e.

$$\big|\ y^{(i)}(\zeta) - \|z^{(i)}(\zeta)\|_{\kappa^{(i)}}\ \big| \le \frac{1}{4}\|z^{(i)}(\zeta)\|_{\kappa^{(i)}} \quad .$$

Similarly, in the case $y^{(i)}(\zeta) < \|z^{(i)}(\zeta)\|_{\kappa^{(i)}}$, we get from (13.8)

$$\big|\ y^{(i)}(\zeta) - \|z^{(i)}(\zeta)\|_{\kappa^{(i)}}\ \big| \ \le K' \ \frac{\|z^{(i)}(\zeta)\|^3_{\kappa^{(i)}}}{\|z^{(i)}(\zeta)\|_{\kappa^{(i)}}} \ \le \ \frac{1}{4}\|z^{(i)}(\zeta)\|_{\kappa_{(i)}} \quad .$$

$\square$

One can construct modified basins of attractions using Lemma 13.9 as follows.

Step 1:

Let $\tilde{R}$ as in Lemma 13.9. Take $R := \frac{1}{4}\tilde{R}$ and $r_0 > 0$ sufficiently small such that for $i, j = 2, \ldots, m_0$

(i) $\Big(\ \mathcal{B}_i \ \cap \ \mathcal{B}_j \ = \ \emptyset\ \Big) \ \Rightarrow \ \Big(\ B_{r_0}(\mathcal{B}_i) \ \cap \ B_{r_0}(\mathcal{B}_j) \ = \ \emptyset\ \Big)$

(ii) $\Big(\ \mathcal{B}_i \ \subset \ \mathring{\mathcal{B}}_j\ \Big) \ \Rightarrow \ \Big(\ B_{r_0}(\mathcal{B}_i) \ \subset \ \mathring{\mathcal{B}}_j\ \Big)$

(iii) $f(\zeta) \ > \ f(\zeta_i^{(1)})$ for every $\zeta \in \big(\ B_{r_0}(\mathcal{B}_i) \setminus \mathcal{B}_i\ \big) \ \cap \ Q^c_{i,\tilde{R}}$

Note that (iii) can be achieved thanks to Assumption III.2 (i), which implies that there is no critical point of f on $\partial\mathcal{B}_i \cap Q^c_{i,\tilde{R}}$.

Step 2:

Construct for every $i = 2, \ldots, m_0$ a compact n-dimensional smooth submanifold $\tilde{\mathcal{B}}_i$ of M satisfying for some $0 < r_1 < r_0$

(i) $B_{r_1}(\mathcal{B}_i) \cap Q^c_{i,\tilde{R}} \ \subset \ \tilde{\mathcal{B}}_i \cap Q^c_{i,\tilde{R}} \ \subset \ B_{r_0}(\mathcal{B}_i) \cap Q^c_{i,\tilde{R}}$

(ii) $\tilde{\mathcal{B}}_i \cap Q_{i,\tilde{R},2R} \ = \ \Big\{\zeta \in M : \ \ 0 \le y^{(i)}(\zeta) \le \tilde{R} \ \text{ and } \ \|z(\zeta)\|_{\kappa^{(i)}} \le 2R\ \Big\}$

(iii) $f(\zeta) > f(\zeta_i^{(1)})$ if ζ is both in $Q_{i,\tilde{R}} \cap Q^c_{i,\tilde{R},2R}$ and in $\tilde{\mathcal{B}}_i \cap \mathcal{B}_i^c$

This is possible thanks to Lemma 13.9 and it is straightforward to check that the thus constructed $\tilde{\mathcal{B}}_i$'s are modified basins of attraction.

Remark 13.10. *If $\tilde{\mathcal{B}}_i$ is a modified basin of attraction property (i) b) appearing in Definition 13.8 can be improved in the following sense: for $r > 0$*

sufficiently small

$$f(\zeta) \;>\; f(\zeta_i^{(1)}) \quad \textit{for every} \quad \zeta \in B_r(\partial\tilde{\mathcal{B}}_i) \;\setminus\; Q_{i,2r} \quad .$$

This can be seen using Lemma 13.9.

Remark 13.11.

Let $\tilde{\mathcal{B}}_i$ *be a modified basin of attraction. Since* $\tilde{\mathcal{B}}_i$ *is smooth, the inward unitary normal vector* $\mathbf{n} = \mathbf{n}(\eta)$ *of* $\tilde{\mathcal{B}}_i$ *is well defined at every point* $\eta \in \partial\tilde{\mathcal{B}}_i$. *For* r *sufficiently small we shall consider on the set* $B_r(\partial\tilde{\mathcal{B}}_i)$ *the coordinates* $\zeta \mapsto \big(\eta(\zeta), \iota(\zeta)\big) \in \partial\tilde{\mathcal{B}}_i \times (0, r)$ *defined by*

$$\zeta \;=\; \eta(\zeta) \;+\; \iota(\zeta)\; \mathbf{n}(\zeta) \quad .$$

We shall also write $\mathbf{n}_i, \eta_i$ *and* ι_i *to stress the dependence on* i.

14. Quasimodes

Following [42] we attach to every local minimum of f a quasimode for $\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$ and to every critical point of index 1 of f a quasimode for $\mathcal{H}^{(1)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$. The former is obtained by cutting the ground state $e^{-\frac{f}{\varepsilon}}$ outside the basin of attraction of the considered local minimum; the latter by using a WKB-expansion around a small neigbourhood of the considered saddle point.

To make this precise we introduce now suitable cut-off functions: the cut-off function $\chi^{(0)}_{i,s,\varepsilon}$ attached to $\zeta^{(0)}_i$ will be supported in a small neigbourhood of the modified basin of attraction $\tilde{\mathcal{B}}_i$ and will depend both on ε and a second parameter $s > 0$, which can be thought as fixed throughout. Every choice of $s \in [\frac{1}{2}, 1)$ will be fine to obtain asymptotic expressions for the low-lying eigenvalues of $\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$, with $s = \frac{1}{2}$ giving the best (but not optimal) error estimate, see Proposition 15.1 in Section 15. Therefore, up to Section 16 included, one can think of $s = \frac{1}{2}$. The convenience of developing the theory also for different values of s will show up only in Section 17, where comparing two possible choices of s (say $s = \frac{1}{2}$ and $s = \frac{\sqrt{2}}{2}$) one can easily get rid of the fictitious dependence on s of the results and thus obtain optimal error estimates.

Definition 14.1. *[Cut-off function corresponding to a local minimum]*
Let $i = 2, \dots, m_0$ and let $s > 0$. A cut-off function (of order s) corresponding to the local minimum $\zeta^{(0)}_i$ is a function $\chi^{(0)}_{i,s,\varepsilon} \in C^\infty(M;\mathbb{R})$ also depending on $\varepsilon > 0$, satisfying for ε sufficiently small

$$\chi^{(0)}_{i,s,\varepsilon}(\zeta) \;=\; \begin{cases} 1 & \text{if } \zeta \in \tilde{\mathcal{B}}_i \setminus B_{\varepsilon^s}(\partial\tilde{\mathcal{B}}_i) \\ \theta\left(\frac{\iota_i(\zeta)}{\varepsilon^s}\right) & \text{if } \zeta \in B_{\varepsilon^s}(\partial\tilde{\mathcal{B}}_i) \\ 0 & \text{if } \zeta \in M \setminus B_{\varepsilon^s}(\tilde{\mathcal{B}}_i) \end{cases} ,$$

where $\tilde{\mathcal{B}}_i$ is a modified basin of attraction as in Definition 13.8, $\zeta \mapsto \iota_i(\zeta)$ is the coordinate introduced in Remark 13.11 and $\theta \in C^\infty(\mathbb{R};\mathbb{R})$ satisfies

$$\theta(t) = \begin{cases} 1 & \text{if } t \geq 1 \\ 0 & \text{if } t \leq -1 \end{cases} .$$

Moreover, in the case $i = 1$ we set for $s, \varepsilon > 0$

$$\chi^{(0)}_{1,s,\varepsilon} \equiv 1 \quad .$$

Remark 14.2.

Recall the definition of the scaling operator Ψ_ε given in (9.2)*. Let $i = 2, \ldots, m_0$ and $s > 0$. Observe that for $\zeta \in M$, $v \in V$ and $\varepsilon > 0$*

$$\Psi_\varepsilon\ \tau_*\ \delta\ \chi^{(0)}_{i,s,\varepsilon}\ (\zeta, v)\ =\ \chi^{(0)}_{i,s,\varepsilon}(\zeta + \varepsilon v) - \chi^{(0)}_{i,s,\varepsilon}(\zeta) \quad ,$$

so that a Taylor expansion gives

$$\Psi_\varepsilon\ \tau_*\ \delta\ \chi^{(0)}_{i,s,\varepsilon}\Big|_{Q_{i,R}}\ \sim\ \sum_{k=1}^{\infty} \varepsilon^{(1-s)k}\ \ \frac{1}{k!}\theta^{(k)}\big(\ \frac{y^{(i)}}{\varepsilon^s}\ \big)\ e_1^* \quad , \tag{14.1}$$

where $\theta^{(k)}$ denotes the k-th derivative of the function $\theta \in C^\infty(\mathbb{R};\mathbb{R})$ appearing in definition 14.1 and $R > 0$ is sufficiently small such that $\iota_i(\zeta) = y^{(i)}(\zeta)$ for $\zeta \in Q_{i,R}$ (recall the definition of the latter in (13.4)*).*

We shall also use in the sequel that for every $k \in \mathbb{N}_0$ there exists a constant $C > 0$ such that for every ζ in M and $\varepsilon > 0$

$$\|\nabla^k \chi_{i,s,\varepsilon}(\zeta)\|_\mu\ \le C\ \varepsilon^{-ks} \quad . \tag{14.2}$$

Moreover, for $s \in (0,1)$ and ε sufficiently small

$$\operatorname{supp}\ \|\tau_*\ \delta\chi^{(0)}_{i,s,\varepsilon}\|_{\mu_\varepsilon}\ \subset\ B_{2\varepsilon^s}(\partial\tilde{\mathcal{B}}_i) \quad .$$

Finally note that from Remark 13.10 it follows that for $s \in (0,1)$ there exists a constant $C > 0$ such that for $\varepsilon > 0$ sufficiently small

$$\max_{\operatorname{supp}\|\tau_*\ \delta\chi^{(0)}_{i,s,\varepsilon}\|_{\mu_\varepsilon}} [\ f(\zeta_i^{(1)}) - f\ ]\ \le\ C\ \varepsilon^{2s} \quad . \tag{14.3}$$

The cut-off function $\chi_i^{(1)}$ attached to the saddle point $\zeta_j^{(1)}$ will be supported in an ε-independent but suitably small neighbourhood of $\zeta_j^{(1)}$. Recall for this purpose the definitions of $Q_{i,R,r}$ and $Q_{i,R}$ given in (13.4).

Remark 14.3. *Let $i = 2, \ldots, m_1 + 1$ and let $\varphi_i^{(1)} \in C^\infty(M;\mathbb{R})$ be a phase function corresponding to the critical point $\zeta_i^{(1)}$ as constructed in Theorem 11.1. Since in particular*

$$\varphi_i^{(1)}(\zeta_i^{(1)}) = 0 \quad , \quad \nabla\varphi_i^{(1)}(\zeta_i^{(1)}) \equiv 0 \quad \textit{and} \quad \nabla^2_{e_l,e_j}\varphi_i^{(1)}(\zeta_i^{(1)}) = |\kappa_j^{(i)}|\ 1_{l,j} \quad ,$$

it follows that for sufficiently small $R, \gamma > 0$ the estimates

$$\varphi_i^{(1)}(\zeta)\ \ge\ \gamma|y^{(i)}(\zeta)|^2 + \gamma\|z^{(i)}(\zeta)\|^2_{\kappa^{(i)}} \tag{14.4}$$

and

$$f(\zeta) - f(\zeta_i^{(1)}) + \varphi_i^{(1)}(\zeta)\ \ge\ -\gamma|y^{(i)}(\zeta)|^2 + \gamma\|z^{(i)}(\zeta)\|^2_{\kappa^{(i)}} \tag{14.5}$$

hold for every $\zeta \in Q_{i,R}$. *To see* (14.5) *observe that for every* $\gamma' > 0$ *there exists an* $R_{\gamma'} > 0$ *such that* $f(\zeta) - f(\zeta_i^{(1)}) + \varphi_i^{(1)}(\zeta) + \gamma' |y^{(i)}(\zeta)|^2$ *is strictly positive in* $Q_{i,R_{\gamma'}} \setminus \{0\}$. *It follows that the function defined by*

$$g_i(\zeta) \;:=\; \frac{f(\zeta) - f(\zeta_i^{(1)}) + \varphi_i^{(1)}(\zeta) + \gamma'|y^{(i)}(\zeta)|^2}{\|z^{(i)}(\zeta)\|^2_{\kappa^{(i)}} + \gamma'|y^{(i)}(\zeta)|^2} \quad ,$$

extended by continuity to $\zeta_i^{(1)}$ *is strictly positive in* $Q_{i,R_{\gamma'}}$, *so with* $\gamma := \inf_{\zeta \in Q_{i,R_{\gamma'}}} g_i(\zeta) > 0$ *one gets*

$$f(\zeta) - f(\zeta_i^{(1)}) + \varphi_i^{(1)}(\zeta) \;\geq\; \gamma'(\gamma - 1)|y^{(i)}(\zeta)|^2 + \gamma \|z^{(i)}(\zeta)\|^2_{\kappa^{(i)}} \quad ,$$

giving (14.5) *for sufficiently small* γ'.

Definition 14.4 (Cut-off function corresponding to a saddle point)**.**
Let $i = 2, \ldots, m_1 + 1$. *A cut-off function corresponding to the saddle point* $\zeta_i^{(1)}$ *is a (*ε *- independent) function* $\chi_i^{(1)} \in C^\infty(M;\mathbb{R})$ *satisfying*

$$\chi_i^{(1)} \;\equiv\; 1 \quad \text{on} \quad Q_{i,R} \quad \text{and} \quad \chi_i^{(1)} \;\equiv 0 \quad \text{on } M \setminus Q_{i,2R}$$

for some $R > 0$ *such that* (14.4) *and* (14.5) *hold in* $Q_{i,3R}$ *for some sufficiently small* $\gamma > 0$ *and such that for every sufficiently small* $r > 0$

$$Q_{i,3R} \;\cap\; B_r(\tilde{\mathcal{B}}_i) \;=\; Q_{i,r,3R} \quad .$$

We shall also assume that for $i \neq j$

$$\operatorname{supp} \|\tau_* \chi_i^{(1)}\|_{\mu_\varepsilon} \cap \operatorname{supp} \|\tau_* \chi_j^{(1)}\|_{\mu_\varepsilon} \;=\; \emptyset \quad \text{and} \quad \operatorname{supp} \|\tau_* \chi_i^{(1)}\|_{\mu_\varepsilon} \cap B_r(\partial \tilde{\mathcal{B}}_j) = \emptyset \tag{14.6}$$

for $\varepsilon, r > 0$ *sufficiently small.*

Remark 14.5. *For our purposes one could alternatively define an* ε*-dependent cut-off function* $\chi_{i,\varepsilon}^{(1)} \in C^\infty(M;\mathbb{R})$ *corresponding to the saddle point* $\zeta_i^{(1)}$ *by just requiring that*

$$\chi_{i,\varepsilon}^{(1)} \;\equiv\; 1 \quad \text{on} \quad Q_{i,R_\varepsilon} \quad \text{and} \quad \chi_{i,\varepsilon}^{(1)} \;\equiv 0 \quad \text{on } M \setminus Q_{i,2R_\varepsilon} \quad ,$$

with R_ε *going to zero at least as slowly as* $\sqrt{\varepsilon |\log \varepsilon|}$. *Working with* $\chi_{i,\varepsilon}^{(1)}$ *instead of* $\chi_i^{(1)}$ *would not affect the following results.*

Definition 14.6 (Quasimodes and approximate eigenvalues)**.**

(i) *Let* $i = 1, \ldots, m_0$ *and* $s > 0$. *For* $\varepsilon > 0$ *we define the quasimode* $\psi^{(0)}_{i,s,\varepsilon} \in C^\infty(M;\mathbb{R})$ *corresponding to* $\zeta^{(0)}_i$ *as*

$$\psi^{(0)}_{i,s,\varepsilon}(\zeta) \;:=\; Z^{(0)}_{i,s,\varepsilon}\; \chi^{(0)}_{i,s,\varepsilon}(\zeta)\; e^{-\frac{f(\zeta)-f(\zeta^{(0)}_i)}{\varepsilon}} \quad ,$$

where $Z^{(0)}_{i,s,\varepsilon}$ *is a normalization constant:*

$$Z^{(0)}_{i,s,\varepsilon} \;:=\; \|\chi^{(0)}_{i,\varepsilon}\; e^{-\frac{f-f(\zeta^{(0)}_i)}{\varepsilon}}\|^{-1}_{\Lambda_{\mu_\varepsilon}}$$

and $\chi^{(0)}_{i,s,\varepsilon}$ *is a cut-off function corresponding to* $\zeta^{(0)}_i$ *(see Definition 14.1).*

(ii) *Let* $i = 2, \ldots, m_1+1$. *For* $\varepsilon > 0$ *we define the quasimode* $\psi^{(1)}_{i,\varepsilon} \in C^\infty(M;\mathbb{R}^{V,\mu_\varepsilon}_a)$ *corresponding to* $\zeta^{(1)}_i$ *as*

$$\psi^{(1)}_{i,\varepsilon}(\zeta) \;:=\; Z^{(1)}_{i,\varepsilon}\; \chi^{(1)}_i(\zeta)\; a^{(1)}_{i,\varepsilon}(\zeta)\; e^{-\frac{\varphi^{(1)}_i(\zeta)}{\varepsilon}} \quad ,$$

where $Z^{(1)}_{i,\varepsilon}$ *is a normalization constant:*

$$Z^{(1)}_{i,\varepsilon} \;:=\; \|\chi^{(1)}_i\; a^{(1)}_{i,\varepsilon}\; e^{-\frac{\varphi^{(1)}_i}{\varepsilon}}\|^{-1}_{\Lambda_{\mu_\varepsilon}} \quad ,$$

$\chi^{(1)}_i$ *is a cut-off function corresponding to* $\zeta^{(1)}_i$ *(see Definition 14.4) and* $a^{(1)}_{i,\varepsilon}\; e^{-\frac{\varphi^{(1)}_i}{\varepsilon}} \in C^\infty(M;\mathbb{R}^{V,\mu_\varepsilon}_a)$ *is a WKB quasimode around* $\zeta^{(1)}_i$, *i.e.* $\Psi_\varepsilon\; a^{(1)}_{i,\varepsilon}$ *and* $\varphi^{(1)}_i$ *have the properties of the amplitude and phase appearing in Theorem 11.1, with critical point* $\zeta^{(1)}_i$. *Moreover, by possibly changing sign, we shall assume that* $\Psi_\varepsilon a^{(1)}_{i,0}(\zeta^{(1)}_i) = e^*_1$, *with* e^*_1 *as in Definition 13.6.*

(iii) *Let* $i = 2, \ldots, m_0$ *and* $s > 0$. *For* $\varepsilon > 0$ *we define the approximate eigenvalues* $\nu^{app}_{i,s,\varepsilon} \in \mathbb{R}$ *as*

$$\nu^{app}_{i,s,\varepsilon} \;:=\; \left|\langle \psi^{(1)}_{i,\varepsilon}, \delta_{\rho_\varepsilon}\; \psi^{(0)}_{i,s,\varepsilon}\rangle_{\Lambda_{\mu_\varepsilon}}\right|^2 \quad . \tag{14.7}$$

Given $\zeta \in M$ we shall denote in the sequel by $\mathrm{Hess}_\mu f(\zeta)$ the Hessian of f with respect to μ at ζ, defined via the identity

$$\nabla^2_{v,w} f(\zeta) \;=\; \langle \mathrm{Hess}_\mu f(\zeta)\; v, w\rangle_\mu \quad .$$

Remark 14.7. *It follows from the discrete Laplace method (see Corollary C.2 in the appendix) that for $i = 1, \ldots, m_0$ and $s > 0$*

$$Z^{(0)}_{i,s,\varepsilon} \;\sim\; \varepsilon^{n/4} \sum_{k=0}^{\infty} \varepsilon^k \;\; \hat{Z}^{(0)}_{i,k} \tag{14.8}$$

for some s-independent sequence $(\hat{Z}^{(0)}_{i,k})_{k\in\mathbb{N}_0}$ in $\mathbb{R}$ with

$$\hat{Z}^{(0)}_{i,0} \;=\; \frac{\big(\det \mathrm{Hess}_\mu f(\zeta^{(0)}_i)\big)^{\frac{1}{4}}}{\pi^{\frac{n}{4}}} \quad .$$

Similarly for $i = 2, \ldots, m_1 + 1$

$$Z^{(1)}_{i,\varepsilon} \;\sim\; \varepsilon^{n/4} \sum_{k=0}^{\infty} \varepsilon^k \;\; \hat{Z}^{(1)}_{i,k} \quad . \tag{14.9}$$

Here $(\hat{Z}^{(1)}_{i,k})_{k\in\mathbb{N}_0}$ is a sequence in $\mathbb{R}$ with

$$\hat{Z}^{(1)}_{i,0} \;=\; \frac{|\det \mathrm{Hess}_\mu f(\zeta^{(1)}_i)|^{\frac{1}{4}}}{\pi^{\frac{n}{4}}} \quad . \tag{14.10}$$

Remark 14.8. *Observe that by definition of $\delta_{\rho_\varepsilon}$ (Definition 8.1) for every $i = 1, \ldots, m_0$ and $s, \varepsilon > 0$*

$$\delta_{\rho_\varepsilon}\; \psi^{(0)}_{i,s,\varepsilon} \;=\; Z^{(0)}_{i,s,\varepsilon}\; e^{-\frac{f - f(\zeta^{(0)}_i)}{\varepsilon}}\; \delta\; \chi^{(0)}_{i,s,\varepsilon} \quad .$$

In particular

$$\delta_{\rho_\varepsilon}\; \psi^{(0)}_{1,s,\varepsilon} \;=\; 0 \quad .$$

Note also that by Remark 10.4 we have $\psi^{(0)}_{1,s,\varepsilon} \in D(\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}})$, implying that $\psi^{(0)}_{1,s,\varepsilon}$ is a normalized eigenfunction of $\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$ with eigenvalue 0.

The next two propositions establish crucial properties of the quasimodes.

Proposition 14.9. *Let $i, j = 1, \ldots, m_0$ and $s \in [0, 1)$.*

(i) *There exists a constant $\gamma > 0$ s.t. for sufficiently small $\varepsilon > 0$*

$$\langle \psi^{(0)}_{i,s,\varepsilon}, \psi^{(0)}_{j,s,\varepsilon} \rangle_{\Lambda_{\mu_\varepsilon}} \;=\; 1_{i,j} \;+\; \mathcal{O}(e^{-\gamma/\varepsilon}) \quad .$$

(ii) *If $s \in [\frac{1}{2}, 1)$, there exists a constant $C > 0$ s.t. for sufficiently small $\varepsilon > 0$*

$$\langle \mathcal{H}_{\rho_\varepsilon,\mu_\varepsilon} \psi^{(0)}_{j,\varepsilon}, \psi^{(0)}_{j,\varepsilon} \rangle_{\Lambda_{\mu_\varepsilon}} \;\leq\; C\; e^{-2[f(\zeta^{(1)}_j) - f(\zeta^{(0)}_j)]/\varepsilon} \quad .$$

Remark 14.10. *In fact all we need in the sequel from Proposition 14.9 is property (i) together we the following weak version of property (ii): if* $s \in [\frac{1}{2}, 1)$ *there exist constants* $C > 0$ *and* $N \in \mathbb{N}_0$ *s.t. for sufficiently small* $\varepsilon > 0$

$$\langle \mathcal{H}_{\rho_\varepsilon,\mu_\varepsilon} \psi^{(0)}_{j,s,\varepsilon}, \psi^{(0)}_{j,s,\varepsilon} \rangle_{\Lambda_{\mu_\varepsilon}} \;\leq\; C\ \varepsilon^{-N}\ e^{-2[f(\zeta^{(1)}_j) - f(\zeta^{(0)}_j)]/\varepsilon} \quad .$$

Proof of Prop.14.9.
(i): the case $i = j$ is clear since the quasimodes are normalized by definition. Assume now $i \neq j$. Observe that supp $\chi^{(0)}_{l,s,\varepsilon} \subset B_{2\varepsilon^s}(\tilde{B}_l)$ for $l = i, j$ and recall Proposition 13.5 (ii). In the case $\mathcal{B}_i \cap \mathcal{B}_j = \emptyset$, it follows from property (ii) in Definition 13.8 that supp $\chi^{(0)}_{i,s,\varepsilon} \cap$ supp $\chi^{(0)}_{j,s,\varepsilon} = \emptyset$ for sufficiently small ε, so $\langle \psi^{(0)}_{i,s,\varepsilon}, \psi^{(0)}_{j,s,\varepsilon} \rangle_{\Lambda_{\mu_\varepsilon}} = 0$. In the case $\mathcal{B}_j \subset \mathring{\mathcal{B}}_i$ we have supp $\chi^{(0)}_{j,s,\varepsilon} \subset$ supp $\chi^{(0)}_{i,s,\varepsilon}$ for sufficiently small ε and

$$f(\zeta^{(0)}_j) > f(\zeta^{(0)}_i)$$

holds by Proposition 13.5 (i). The latter also gives $f > f(\zeta^{(0)}_j)$ on supp $\chi^{(0)}_{j,s,\varepsilon} \setminus \{\zeta^{(0)}_j\}$. It follows now from the discrete Laplace method (see Corollary C.2) and from (14.8), that

$$\begin{aligned} \langle \psi^{(0)}_{i,s,\varepsilon}, \psi^{(0)}_{j,s,\varepsilon} \rangle_{\Lambda_{\mu_\varepsilon}} \;&=\\ = \; e^{\frac{f(\zeta^{(0)}_i) - f(\zeta^{(0)}_j)}{\varepsilon}}\ Z^{(0)}_{i,s,\varepsilon}\ Z^{(0)}_{j,s,\varepsilon}\ \int_M \chi^{(0)}_{i,s,\varepsilon}\ \chi^{(0)}_{j,s,\varepsilon}\ e^{\frac{-2[f(\zeta) - f(\zeta^{(0)}_j)]}{\varepsilon}} \;&\leq \\ \leq\ \text{Const}\ \times\ e^{\frac{f(\zeta^{(0)}_i) - f(\zeta^{(0)}_j)}{\varepsilon}} \quad . \end{aligned}$$

The case $\mathcal{B}_i \subset \mathcal{B}_j$ is analogous.

Proof of (ii): we show the stronger statement that for every $s \in (0, 1)$ there exists a constant $C > 0$ s.t. for sufficiently small $\varepsilon > 0$

$$\langle \mathcal{H}_{\rho_\varepsilon,\mu_\varepsilon} \psi^{(0)}_{j,s,\varepsilon}, \psi^{(0)}_{j,s,\varepsilon} \rangle_{\Lambda_{\mu_\varepsilon}} \;\leq\; C\ \varepsilon^{n/2+2-s}\ e^{C\varepsilon^{2s-1}}\ e^{-2[f(\zeta^{(1)}_j) - f(\zeta^{(0)}_j)]/\varepsilon} \quad .$$

By Remark 14.8 and using (14.8) we get

$$\langle \mathcal{H}_{\rho_\varepsilon,\mu_\varepsilon}\ \psi^{(0)}_{j,s,\varepsilon}, \psi^{(0)}_{j,s,\varepsilon}\rangle_{\Lambda_{\mu_\varepsilon}} \ = \ \big\|\delta_{\rho_\varepsilon}\ \psi^{(0)}_{j,s,\varepsilon}\big\|^2_{\Lambda_{\mu_\varepsilon}} \ =$$

$$= \ \big(Z^{(0)}_{i,s,\varepsilon}\big)^2\ \big\|e^{-\frac{f-f(\zeta_i^{(0)})}{\varepsilon}}\ \delta\ \chi^{(0)}_{i,s,\varepsilon}\big\|^2_{\Lambda_{\mu_\varepsilon}} \ =$$

$$= \ e^{-\frac{2[f(\zeta_i^{(1)})-f(\zeta_i^{(0)})]}{\varepsilon}}\ \big(Z^{(0)}_{i,s,\varepsilon}\big)^2\ \big\|e^{-\frac{f-f(\zeta_i^{(1)})}{\varepsilon}}\ \delta\ \chi^{(0)}_{i,s,\varepsilon}\big\|^2_{\Lambda_{\mu_\varepsilon}} \ \le$$

$$\le \ \text{Const}\ \varepsilon^{n/2}\ e^{-\frac{2[f(\zeta_i^{(1)})-f(\zeta_i^{(0)})]}{\varepsilon}}\ \big\|e^{-\frac{f-f(\zeta_i^{(1)})}{\varepsilon}}\ \delta\ \chi^{(0)}_{i,s,\varepsilon}\big\|^2_{\Lambda_{\mu_\varepsilon}} \quad .$$

Moreover for $\varepsilon > 0$ sufficiently small

$$\big\|e^{-\frac{f-f(\zeta_i^{(1)})}{\varepsilon}}\ \delta\ \chi^{(0)}_{i,s,\varepsilon}\big\|^2_{\Lambda_{\mu_\varepsilon}} \ =$$

$$= \ \int_M\int_V \big(\ \chi^{(0)}_{i,s,\varepsilon}(\zeta+\varepsilon v) - \chi^{(0)}_{i,s,\varepsilon}(\zeta)\ \big)^2\ e^{-\frac{2[f(\zeta+\varepsilon v/2)-f(\zeta_i^{(1)})]}{\varepsilon}}\ \Lambda(d\zeta)\mu(dv) \ =$$

$$= \ \varepsilon^2 \int_{B_{2\varepsilon^s(\partial\tilde{\mathcal{B}}_i)}}\int_V \Big(\ \int_0^1 \nabla_v\chi^{(0)}_{i,\varepsilon}(\zeta+\varepsilon t v)\ dt\ \Big)^2\ e^{-\nabla_v f(\zeta)}\ e^{-\frac{2[f(\zeta)-f(\zeta_i^{(1)})]}{\varepsilon}}\ \Lambda(d\zeta)\mu(dv)\ \big(\ 1+\mathcal{O}(\varepsilon)\ \big) \ \le$$

$$\le \ \text{Const}\,\varepsilon^{2-s}\ e^{\text{Const}\,\varepsilon^{2s-1}} \quad .$$

Note that for the last inequality we used $\text{Vol}(B_{2\varepsilon^s(\partial\tilde{\mathcal{B}}_i)}) \le \text{Const}\,\varepsilon^s$, and the estimates (14.2) (with $k=1$) and (14.3). □

Proposition 14.11. *For $i,j = 1,\dots,m_1$ and ε small enough*

(i)

$$\langle \psi^{(1)}_{i,\varepsilon}, \psi^{(1)}_{i,\varepsilon}\rangle_{\Lambda_{\mu_\varepsilon}} \ = \ 1_{i,j} \quad .$$

(ii)

$$\langle \mathcal{H}_{\rho_\varepsilon,\mu_\varepsilon}\ \psi^{(1)}_{j,\varepsilon}, \psi^{(1)}_{j,\varepsilon}\rangle_{\Lambda_{\mu_\varepsilon}} \ = \ \mathcal{O}(\varepsilon^\infty) \quad .$$

Proof. (i) follows immediately from the definition of the $\psi^{(1)}_{i,\varepsilon}$'s and the fact that cut-off functions corresponding to different saddle points have disjoint supports.

(ii): by Cauchy-Schwarz it suffices to show that

$$\big\|\mathcal{H}_{\rho_\varepsilon,\mu_\varepsilon}\ \psi^{(1)}_{j,\varepsilon}\big\|_{\Lambda_{\mu_\varepsilon}} \ = \ \mathcal{O}(\varepsilon^\infty) \quad .$$

This can be shown using (i) of Theorem 11.1 and then proceeding as in Remark 11.7. □

15. Computation of approximate small eigenvalues

In this section we analyze the asymptotic behaviour as $\varepsilon \to 0$ of the (square root of the) approximate eigenvalues $\nu_{i,s,\varepsilon}^{\text{app}}$, defined in Definition 14.6. Recall that $\kappa_{f,\mu,1}^{(i)}$ denotes the negative eigenvalue of $\text{Hess}_\mu f(\zeta_i^{(1)})$.

Proposition 15.1. *Let $i = 2, \dots, m_0$ and $s \in [\frac{1}{2}, 1)$. Then for $\varepsilon > 0$*

$$\langle \psi_{i,\varepsilon}^{(1)}, \delta_{\rho_\varepsilon} \ \psi_{i,s,\varepsilon}^{(0)} \rangle_{\Lambda_{\mu_\varepsilon}} \ = \ \sqrt{\varepsilon} \ \ P_i \ \ e^{-\frac{f(\zeta_i^{(1)}) - f(\zeta_i^{(0)})}{\varepsilon}} \ \ \Big(\ 1 + \mathcal{E}_{i,s,\varepsilon} \ \Big) \quad , \tag{15.1}$$

with

$$P_i \ := \ \sqrt{\frac{|\kappa_{f,\mu,1}^{(i)}|}{\pi}} \ \frac{\big[\det \text{Hess}_\mu f(\zeta_i^{(0)}) \big]^{\frac{1}{4}}}{|\det \text{Hess}_\mu f(\zeta_i^{(1)})|^{\frac{1}{4}}} \tag{15.2}$$

and with $\mathcal{E}_{i,s,\varepsilon} \in \mathbb{R}$ satisfying

$$\mathcal{E}_{i,s,\varepsilon} \ = \ \mathcal{O}(\varepsilon^{1-s}) \quad . \tag{15.3}$$

Moreover for each $j = 2, \dots, m_1 + 1$ with $j \neq i$

$$\langle \psi_{j,\varepsilon}^{(1)}, \delta_{\rho_\varepsilon} \ \psi_{i,s,\varepsilon}^{(0)} \rangle_{\Lambda_{\mu_\varepsilon}} \ = \ 0 \quad . \tag{15.4}$$

Remark 15.2. *In fact we will show in the proof below that the $\mathcal{E}_{i,s,\varepsilon}$ appearing in Proposition 15.1 has the following property: there exists a sequence $(\hat{\mathcal{E}}_{i,\mathbf{k}})_{\mathbf{k}=(k_1,\dots,k_4)\in\mathbb{N}_0^4}$ in $\mathbb{R}$ with $\hat{\mathcal{E}}_{i,(0,0,0,0)} = \hat{\mathcal{E}}_{i,(0,0,k_3,k_4)} = 0$ for every $k_3 \in \mathbb{N}_0$ and every $k_4 \in \mathbb{N}_*$, such that*

$$1 \ + \ \mathcal{E}_{i,s,\varepsilon} \ \sim \sum_{\mathbf{k}=(k_1,\dots,k_4)\in\mathbb{N}_0^4} \varepsilon^{k_1 + sk_2 + (1-s)k_3 + (2s-1)k_4} \ \ \hat{\mathcal{E}}_{i,\mathbf{k}} \quad .$$

Note that this implies in particular (15.3)*, since for every choice of $s \in [\frac{1}{2}, 1)$ the biggest terms appearing in the expansion correspond to $\mathbf{k} = (0,0,1,0)$, $\mathbf{k} = (0,1,0,0)$ and $\mathbf{k} = (0,1,0,1)$.*

Proof.

Observe that by definition of $\psi_{i,s,\varepsilon}^{(0)}$ and $\psi_{i,\varepsilon}^{(1)}$ (see Definition 14.6) and Remark 14.8 we have

$$\langle \psi_{i,\varepsilon}^{(1)}, \delta_{\rho_\varepsilon} \ \psi_{i,s,\varepsilon}^{(0)} \rangle_{\Lambda_{\mu_\varepsilon}} \ = \ Z_{i,s,\varepsilon}^{(0)} \ Z_{i,\varepsilon}^{(1)} \ I_{i,s,\varepsilon} \quad , \tag{15.5}$$

with the interaction integral $I_{i,s,\varepsilon}$ defined as

$$I_{i,s,\varepsilon} \;:=\; \langle \chi_i^{(1)} \; a_{i,\varepsilon}^{(1)} \; e^{-\varphi_i^{(1)}/\varepsilon}, e^{-(f-f(\zeta_i^{(0)}))/\varepsilon} \; \delta\chi_{i,s,\varepsilon}^{(0)} \rangle_{\Lambda_{\mu_\varepsilon}} \quad . \tag{15.6}$$

Statement (15.4) follows now from the second property in (14.6) giving for $i \neq j$ and for sufficiently small ε

$$\operatorname{supp} \|\tau_* \; \chi_j^{(1)}\|_{\mu_\varepsilon} \;\cap\; \operatorname{supp} \|\tau_* \; \delta\chi_{i,s,\varepsilon}^{(0)}\|_{\mu_\varepsilon} \;=\; \emptyset \quad .$$

To prove (15.1) we proceed as follows.

Step 1

Taking out in (15.6) the exponential factor appearing in (15.1) gives

$$I_{i,s,\varepsilon} \;=\; e^{-\frac{f(\zeta_i^{(1)})-f(\zeta_i^{(0)})}{\varepsilon}} \; \tilde{I}_{i,s,\varepsilon} \quad , \tag{15.7}$$

with

$$\tilde{I}_{i,s,\varepsilon} \;:=\; \int_{M\times V} \tau_* \; \chi_i^{(1)} \; a_{i,\varepsilon}^{(1)} \; e^{-\frac{f-f(\zeta_i^{(1)})+\varphi_i^{(1)}}{\varepsilon}} \; \delta \; \chi_{i,s,\varepsilon}^{(0)} \;\; d\Lambda_\varepsilon \otimes d\mu_\varepsilon \;=$$

$$= \int_{M\times V} \chi_i^{(1)}(\zeta+\varepsilon v/2) \; a_{i,\varepsilon}^{(1)}(\zeta+\varepsilon v/2, \varepsilon v) \; e^{-\frac{f(\zeta+\varepsilon v/2)-f(\zeta_i^{(1)})+\varphi_i^{(1)}(\zeta+\varepsilon v/2)}{\varepsilon}} \\ \times \big(\; \chi_{i,s,\varepsilon}^{(0)}(\zeta+\varepsilon v) - \chi_{i,s,\varepsilon}^{(0)}(\zeta) \; \big) \;\; \Lambda_\varepsilon(d\zeta) \otimes \mu(dv) \quad .$$

Taylor expanding around every ζ the term

$$\chi_i^{(1)}(\zeta+\varepsilon v/2) \; a_{i,\varepsilon}^{(1)}(\zeta+\varepsilon v/2, \varepsilon v) \; e^{-\frac{f(\zeta+\varepsilon v/2)-f(\zeta_i^{(1)})+\varphi_i^{(1)}(\zeta+\varepsilon v/2)}{\varepsilon}}$$

and using that for some sequence $(\hat{a}_{i,k})_{k\in\mathbb{N}_0}$ in $C^\infty(M;\mathbb{R}_a^{V,\mu})$

$$\Psi_\varepsilon \; a_{i,\varepsilon}^{(1)} \;\sim\; \sum_{k=0}^{\infty} \varepsilon^k \;\; \hat{a}_{i,k}$$

we get

$$\tilde{I}_{i,s,\varepsilon} \;\sim\; \sum_{k=0}^{\infty} \varepsilon^k \;\; J_{i,s,k,\varepsilon} \quad , \tag{15.8}$$

with

$$J_{i,s,k,\varepsilon} \;:=\; \int_M \langle A_{i,k} \;,\; \Psi_\varepsilon \tau_* \; \delta \; \chi_{i,s,\varepsilon}^{(0)} \rangle_\mu \;\; e^{-F_i/\varepsilon} \; \Lambda_\varepsilon(d\zeta) \quad ,$$

i.e., more explicitly,

$$J_{i,s,k,\varepsilon} \;:=\; \int_{M\times V} A_{i,k}(\zeta,v) \, e^{-F_i(\zeta)/\varepsilon} \, \big(\, \chi_{i,s,\varepsilon}^{(0)}(\zeta+\varepsilon v) - \chi_{i,s,\varepsilon}^{(0)}(\zeta) \, \big) \;\; \Lambda_\varepsilon(d\zeta) \otimes \mu(dv) \;\; .$$

Here $(A_{i,k})_{k\in\mathbb{N}_0}$ is an ε-independent sequence of functions in $C^\infty(M;\mathbb{R}^{V,\mu})$ having compact support, with

$$A_{i,0}(\zeta,v) \ := \ \chi_i^{(1)}(\zeta)\ e^{-\frac{1}{2}[\nabla_v f(\zeta)-\nabla_v\varphi(\zeta)]}\ \hat{a}_{i,0}(\zeta,v) \tag{15.9}$$

and

$$F_i(\zeta) \ := \ f(\zeta)-f(\zeta_i^{(1)})+\varphi_i^{(1)}(\zeta) \quad .$$

For the sake of clarity, we stress that (15.8) actually means that there exists for $\varepsilon>0$ and every $N\in\mathbb{N}_0$ an $A_{i,\varepsilon}^{(N+1)}\in C^\infty(M;\mathbb{R}^{V,\mu})$ with compact support such that $A_{i,\varepsilon}^{(N+1)}=\mathcal{O}(1)$ and

$$\tilde{I}_{i,s,\varepsilon} \ = \ \sum_{k=0}^{N}\varepsilon^k \ \ J_{i,s,k,\varepsilon} \ + \ \varepsilon^{N+1} \ \ J_{i,s,\varepsilon}^{(N+1)} \quad ,$$

with

$$J_{i,s,\varepsilon}^{(N+1)} \ := \ \int_{M\times V} A_{i,\varepsilon}^{(N+1)}(\zeta,v)\, e^{-F_i(\zeta)/\varepsilon}\,\big(\,\chi_{i,s,\varepsilon}^{(0)}(\zeta+\varepsilon v)-\chi_{i,s,\varepsilon}^{(0)}(\zeta)\,\big)\ \Lambda_\varepsilon(d\zeta)\otimes\mu(dv) \ .$$

Observe that by definition of $\chi_i^{(1)}$ and $\chi_{i,s,\varepsilon}^{(0)}$ (see Def.14.1 and 14.4) there exists an $R>0$ such that for every $k\in\mathbb{N}_0$

$$\text{supp}\ \langle A_{i,k}\ ,\ \Psi_\varepsilon\tau_*\ \delta\ \chi_{i,s,\varepsilon}^{(0)}\rangle_\mu \ \subset \ Q_{i,2\varepsilon^s,R} \tag{15.10}$$

and

$$\chi_{i,s,\varepsilon}^{(0)}(\zeta+\varepsilon v)-\chi_{i,s,\varepsilon}^{(0)}(\zeta)\ \Big|_{Q_{i,2\varepsilon^s,R}} \ = \ \theta\Big(\frac{y^{(i)}(\zeta)+\varepsilon e_1^*(v)}{\varepsilon^s}\Big)-\theta\Big(\frac{y^{(i)}(\zeta)}{\varepsilon^s}\Big) \quad ,$$

where $\theta\in C^\infty(\mathbb{R};\mathbb{R})$ satisfies

$$\theta(t)=\begin{cases}1 & \text{if } t\geq 1\\ 0 & \text{if } t\leq -1\end{cases} \quad . \tag{15.11}$$

Step 2

Consider the coordinates x adapted to the lattice and write $J_{i,s,k,\varepsilon}$ as

$$J_{i,s,k,\varepsilon} \ = \ \sum_{x\in\sqrt{\varepsilon}\mathbb{Z}^n} B_{i,s,k,\varepsilon}(x)\ e^{-F_{i,\varepsilon}(x)} \quad ,$$

where

$$B_{i,s,k,\varepsilon}(x) \ := \ \int_V A_{i,k}(\sqrt{\varepsilon}x,v)\ \big(\ \chi_{i,s,\varepsilon}^{(0)}(\sqrt{\varepsilon}x+\varepsilon v)-\chi_{i,s,\varepsilon}^{(0)}(\sqrt{\varepsilon}x)\ \big)\ \ \mu(dv)$$

and

$$F_{i,\varepsilon}(x) \ := \ \varepsilon^{-1} \ F_i(\sqrt{\varepsilon} x)$$

(with standard abuse of notation we do not distinguish between a function on M and the corresponding function on coordinate space).

In terms of $h := \sqrt{\varepsilon}$ we are thus reduced to computing

$$J_{i,s,k,h^2} \ = \ \sum_{x \in h\mathbb{Z}^n} G_{i,s,k,h}(x) \quad ,$$

where

$$G_{i,s,k,h}(x) \ := \ B_{i,s,k,h^2}(x) \ e^{-F_{i,h^2}(x)} \quad .$$

In view of applying Proposition C.1 to $G_{i,s,k,h}$, we check that for every multiindex α there exists an h-independent constant $C_\alpha > 0$ such that for $h > 0$

$$\int_{\mathbb{R}^n} |\partial^\alpha G_{i,s,k,h}(x)| \ dx \ \leq \ C^\alpha \quad , \tag{15.12}$$

where ∂^α denotes derivation with respect to x. Indeed, note that $|\partial^\alpha G_{i,s,k,h}(x)|$ can be expressed as a sum of terms of the type

$$|\partial^{\alpha'} B_{i,s,k,h^2}|^{k'} \ |\partial^{\alpha''} F_{i,h}|^{k''} \ e^{-F_{i,h}} \tag{15.13}$$

and that (recall Def. 13.6 for the coordinates $(y,z) = (y^{(i)}, z^{(i)})$ and (15.10))

$$\operatorname{supp} B_{i,s,k,h^2} \ \subset \ \Big\{ \ h|y| \leq 2h^{2s-1} \ \text{ and } \ \|hz\|_{\kappa^{(i)}} \leq R \ \Big\} \ \subset \ \Big\{ \ |y| \leq 2 \ \text{ and } \ \|hz\|_{\kappa^{(i)}} \leq R \ \Big\} \quad .$$

Due to Def. 14.4, R can be taken small enough such that for some $\gamma > 0$

$$F_{i,h}(y,z) \ \geq \ -\gamma|y|^2 + \gamma\|z\|^2_{\kappa^{(i)}} \ \text{ if } \ |hy|, \|hz\|_{\kappa^{(i)}} \leq R \quad . \tag{15.14}$$

In particular, for h sufficiently small, the estimate(15.14) holds on supp B_{i,s,k,h^2}.

Moreover for every multiindex α there exists a constant $C_\alpha > 0$ (independent on h, s and x) such that

a)

$$|\partial^\alpha B_{i,s,k,h}(x)| \leq C_\alpha \quad \text{for} \ \ h > 0 \ \text{ and every } \ x \in \mathbb{R}^n \quad .$$

b) denoting by $B_1(0)$ the unit ball centered at the origin

$$|\partial^\alpha F_{i,h}(x)| \leq C_\alpha \quad \text{for} \ \ h > 0 \ \text{ and every } x \in B_1(0)$$

and

$$|\partial^\alpha F_{i,h}(x)| \leq C_\alpha |x|^2 \quad \text{for} \ \ h > 0 \ \text{ and every } x \in B_1^c(0) \cap B_{C/h}(0)$$

for every $C > 0$. The estimate $a)$ follows from the estimates (14.2).

The estimates in $b)$ can be easily obtained from the Taylor expansion

$$\partial^\alpha F_{i,h}(x) \;=\; h^{|\alpha|-2}\partial^\alpha F_{i,h}(hx) \;=$$

$$= \; h^{|\alpha|-2}\partial^\alpha F_{i,h}(0) \;+\; h^{|\alpha|-1}\langle \nabla\partial^\alpha F_{i,h}(0), x\rangle \;+\; h^{|\alpha|}\int_0^1 \frac{(1-t)^2}{2}\langle \mathrm{Hess}\,\partial^\alpha F_{i,h}(htx)x, x\rangle\; dt$$

using, in the cases $|\alpha| = 0, 1$, that $F_{i,h}(0) = \nabla F_{i,h}(0) = 0$.

Using (15.13), (15.14) and the estimates a),b) above (in fact from b) we need only the case $|\alpha| > 0$) we can conclude that for $h > 0$, $s \in [\frac{1}{2}, 1)$ and every multiindex α there exist $k' \in \mathbb{N}_0$ and $\gamma > 0$ such that

$$\int_{\mathbb{R}^n} |\partial^\alpha G_{i,s,k,h}\;(x)|\; dx \;= \int_{\mathrm{supp}\, B_{i,s,k,h}} |\partial^\alpha G_{i,s,k,h}\;(x)|\; dx \;\leq$$

$$\leq\; \mathrm{Const}\; \int_{B_1(0)} dx \;+\; \mathrm{Const}\; \int_{\mathbb{R}^{n-1}} \|z\|^{k'}\; e^{-\gamma\|z\|^2}\; dz \;\leq\; \mathrm{Const} \quad .$$

Having checked (15.12), it follows from Proposition C.1 that

$$J_{i,s,k,h^2} \;=\; h^{-n}\int_{\mathbb{R}^n} G_{i,s,k,h}(x)\; dx \quad +\; \mathcal{O}(h^\infty) \quad . \tag{15.15}$$

Step 3

We compute now the integral $\int_{\mathbb{R}^n} G_{i,s,k,h}(x)\; dx$: first note that

$$\int_{\mathbb{R}^n} G_{i,s,k,h}(x)\, dx \;=\; \int_{\mathbb{R}^n} G_{i,s,k,h}(y,z)\, dy\, dz \;=\; h^{2s-1}\; h^{-(n-1)} \int_{\mathbb{R}^n} G_{i,s,k,h}(h^{2s-1}y, \frac{z}{h})\, dy\, dz \quad . \tag{15.16}$$

Moreover

$$G_{i,s,k,h}(h^{2s-1}y, \frac{z}{h}) \;=\; B_{i,s,k,h^2}(h^{2s-1}y, \frac{z}{h})\;\; e^{-F_i(h^{2s}y,z)/h^2} \;=$$

$$=\; \langle A_{i,k}\;,\; \Psi_{h^2\tau_*}\;\delta\; \chi^{(0)}_{i,s,h^2}\rangle_\mu\; (h^{2s}y, z)\;\; e^{-F_i(h^{2s}y,z)/h^2} \quad .$$

In particular, by (15.10), the last integral in (15.16) can be restricted to the set $\mathcal{Q}_{i,2,R} := \big\{\; (y,z) \in \mathbb{R}\times\mathbb{R}^{n-1} :\; |y| \leq 2 \;\text{ and }\; \|z\|_{\kappa^{(i)}} \leq R\;\big\}$. On the latter we have

$$\Psi_{h^2\tau_*}\;\delta\;\chi^{(0)}_{i,s,h^2}\;(h^{2s}y, z) \;=\; \theta(y + h^{2(1-s)}\mathfrak{e}^*_1) - \theta(y) \quad .$$

A Taylor expansion at $y = 0$ for every fixed z of the function $y \mapsto A_{i,k}(h^{2s}y, z)$ and a Taylor expansion at every y for every fixed $v \in V$ of the function $y \mapsto \theta(y + h^{2(1-s)}\mathfrak{e}_1^*(v)) - \theta(y)$ gives

$$\int_{\mathbb{R}^n} G_{i,s,k,h}(x)\ dx \ \sim\ h^{2s-1}\ h^{-(n-1)} \sum_{k_1=0}^{\infty} \sum_{k_2=1}^{\infty} h^{2sk_1+2(1-s)k_2} \ \times$$

$$\times\ \frac{1}{k_1!k_2!} \int_{\mathcal{Q}_{i,2,R}} \theta^{(k_2)}(y)\ y^{k_1}\ \ \langle A_{i,k}^{(k_1)}(0,z)\ ,\ \mathfrak{e}_1^* \rangle_\mu\ \ e^{-F_i(h^{2s}y,z)/h^2}\ dydz \quad . \tag{15.17}$$

A change in the summation index in (15.17) gives

$$\int_{\mathbb{R}^n} G_{i,s,k,h}(x)\ dx \ \sim\ h\ h^{-(n-1)} \sum_{k_1,k_2=0}^{\infty} h^{2sk_1+2(1-s)k_2} \ \times$$

$$\times\ \frac{1}{k_1!(k_2+1)!} \int_{\mathcal{Q}_{i,2,R}} \theta^{(k_2+1)}(y)\ y^{k_1}\ \ \langle A_{i,k}^{(k_1)}(0,z)\ ,\ \mathfrak{e}_1^* \rangle_\mu\ \ e^{-F_i(h^{2s}y,z)/h^2}\ dydz \quad . \tag{15.18}$$

For the exponential term $e^{-F_i(h^{2s}y,z)/h^2}$ we write

$$e^{-F_i(h^{2s}y,z)/h^2} \ =\ e^{-F_i(0,z)/h^2}\ e^{-h^{2s-2}F_i^{(1)}(0,z)y}\ e^{-h^{4s-2}F_i^{(2)}(0,z)y^2}\ R_h(y,z) \quad , \tag{15.19}$$

with $R_h \in C^\infty(\mathbb{R}^n, \mathbb{R})$ given by

$$\log R_h(y,z) \ :=\ -h^{-2}F_i(h^{2s}y,z) + h^{2s-2}F_i^{(1)}(0,z)y + h^{4s-2}F_i^{(2)}(0,z)y^2 \quad .$$

Expanding the second and third exponential on the right hand side of (15.19) and using that for some sequence $(L_{i,k_5,k_6})_{k_5,k_6\in\mathbb{N}_0}$ in $C^\infty(\mathbb{R}^n;\mathbb{R})$ with $L_{i,0,0} = 1$ and $L_{i,0,k_6} = 0$ for $k_6 \geq 1$

$$R_h \ \sim \sum_{k_5,k_6=0}^{\infty} h^{2[sk_5+(2s-1)k_6]}\ \ L_{i,k_5,k_6} \quad ,$$

we get from (15.18)

$$h^{-1}\ h^{(n-1)} \int_{\mathbb{R}^n} G_{i,s,k,h}(x)\ dx \ \sim \tag{15.20}$$

$$\sim \sum_{\mathbf{k}\in\mathbb{N}_0^6} h^{2[sk_1+(1-s)k_2+k_3(s-1)+k_4(2s-1)+sk_5+k_6(2s-1)}\ \frac{(-1)^{k_3+k_4}}{k_1!(k_2+1)!k_3!k_4!} \int_{Q_{i,2,R}} \theta^{(k_2+1)}(y) \ \times$$

$$\times\ y^{k_1+k_3+k_4}\ L_{i,k_5,k_6}(y,z)\ [F_i^{(1)}(0,z)]^{k_3}\ [F_i^{(2)}(0,z)]^{k_4}\ \langle A_{i,k}^{(k_1)}(0,z)\ ,\ \mathfrak{e}_1^* \rangle_\mu\ \ e^{-F_i(0,z)/h^2}\ dydz \quad .$$

For the integral in z we use the classical Laplace asymptotic in dimension $n-1$. For this puropose note that both $z \mapsto F_i^{(1)}(0,z)$ and its first differential vanish at $z=0$, and also $F_i^{(2)}(0,0)=0$, implying that for fixed y

$$z \mapsto \tilde{A}_{i,k,k_1,k_3,k_4,k_5,k_6}(y,z) \ := $$
$$= \ L_{i,k_5,k_6}(y,z) \ [F_i^{(1)}(0,z)]^{k_3} \ [F_i^{(2)}(0,z)]^{k_4} \ \langle A_{i,k}^{(k_1)}(0,z) \ , \ \mathfrak{e}_1^* \rangle_\mu$$

vanishes up to order $2k_3 + k_4 - 1$ in z. The Laplace asymptotics gives therefore

$$h^{-(n-1)} \int_{\|z\|_{\kappa(i)} \le R} \tilde{A}_{i,k,k_1,k_3,k_4,k_5,k_6}(\cdot,z) \ \ e^{-F_i(0,z)/h^2} \ dydz \ \sim \tag{15.21}$$

$$\sim \sum_{k_7=k_3+k_4^*/2}^{\infty} h^{2k_7} \ \ C_{i,k,k_1,k_3,k_4,k_5,k_6,k_7} = \sum_{k_7=0}^{\infty} h^{2[k_7+k_3+k^*4/2]} \ \ C_{i,k,k_1,k_3,k_4,k_5,k_6,k_7+k_3+k_4^*/2} \ \ ,$$

where $k_4^* = k_4$ if k_4 is even and $k_4^* = k_4+1$ if k_4 is odd, and with $C_{i,k_1,k_3,k_4,k_5,k_6,k_7} \in C^\infty(\mathbb{R};\mathbb{R})$.

Putting together (15.20) and (15.21) gives

$$\int_{\mathbb{R}^n} G_{i,s,k,h}(x)dx \ \sim \tag{15.22}$$

$$h \sum_{\mathbf{k}\in\mathbb{N}_0^7} h^{2 \ [\ k_4^*/2+k_7 \ + \ s(k_1+k_3+k_5) \ + \ (1-s) \ k_2 \ + \ (2s-1) \ (k_4+k_6) \ ]} \ \ D_{i,k,\mathbf{k}} \ \ ,$$

with $D_{i,k,\mathbf{k}} \in \mathbb{R}$.

Finally, (15.8) of Step 1 and (15.15) of Step 2, together with (15.22) give by suitably rearranging summation indices

$$\tilde{I}_{i,s,\varepsilon} \ \sim \ \varepsilon^{-n/2} \sqrt{\varepsilon} \sum_{\mathbf{k}\in\mathbb{N}_0^4} \varepsilon^{[\ k_1 \ + \ sk_2 \ + \ (1-s)k_3 \ + \ (2s-1)k_4 \ ]} \ \ K_{i,\mathbf{k}} \ \ ,$$

with $K_{i,\mathbf{k}} \in \mathbb{R}$ having the property that for every $k_3 \in \mathbb{N}_0$ and $k_4 \in \mathbb{N}_*$

$$K_{i,0,0,k_3,k_4} \ = \ 0 \ \ .$$

On the other hand, for the normalization constants we have the expansions (see Remark 14.7)

$$Z_{i,\varepsilon}^{(0)} \ \sim \ \varepsilon^{n/4} \sum_{k=\infty}^{\infty} \varepsilon^k \ \ \hat{Z}_{i,k}^{(0)}$$

and

$$Z_{i,\varepsilon}^{(1)} \ \sim \ \varepsilon^{n/4} \sum_{k=0}^{\infty} \varepsilon^k \ \ \hat{Z}_{i,k}^{(1)} \ \ ,$$

with $(\hat{Z}^{(0)}_{i,k})_{k\in\mathbb{N}_0}$, $(\hat{Z}^{(1)}_{i,k})_{k\in\mathbb{N}_0}$ sequences in $\mathbb{R}$.

Recalling (15.5) and (15.7) this concludes the proof of the expansion of $\langle \psi^{(1)}_{i,\varepsilon}, \delta_{\rho_\varepsilon}\ \psi^{(0)}_{i,s,\varepsilon}\rangle_{\Lambda_{\mu_\varepsilon}}$ in the strong form stated in Remark 15.2.

In order to show the explicit formula (15.2) for the leading term of the prefactor, note that

$$\hat{Z}^{(0)}_{i,0} \ = \ \frac{\big(\det \mathrm{Hess}_\mu f(\zeta^{(0)}_i)\big)^{\frac{1}{4}}}{\pi^{\frac{n}{4}}} \quad \text{and} \quad \hat{Z}^{(1)}_{i,0} \ = \ \frac{|\det \mathrm{Hess}_\mu f(\zeta^{(1)}_i)|^{\frac{1}{4}}}{\pi^{\frac{n}{4}}} \quad .$$

Moreover

$$\int_{\mathbb{R}^n} G_{i,s,0,h}(x)\ dx \ =$$

$$= \ h\ h^{-(n-1)} \int_{\mathcal{Q}_{i,2,R}} \theta^{(1)}(y)\ \langle A_{i,0}(0,z), \mathfrak{e}^*_1\rangle_\mu \quad e^{-F_i(0,z)/h^2}\ dydz \quad \Big(\ 1 + \mathcal{O}(h^{2(1-s)})\ \Big) \ =$$

$$= \ h\ \langle A_{i,0}(0,0), \mathfrak{e}^*_1\rangle_\mu\ \frac{\pi^{\frac{n-1}{2}}}{\sqrt{\prod_{j=2}^n \kappa^{(i)}_j}}\ \int_{-2}^{2} \theta^{(1)}(y)dy \quad \Big(\ 1 + \mathcal{O}(h^{2(1-s)})\ \Big) \ =$$

$$= \quad h\ \frac{\pi^{\frac{n-1}{2}}}{\sqrt{\prod_{j=2}^n \kappa^{(i)}_j}} \quad \Big(\ 1 + \mathcal{O}(h^{2(1-s)})\ \Big) \quad .$$

For the last equality we used that $A_{i,0}(0,0) = \hat{a}_{i,0}(0)$ by (15.9), that $\hat{a}_{i,0}(0) = \mathfrak{e}^*_1$ by (iii) in Theorem 11.1, and that $\int_{-2}^{2}\theta^{(1)}(y)dy = \theta(2) - \theta(-2) = 1$ by (15.11). $\square$

16. Comparison between exact and approximate small eigenvalues

In this section we establish the following theorem, which gives a sharp asymptotic relation between the approximate eigenvalues defined in (14.7) and the actual small eigenvalues $\nu_{2,\varepsilon}, \ldots, \nu_{m_0,\varepsilon}$ of $\mathcal{H}^{(0)}_{\Lambda_{\rho_\varepsilon,\mu_\varepsilon}}$. Recall that we already know that $\nu_{1,\varepsilon} = 0$.

Theorem 16.1. *For $i = 2, \ldots, m_0$*

$$\nu_{i,\varepsilon} \;=\; \nu^{\mathrm{app}}_{i,s,\varepsilon} \quad \big(\, 1 + \mathcal{O}(\varepsilon^\infty) \;\big) \quad .$$

Proof. This follows (after suitable relabelling of indices) immediately from Remark 10.5, Theorem D.1 in the appendix and Proposition 16.2 below. □

In the sequel we use the short notation $b_i := f(\zeta_i^{(1)}) - f(\zeta_i^{(0)})$ for $i = 2, \ldots, m_0$. Moreover we set for $i = 1, \ldots, m_0$ and $s \in [\frac{1}{2}, 1)$

$$u_{i,s,\varepsilon} \;:=\; 1_{[0,\varepsilon^{6/5})}(\mathcal{H}^{(0)}_{\Lambda_{\rho_\varepsilon,\mu_\varepsilon}})\; \psi^{(0)}_{i,s,\varepsilon}$$

and for $i = 2, \ldots, m_1 + 1$

$$\alpha_{i,\varepsilon} \;:=\; 1_{[0,\varepsilon^{6/5})}(\mathcal{H}^{(1)}_{\Lambda_{\rho_\varepsilon,\mu_\varepsilon}})\; \psi^{(1)}_{i,\varepsilon} \quad .$$

Proposition 16.2. *Fix $s \in [\frac{1}{2}, 1)$. Then*

(i) *for $i, j = 1, \ldots, m_0$*

$$\langle u_{i,s,\varepsilon}, u_{j,s,\varepsilon}\rangle_{\Lambda_{\mu_\varepsilon}} \;=\; 1_{i,j} \;+\; \mathcal{O}(\varepsilon^\infty)$$

and for $i, j = 2, \ldots, m_1 + 1$

$$\langle \alpha_{i,\varepsilon}, \alpha_{j,\varepsilon}\rangle_{\Lambda_{\mu_\varepsilon}} \;=\; 1_{i,j} \;+\; \mathcal{O}(\varepsilon^\infty) \quad .$$

(ii) *for $i = 2, \ldots, m_0$ we have*

a) *for $\varepsilon > 0$ sufficiently small*

$$\varepsilon^2\, e^{-b_i/\varepsilon} \;\le\; |\langle \alpha_{i,\varepsilon}, \delta_{\rho_\varepsilon}\; u_{i,s,\varepsilon}\rangle_{\Lambda_{\mu_\varepsilon}}| \;\le\; \varepsilon^{-2}\, e^{-b_i/\varepsilon} \quad .$$

b) *for $j = 2, \cdots, m_1 + 1$ with $j \ne i$*

$$|\langle \alpha_{j,\varepsilon}, \delta_{\rho_\varepsilon}\; u_{i,s,\varepsilon}\rangle_{\Lambda_{\mu_\varepsilon}}| \;\le\; \mathcal{O}(\varepsilon^\infty)\; e^{-b_i/\varepsilon} \quad .$$

(iii) $\delta_{\rho_\varepsilon}\ u_{1,s,\varepsilon} = 0$ *and for* $i = 2, \ldots, m_0$

$$|\langle \alpha_{i,\varepsilon}, \delta_{\rho_\varepsilon}\ u_{i,s,\varepsilon}\rangle_{\Lambda_{\mu_\varepsilon}}|^2 \ = \ \nu^{\text{app}}_{i,s,\varepsilon} \ \Big(\ 1 + \mathcal{O}(\varepsilon^\infty) \ \Big) \quad .$$

In the proof of Proposition 16.2 the following Markov-type inequality is used repeatedly.

Lemma 16.3. *Let T be a selfadjoint nonnegative operator on a Hilbert space H with domain D. Then for every $u \in D$ and every $b > 0$*

$$\|1_{[b,\infty)}(T)u\|^2 \leq \frac{\langle Tu, u\rangle}{b} \quad .$$

Proof. As a consequence of the spectral theorem,

$$\begin{aligned} \|1_{[b,\infty)}(T)u\|^2 \ &= \ \langle 1_{[b,\infty)}(T)u, 1_{[b,\infty)}(T)u\rangle \ = \ \langle 1_{[b,\infty)}(T)u, u\rangle \ = \\ = \ \int_b^\infty d\langle 1_\lambda(T)u, u\rangle \ &\leq \ \int_b^\infty \frac{\lambda}{b}\ d\langle 1_\lambda(T)u, u\rangle \ \leq \ \int_0^\infty \frac{\lambda}{b}\ d\langle 1_\lambda(T)u, u\rangle \ = \\ &= \ \frac{\langle Tu, u\rangle}{b} \quad . \end{aligned}$$

□

Proof of Proposition16.2. Statement (i) follows easily from Propositions 14.9 and 14.11 and Lemma 16.3. Indeed, for the $u_{i,s,\varepsilon}$'s we have

$$\begin{aligned} \langle u_{i,s,\varepsilon}, u_{j,s,\varepsilon}\rangle_{\Lambda_{\mu_\varepsilon}} \ = \ \langle \psi^{(0)}_{i,s,\varepsilon}, \psi^{(0)}_{j,s,\varepsilon}\rangle_{\Lambda_{\mu_\varepsilon}} \ + \ \langle u_{i,s,\varepsilon} - \psi^{(0)}_{i,s,\varepsilon}, u_{j,s,\varepsilon} - \psi^{(0)}_{j,s,\varepsilon}\rangle_{\Lambda_{\mu_\varepsilon}} \ + \\ + \ \langle u_{i,s,\varepsilon} - \psi^{(0)}_{i,s,\varepsilon}, \psi^{(0)}_{j,s,\varepsilon}\rangle_{\Lambda_{\mu_\varepsilon}} \ + \ \langle \psi^{(0)}_{i,s,\varepsilon}, u_{j,s,\varepsilon} - \psi^{(0)}_{j,s,\varepsilon}\rangle_{\Lambda_{\mu_\varepsilon}} \quad . \end{aligned}$$

Note that by definition $u_{i,s,\varepsilon} - \psi^{(0)}_{i,s,\varepsilon} = 1_{[\varepsilon^{6/5},\infty)}(\mathcal{H}^{(0)}_{\Lambda_{\rho_\varepsilon,\mu_\varepsilon}})\ \psi^{(0)}_{i,s,\varepsilon}$, so by Lemma 16.3 and Proposition 14.9 (ii), we get for some $\gamma > 0$

$$\|u_{i,s,\varepsilon} - \psi^{(0)}_{i,s,\varepsilon}\| \ \leq e^{-\gamma/\varepsilon} \quad .$$

Together with Proposition 14.9 (i) we can conclude that the $u_{i,s,\varepsilon}$'s are orthonormal up to an additive error which is even exponentially small in ε. The case of the $\alpha_{i,\varepsilon}$'s is analogous, but note that here Proposition 14.11 permits only to get an $\mathcal{O}(\varepsilon^\infty)$ error in the end.

Proof of (ii): for $j = 2, \ldots, m_1 + 1$ and $i = 2, \ldots, m_0$ we have

$$\langle \alpha_{j,\varepsilon}, \delta_{\rho_\varepsilon}\ u_{i,s,\varepsilon} \rangle_{\Lambda_{\mu_\varepsilon}} \ =\ \langle \alpha_{j,\varepsilon}, \delta_{\rho_\varepsilon}\ 1_{[\varepsilon^{6/5},\infty)}(\mathcal{H}^{(0)}_{\Lambda_{\rho_\varepsilon,\mu_\varepsilon}})\ \psi^{(0)}_{i,s,\varepsilon} \rangle_{\Lambda_{\mu_\varepsilon}} \ =$$
$$=\ \langle \alpha_{j,\varepsilon}, 1_{[\varepsilon^{6/5},\infty)}(\mathcal{H}^{(1)}_{\Lambda_{\rho_\varepsilon,\mu_\varepsilon}})\ \delta_{\rho_\varepsilon}\ \psi^{(0)}_{i,s,\varepsilon} \rangle_{\Lambda_{\mu_\varepsilon}} \ =\ \langle \alpha_{j,\varepsilon}, \delta_{\rho_\varepsilon}\ \psi^{(0)}_{i,s,\varepsilon} \rangle_{\Lambda_{\mu_\varepsilon}} \quad ,$$

where in the second equality we used the intertwining property, given in Proposition 8.4, and in the last equality we used that $1_{[\varepsilon^{6/5},\infty)}(\mathcal{H}^{(1)}_{\Lambda_{\rho_\varepsilon,\mu_\varepsilon}})$ is selfadjoint and equal to its square.

It follows that

$$\langle \alpha_{j,\varepsilon}, \delta_{\rho_\varepsilon}\ u_{i,s,\varepsilon} \rangle_{\Lambda_{\mu_\varepsilon}} \ =\ \langle \psi^{(1)}_{i,\varepsilon}, \delta_{\rho_\varepsilon}\ \psi^{(0)}_{i,s,\varepsilon} \rangle_{\Lambda_{\mu_\varepsilon}} \ +\ \langle \alpha_{i,\varepsilon} - \psi^{(1)}_{i,\varepsilon}, \delta_{\rho_\varepsilon}\ \psi^{(0)}_{i,s,\varepsilon} \rangle_{\Lambda_{\mu_\varepsilon}} \quad . \tag{16.1}$$

Now observe that by Propostion 15.1,

$$\varepsilon\ e^{-b_i/\varepsilon}\ \leq\ |\langle \psi^{(1)}_{j,\varepsilon}, \delta_{\rho_\varepsilon}\ \psi^{(0)}_{i,s,\varepsilon} \rangle_{\Lambda_{\mu_\varepsilon}}|\ \leq\ \varepsilon^{-1}\ e^{-b_i/\varepsilon} \tag{16.2}$$

if $j = i$ and

$$\langle \psi^{(1)}_{j,\varepsilon}, \delta_{\rho_\varepsilon}\ \psi^{(0)}_{i,s,\varepsilon} \rangle_{\Lambda_{\mu_\varepsilon}} \ =\ 0$$

if $j \neq i$.

Moreover, in both cases, by Proposition 14.11 (ii), Lemma16.3 and Proposition 14.9

$$\langle \alpha_{j,\varepsilon} - \psi^{(1)}_{j,\varepsilon}, \delta_{\rho_\varepsilon}\ \psi^{(0)}_{i,s,\varepsilon} \rangle_{\Lambda_{\mu_\varepsilon}} \ = \mathcal{O}(\varepsilon^\infty)\ e^{-b_i/\varepsilon} \quad . \tag{16.3}$$

Statement (iii) follows from Remark 14.8 in the case $i = 1$. For $i > 1$ it is a consequence of (16.1), (16.2), (16.3), recalling that by definition

$$\nu^{\mathrm{app}}_{i,s,\varepsilon} \ =\ |\langle \psi^{(1)}_{j,\varepsilon}, \delta_{\rho_\varepsilon}\ \psi^{(0)}_{i,s,\varepsilon} \rangle_{\Lambda_{\mu_\varepsilon}}|^2 \quad .$$

□

Combining the results of Section 15 and Section 16 leads now easily to complete expansions of the first m_0 eigenvalues of $\mathcal{H}^{(0)}_{\Lambda_{\rho_\varepsilon,\mu_\varepsilon}}$, denoted by

$$\nu_{1,\varepsilon} \leq \ \ldots \ \leq \ \nu_{m_0,\varepsilon} \quad .$$

Recall that we work under Assumptions III.1 and III.2, implying in particular that $\nu_{1,\varepsilon} = 0$. Recall also that $\kappa^{(i)}_{f,\mu,1}$ denotes for each $i = 1, \ldots, m_0$ the negative eigenvalue of $\mathrm{Hess}_\mu f(\zeta_i^{(1)})$.

Theorem 17.1. *For each $i = 2, \ldots, m_0$ there exists a sequence $(P_{i,k})_{k\in\mathbb{N}_0}$ in $\mathbb{R}$ with*

$$P_{i,0} \ = \ \frac{|\kappa^{(i)}_{f,\mu,1}|}{\pi} \ \frac{\left[\det \mathrm{Hess}_{mu} f(\zeta_i^{(0)})\right]^{\frac{1}{2}}}{|\det \mathrm{Hess}_\mu f(\zeta_i^{(1)})|^{\frac{1}{2}}}$$

such that

$$\nu_{i,\varepsilon} \ \sim \ \ \varepsilon \ e^{-\frac{2[f(\zeta_i^{(1)})-f(\zeta_i^{(0)})]}{\varepsilon}} \quad \sum_{k=0}^{\infty} \varepsilon^k \quad P_{i,k} \quad .$$

Proof. By Theorem 16.1 we have for every $s \in [\frac{1}{2}, 1)$

$$\nu_{i,\varepsilon} \ = \ \nu^{\mathrm{app}}_{i,s,\varepsilon} \quad \left(\ 1 + \mathcal{O}(\varepsilon^\infty) \ \right) \quad .$$

Taking in particular $s_1 = \frac{1}{2}$ and $s_2 = \frac{\sqrt{2}}{2}$, it follows from Proposition 15.1 and Remark 15.1 that for $l = 1, 2$ there exist sequences $(P^{(s_l)}_{i,\mathbf{k}})_{k\in\mathbb{N}_4}$ in $\mathbb{R}$ with $P^{(s_l)}_{i,0} = 0$ such that

$$\sqrt{\nu_{i,\varepsilon}} \ \sim$$

$$\sim \quad \sqrt{\varepsilon \ P_{i,0}} \ e^{-\frac{f(\zeta_i^{(1)})-f(\zeta_i^{(0)}}{\varepsilon}} \quad \Bigg(\ 1 + \sum_{\mathbf{k}=(k_1,\ldots,k_4)\in\mathbb{N}_0^4} \varepsilon^{k_1+s_lk_2+(1-s_l)k_3+(2s_l-1)k_4} \quad P^{(s_l)}_{i,k} \ \Bigg) \quad .$$

It follows that for $l = 1, 2$ it can be $P^{(s_l)}_{i,(k_1,k_2,k_3,k_4)} \neq 0$ only if $k_2 = k_3 = k_4 = 0$. $\square$

Part IV. Appendix

Appendix A. Singular transport equations

Let $\Omega \subset \mathbb{R}^n$ be an open neighbourhood of 0 and H a Hilbert space with scalar product $\langle \cdot, \cdot \rangle_H$. We denote in the sequel by $C^\infty(\Omega; H)$ (resp. $C^\infty(\Omega; \mathscr{B}(H))$) the space of smooth functions defined on Ω with values in H (resp. with values in $\mathscr{B}(H)$, the space of bounded linear operators on H). Moreover, for $j = 1, \ldots, n$, we use $\frac{\partial}{\partial x_j}$ to denote the j-th partial derivative acting on smooth functions on Ω.

Consider for an unknown $\alpha \in C^\infty(\Omega; H)$ the problem:

$$\begin{cases} \mathcal{T}\alpha\ (x) = q(x) & \text{for every } x \in \Omega \\ \alpha(0) = \omega \end{cases} \quad . \tag{A.1}$$

Here $q \in C^\infty(\Omega; H)$ (the "inhomogeneity"), $\omega \in H$ (the "initial value") and $\mathcal{T} : C^\infty(\Omega; H) \to C^\infty(\Omega; H)$ is a linear first order differential operator (the "transport operator") of the form

$$\mathcal{T}\alpha\ (x) := \sum_{j=1}^{n} \mathcal{V}_j(x) \frac{\partial}{\partial x_j} \alpha\ (x) + A(x)\alpha(x) \quad ,$$

with the $\mathcal{V}_j$'s in $C^\infty(\Omega; \mathbb{R})$ and $A \in C^\infty(\Omega; \mathscr{B}(H))$. Moreover we assume throughout that

(1) $\mathcal{V}_j(0) = 0$ for every $j = 1, \ldots, n$ and the matrix $\left(\frac{\partial \mathcal{V}_j}{\partial x_l}(0) \right)_{l,j}$ is diagonal with strictly positive eigenvalues.
(2) $A(0)$ is nonnegative, i.e. $A(0)$ is selfadjoint and $\langle A(0)u, u \rangle_H \geq 0$ for every $u \in H$.

Oberve that if a solution α of (A.1) exists under the above assumptions then necessarily

$$A(0)\omega = q(0) \quad . \tag{A.2}$$

In fact this compatibility condition is also sufficient for local existence as stated in the following theorem. In the case $H = \mathbb{R}$ this is a classical result which is proved for example in [27] or [40]. The higher-dimensional result requires only minor modifications to the proof and is used for example (with $H = \mathbb{R}^n$) in [48]. For the sake of the reader we give here a complete proof in the general case adapting the one of [27].

Theorem A.1.

If the compatibility condition (A.2) *holds and* Ω *is sufficiently small, there exists a unique* $\alpha \in C^\infty(\Omega; H)$ *solving the problem* (A.1)*. Moreover the restriction on* Ω *is independent of the inhomogenity.*

Proof. The idea is to solve the equation first in the sense of formal power series (see Step 1 and 2 below). Here one works only with the principal part $\mathcal{T}_0$ of $\mathcal{T}$ (obtained by linearizing $\mathcal{V}$ and taking just $A(0)$ as 0-th order term), and regards the difference $\mathcal{T} - \mathcal{T}_0$ as an additional inhomogeneity. Then (Step 3) the equation is solved by the method of characteristics in the space of functions vanishing at infinite order in 0. The final result is then easily achieved through a Borel summation (Step 4).

Step 1

By assumption on the $\mathcal{V}_j$'s we have for $j = 1, \ldots, n$ and x in a sufficiently small neighbourhood of 0

$$\mathcal{V}_j(x) = \sum_m \frac{\partial \mathcal{V}_j}{\partial x_m}(0)\; x_m + \mathcal{O}(\|x\|^2) = \lambda_j x_j + \mathcal{O}(\|x\|^2) \quad ,$$

with $\lambda_j > 0$ for every $j = 1, \ldots, n$.

Let $\mathcal{T}_0 : C^\infty(\mathbb{R}^n; H) \to C^\infty(\mathbb{R}^n; H)$ be defined as

$$\mathcal{T}_0 := \mathcal{V}_{\text{lin}} + A(0) \quad ,$$

with

$$\mathcal{V}_{\text{lin}} := \sum_j \lambda_j x_j \frac{\partial}{\partial x_j} \quad .$$

We shall now consider for $r \geq 0$ the Hilbert space $\mathcal{P}^r_{\text{hom}}(\mathbb{R}^n; H)$ of homogeneous polynomials of degree r in $\mathbb{R}^n$ with values in H. A generic element $\alpha \in \mathcal{P}^r_{\text{hom}}(\mathbb{R}^n; H)$ has the form

$$\alpha(x) = \sum_{\substack{\mathbf{r}=(r_1,\ldots,r_n)\in\mathbb{N}_0^n \\ \sum r_j = r}} \alpha_{\mathbf{r}} x^{\mathbf{r}} \quad ,$$

with $\alpha_{\mathbf{r}} \in H$ for every $\mathbf{r}$ and the scalar product $\langle \cdot, \cdot \rangle_r$ in $\mathcal{P}^r_{\mathrm{hom}}(\mathbb{R}^n; H)$ is defined as

$$\langle \alpha, \beta \rangle_r := \sum_{\substack{\mathbf{r}=(r_1,\dots,r_n)\in\mathbb{N}_0^n \\ \sum r_j = r}} \langle \alpha_{\mathbf{r}}, \beta_{\mathbf{r}} \rangle_H \quad .$$

Define for every $r \geq 0$ the bounded linear operators

$$\mathcal{T}_0^{(r)}, \mathcal{V}_{\mathrm{lin}}^{(r)}, A^{(r)}(0) : \mathcal{P}^r_{\mathrm{hom}}(\mathbb{R}^n; H) \to \mathcal{P}^r_{\mathrm{hom}}(\mathbb{R}^n; H)$$

by restricting the corresponding operators to $\mathcal{P}^r_{\mathrm{hom}}(\mathbb{R}^n; H)$.

Since for every $\alpha, \beta \in \mathcal{P}^r_{\mathrm{hom}}(\mathbb{R}^n; H)$

$$\langle \mathcal{V}_{\mathrm{lin}}^{(r)} \alpha, \beta \rangle_r = \sum_{\substack{\mathbf{r}=(r_1,\dots,r_n)\in\mathbb{N}_0^n \\ \sum r_j = r}} \sum_j r_j \lambda_j \; \langle \alpha_{\mathbf{r}}, \beta_{\mathbf{r}} \rangle_H \quad ,$$

one sees that $\mathcal{V}_{\mathrm{lin}}^{(r)}$ is selfadjoint and, using also the assumption $\lambda_j > 0$ for every j, that for $r > 0$

$$\inf_{\alpha \neq 0} \frac{\langle \mathcal{V}_{\mathrm{lin}}^{(r)} \alpha, \alpha \rangle_r}{\langle \alpha, \alpha \rangle_r} > 0 \quad .$$

Since by assumption $A(0)$ is nonnegative, it follows that also

$$\inf_{\alpha \neq 0} \frac{\langle \mathcal{T}_0^{(r)} \alpha, \alpha \rangle_r}{\langle \alpha, \alpha \rangle_r} > 0 \quad ,$$

implying $0 \notin \mathrm{Spec}(\mathcal{T}_0^{(r)})$. In other words, $\mathcal{T}_0^{(r)}$ is invertible for $r > 0$.

Observe that for $r = 0$ in general we have no invertibility since $\mathcal{T}_0^{(0)} = A(0)$.

Step 2

Define $\alpha^{(0)} := \omega \in \mathcal{P}^0_{\mathrm{hom}}(\mathbb{R}^n; H)$ and then iteratively $\alpha^{(k)} \in \mathcal{P}^k_{\mathrm{hom}}(\mathbb{R}^n; H)$ for every $k \in \mathbb{N}_*$ as the unique solution of

$$\mathcal{T}_0 \; \alpha^{(k)} = Q^{(k)} \quad ,$$

where $Q^{(k)} \in \mathcal{P}^k_{\mathrm{hom}}(\mathbb{R}^n; H)$ is given by

$$Q^{(k)} := \frac{1}{k!} \nabla^k q \; (0) - \sum_{k'=0}^{k-1} \frac{1}{k!} \nabla^k [\; (\mathcal{T} - \mathcal{T}_0) \alpha^{(k')} \;] \; (0) \quad .$$

Here ∇^k denotes the k-th differential operator acting on $C^\infty(\Omega; H)$, which applied to a function and then evaluated at $0 \in \Omega$ yields an element of

$\mathcal{P}^k_{\text{hom}}(\mathbb{R}^n; H)$. The inhomogeneities $Q^{(k)}$ are chosen in such a way that for every $N \in \mathbb{N}_0$

$$\mathcal{T} \sum_{k=0}^{N} \alpha^{(k)} = \sum_{k=0}^{N} \frac{1}{k!} \nabla^k q(0) + R^{(N+1)} \quad , \tag{A.3}$$

with $R^{(N+1)} \in C^\infty(\Omega; H)$ vanishing at order N in 0.[39] In other words $\alpha^{(0)} + \alpha^{(1)} + \ldots$ uniquely solves (A.1) in the sense of formal power series.

Step 3

We shall consider now the space $\mathcal{P}_\infty(\Omega; H)$ of H-valued smooth functions on Ω vanishing at infinite order in 0 and shall show that, if Ω is sufficiently small, there exists for every $Q \in \mathcal{P}_\infty(\Omega; H)$ a unique $\beta \in \mathcal{P}_\infty(\Omega; H)$ such that

$$\mathcal{T} \beta = Q \quad . \tag{A.5}$$

The idea is to show, by means of characteristic equations, that a priori any solution of (A.5) has to equal a certain integral (see formula (A.13) below) and then to check that this integral indeed solves the equation.

A preliminary observation is the following: since the eigenvalues of the linearization of $\mathcal{V}$ around 0 are strictly positive, it follows from standard results (see for example [101]) that there exist constants $C_1, C_2, \gamma > 0$ such that for $\|x\| \leq C_1$ and $t \leq 0$ the flow $\Phi : (t, x) \mapsto \Phi_t(x)$ associated with $\mathcal{V}$ is well defined and satisfies

$$\|\Phi_t(x)\| \leq C_2 e^{-\gamma |t|} \|x\| \quad . \tag{A.6}$$

Here $\| \cdot \|$ denotes the standard norm on $\mathbb{R}^n$. Replacing it by another suitably chosen norm $\| \cdot \|_*$, allows to take $C_2 = 1$ in (A.6). Hence, possibly substituting the original Ω with a 0-centered ball, which is sufficiently small in the norm $\| \cdot \|_*$, we can assume from now on that $\Phi_t(x) \in \Omega$ for every $x \in \Omega$ and $t \leq 0$. Moreover we can assume that Ω is bounded.

[39] By definition a function $R \in C^\infty(\Omega; H)$ vanishes at order $N \in \mathbb{N}_0$ in 0 if $\nabla^k R(0) \equiv 0$ for every $k \leq N$. Equivalently if for every compact subset K of Ω there exists a constant C_K such that for every $x \in K$

$$\|R(x)\|_H \leq C_K \|x\|^N \quad . \tag{A.4}$$

R is said to vanish at infinite order in 0 if $\nabla^k R(0) \equiv 0$ for every $k \in \mathbb{N}_0$, i.e. if there exists a constant $C_{K,N}$ satisfying (A.4) for every compact $K \subset \Omega$ and $N \in \mathbb{N}_0$.

Now, if there exists a solution β of equation (A.5), inserting $u(t,x) := \beta(\Phi_t(x))$ in the equation would give for every $x \in \Omega$ and $t \leq 0$

$$\frac{d}{dt}u(t,x) = -A(\Phi_t(x))u(t,x) + \ Q(\Phi_t(x)) \quad .$$

It would follow by variation of constants that for every t_0, $t \leq 0$ and $x \in \Omega$

$$u(t,x) = B(t,x)B^{-1}(t_0,x)\ u(t_0,x) + B(t,x)\int_{t_0}^{t} B^{-1}(s,x)\ Q(\Phi_s(x))\ ds \quad , \tag{A.7}$$

with $\{B(t,x)\}_{t\leq 0, x\in\Omega}$ a smooth family of bounded linear operators on H uniquely determined by the property that for every $t \leq 0$ and $x \in \Omega$

$$\begin{cases} \frac{d}{dt}B(t,x) = -A(\Phi_t(x))\ B(t,x) \\ B(0,x) = Id \end{cases} \quad . \tag{A.8}$$

Using Gronwall's Lemma one easily gets [40] the existence of a constant $K > 0$ such that for $t \leq 0$

$$\|B(t,x)\|_{\mathscr{B}(H)} + \|B^{-1}(t,x)\|_{\mathscr{B}(H)} \leq 2e^{K|t|} \quad . \tag{A.10}$$

On the other hand it follows from (A.6) that for every function $R \in \mathcal{P}_\infty(\Omega, H)$ and every $N \in \mathbb{N}_0$ there exists a constant C such that for every $x \in \Omega$

$$\|R(\Phi_t(x))\|_H \leq Ce^{-N\gamma|t|}\|x\|^N \quad . \tag{A.11}$$

Using (A.11) with $R = \beta$ and $R = Q$ and the estimate (A.10) we obtain that for every $t \leq 0$ and $x \in \Omega$ the limit for $t_0 \to -\infty$ of the righthand side of (A.7) exists and equals

$$B(t,x)\int_{-\infty}^{t} B^{-1}(s,x)\ Q(\Phi_s(x))\ ds \quad . \tag{A.12}$$

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[40] We give here the argument for completeness: from (A.8) it follows that for $t \geq 0$ and $x \in \Omega$, with $\tilde{B}(t,x) := B(-t,x)$

$$\frac{d}{dt}\tilde{B}(t,x) = A(\Phi_{-t}(x))\ \tilde{B}(t,x) \quad .$$

Hence

$$\frac{d}{dt}\|\tilde{B}(t,x)\|^2_{\mathscr{B}(H)} \leq 2\|A(\Phi_{-t}(x))\|_{\mathscr{B}(H)}\ \|\tilde{B}(t,x)\|^2_{\mathscr{B}(H)} \leq 2\big(\sup_{\substack{s\geq 0\\ y\in\Omega}} \|A(\Phi_{-s}(y))\|_{\mathscr{B}(H)}\big)\ \|\tilde{B}(t,x)\|^2_{\mathscr{B}(H)} \quad .$$

Observing that $\sup_{\substack{s\geq 0\\ y\in\Omega}} \|A(\Phi_{-s}(y))\|_{\mathscr{B}(H)} = \sup_{y\in\Omega}\|A(y)\|_{\mathscr{B}(H)} < K < \infty$ for some $K > 0$ and applying Gronwall's Lemma gives $\|B(-t,x)\|_{\mathscr{B}(H)} = \|\tilde{B}(t,x)\|_{\mathscr{B}(H)} \leq e^{Kt}$ for $t \geq 0$ and $x \in \Omega$. To obtain the same estimate with B^{-1} instead of B observe that from $\frac{d}{dt}[B(t,x)B^{-1}(t,x)] = 0$ it follows that for $t \leq 0$ and $x \in \Omega$

$$\frac{d}{dt}B^{-1}(t,x) = B^{-1}(t,x)\ A(\Phi_t(x)) \quad . \tag{A.9}$$

Now, starting from (A.9) instead of (A.8) we can repeat the same arguments as before.

Letting $t \to 0$ we would get by continuity the representation

$$\beta(x) = u(0,x) = \int_{-\infty}^{0} B^{-1}(s,x)\; Q(\Phi_s(x))\; ds \quad . \tag{A.13}$$

This shows that there can be at most one solution of (A.5).

Now let β be defined by (A.13). It remains to check that $\beta \in \mathcal{P}_\infty(\Omega; H)$ and that β solves (A.5). As far as the former property is concerned, using again (A.10) and (A.11) with $R = Q$, we get that for every $N \in \mathbb{N}_0$ there exists a constant $C > 0$ such that for every $x \in \Omega$

$$\|\beta(x)\|_H \leq C\|x\|^N \int_{-\infty}^{0} e^{K|s|} e^{-N\gamma|s|}\; ds \quad .$$

The integral being finite for N sufficiently large, this implies $\beta \in \mathcal{P}_\infty(\Omega; H)$.

To see that β solves (A.5) observe that for every $x \in \Omega$,

$$\sum_j \mathcal{V}_j(x) \frac{\partial}{\partial x_j} \beta(x) = \frac{d}{dt} u\;(0,x) \quad ,$$

with $u(t,x) := \beta(\Phi_t(x))$. Since, as can be easily checked, $B(t,x) = B^{-1}(s-t,x)B(s,x)$ for every $t,s \leq 0$ and $x \in \Omega$, we have with the integral variable substitution $s' = t + s$ that $u(t,x)$ equals the expression given in (A.12). Differentiating the latter with respect to t and evaluating at $t = 0$ gives the desired result.

Step 4

Let $\alpha^{(k)}$ be defined as in Step 2 and take an $\tilde{\alpha} \in C^\infty(\Omega, H)$ which satisfies $\nabla^k \tilde{\alpha}(0) = \alpha^{(k)}$ for every $k \in \mathbb{N}_0$. The existence of such an $\tilde{\alpha}$ is ensured by Borel's Theorem. [41]

By (A.3) the function $Q^{(\infty)} := q - \mathcal{T}\tilde{\alpha}$ is in $\mathcal{P}_\infty(\Omega; H)$ and by Step 3 there exists a unique $\beta \in \mathcal{P}_\infty(\Omega; H)$ satisfying $\mathcal{T}\beta = Q^\infty$. It follows that

$$\alpha := \tilde{\alpha} + \beta$$

solves (A.1).

Moreover, if α' is another solution then $\alpha' - \alpha$ must be in $\mathcal{P}_\infty(\Omega; H)$ by Step 2. Since

$$\mathcal{T}(\alpha' - \alpha) = 0 \quad ,$$

[41] See for example [82, 1.5.4 on p.30] for real-valued functions. The extension to the Hilbert space case is trivial.

we can conclude $\alpha' - \alpha = 0$ by Step 3.

$\square$

Appendix B. Harmonic approximation

Fix $n, m \in \mathbb{N}_0$. We denote in the following by $\mathcal{M}_m(\mathbb{R})$ the set of real $m \times m$ matrices, by A^t the transposed of $A \in \mathcal{M}_m(\mathbb{R})$, and for every $\gamma \in \mathbb{R}^n$ by τ_γ the translation in direction γ, i.e.

$$\tau_\gamma \ \alpha \ (x) \ := \ \alpha(x + \gamma)$$

if $\alpha : \mathbb{R}^n \to \mathbb{R}^m$. The standard euclidean scalar product and norm in $\mathbb{R}^n$ and $\mathbb{R}^m$ are denoted by $\langle \cdot, \cdot \rangle$ and $\| \cdot \|$. The symbol $\| \cdot \|$ is also used for the operator norm induced by $\langle \cdot, \cdot \rangle$ on the space $\mathcal{M}_m(\mathbb{R})$.

We shall consider for $\varepsilon > 0$ a perturbed discrete Schrödinger operator H_ε, formally defined on the space of functions from $\mathbb{R}^n$ to $\mathbb{R}^m$. More precisely we let

$$H_\varepsilon \ := \ -L_\varepsilon \ + \ V \ + \ \varepsilon \ M_\varepsilon \quad , \tag{B.1}$$

where

- L_ε is a (scalar) discrete Laplacian, given by

$$L_\varepsilon \ := \ \sum_{\gamma \in \mathbb{Z}^n} a_\gamma \ [\ \tau_{\varepsilon\gamma} - 1 \ ]$$

  with the constant coefficients a_γ satisfying: $a_\gamma \geq 0$ for every $\gamma \in \mathbb{Z}^n$, $a_\gamma = a_{-\gamma}$ for every $\gamma \in \mathbb{Z}^n$ and $a_\gamma > 0$ for only finitely many γ's, but for enough γ's such that $\{ \ \gamma : a_\gamma > 0\}$ generates $\mathbb{Z}^n$.
- V is a scalar multiplication operator, identified with a function $V \in C^\infty(\mathbb{R}^n; \mathbb{R})$. We assume throughout that $V \geq 0$.
- the perturbation M_ε is for $\varepsilon > 0$ a matricial translation operator of the form

$$M_\varepsilon \ := \ \sum_{\gamma \in \mathbb{Z}^n} R_{\varepsilon,\gamma} \ \tau_{\varepsilon\gamma} \quad ,$$

  where for $\varepsilon > 0$ and $\gamma \in \mathbb{Z}^n$ the coefficient $R_{\varepsilon,\gamma}$ is in $C^\infty(\mathbb{R}^n; \mathcal{M}_m(\mathbb{R}))$ and $R_{\varepsilon,\gamma} \equiv 0$ for $\varepsilon > 0$ and γ outside a fixed finite subset of $\mathbb{Z}^n$. Moreover
  - for $\varepsilon > 0$ and every $\gamma \in \mathbb{Z}^n$,

$$R_{\varepsilon,\gamma}(x) \ = \ R^t_{\varepsilon,-\gamma}(x + \varepsilon\gamma) \quad . \tag{B.2}$$

  - there exists for every $\gamma \in \mathbb{Z}^n$ an $R_\gamma \in C^\infty(\mathbb{R}^n; \mathcal{M}_m(\mathbb{R}))$ such that

$$R_{\varepsilon,\gamma} \ = \ R_\gamma \ + \ \mathcal{O}(\varepsilon) \quad . \tag{B.3}$$

More explicitly, we have with $R_{\varepsilon,\gamma} = (R_{\varepsilon,\gamma;i,j})_{i,j=1\dots,m}$ and $\alpha := (\alpha_i)_{i=1,\dots,m} : \mathbb{R}^n \to \mathbb{R}^m$ that for every $x \in \mathbb{R}^n$ and $i = 1,\dots,m$

$$\big(\ H_\varepsilon\ \alpha\ \big)_i\ (x) \ = \ \sum_{\gamma\in\mathbb{Z}^n} a_\gamma\ \big[\ \alpha_i(x+\varepsilon\gamma)\ -\ \alpha_i(x)\ \big]\ +\ V(x)\ \alpha_i(x)\ +$$
$$+\ \varepsilon\ \sum_{\gamma\in\mathbb{Z}^n}\sum_{j=1}^m R_{\varepsilon,\gamma;i,j}(x)\ \alpha_j(x+\varepsilon\gamma)\quad .$$

Observe that H_ε is well-defined also as a formal operator on $C(\varepsilon\mathbb{Z}^n;\mathbb{R}^m)$, the set of functions from $\varepsilon\mathbb{Z}^n$ to $\mathbb{R}^m$. Moreover the restriction $H_{\varepsilon,0}$ of H_ε to $C_c(\varepsilon\mathbb{Z}^n;\mathbb{R}^m)$, the space of functions from $\varepsilon\mathbb{Z}^n$ to $\mathbb{R}^m$ with finite support, is symmetric in the Hilbert space

$$\ell^2(\varepsilon\mathbb{Z}^n;\mathbb{R}^m)\ :=\ \Big\{\ (\alpha_i)_{i=1,\dots,m}\in C(\varepsilon\mathbb{Z}^n;\mathbb{R}^m)\quad \text{s.t.}\quad \sum_{x\in\varepsilon\mathbb{Z}^n}\sum_{i=1}^m \alpha_i^2(x)<\infty\ \Big\}$$

whose scalar product and norm we shall denote by $\langle\cdot,\cdot\rangle_{\varepsilon,\ell^2}$ and $\|\cdot\|_{\varepsilon,\ell^2}$.

In general $H_{\varepsilon,0}$ will be unbounded. For its behaviour at infinity we shall henceforth assume the following.

Assumption IV.1. *There exist a compact $K\subset\mathbb{R}^n$ and constants $C', C'' > 0$ such that for every $x\in\mathbb{R}^n\setminus K$, $\varepsilon>0$*

(i) $V(x)\ge C'$.
(ii) $\sum_{\gamma\in\mathbb{Z}^n}\|R_{\varepsilon,\gamma}(x)\|\ \le\ C''\ V(x)$.

Remark B.1. *Note the following implication of Assumption IV.1 and condition* (B.3)*: there exists a constant $C>0$ such that for every $x\in\mathbb{R}^n$, $\varepsilon>0$*

$$\sum_{\gamma\in\mathbb{Z}^n}\|R_{\varepsilon,\gamma}(x)\|\ \le\ C\ (1+V(x))\quad . \tag{B.4}$$

From this it follows that there exists a constant $\tilde C>0$ such that for $\varepsilon>0$ and for every $\alpha\in C_c^\infty(\varepsilon\mathbb{Z}^n;\mathbb{R}^m)$

$$|\langle M_\varepsilon\alpha,\alpha\rangle_{\varepsilon,\ell^2}|\ \le\ \tilde C\ (\|\alpha\|^2_{\varepsilon,\ell^2}+\langle V\alpha,\alpha\rangle_{\varepsilon,\ell^2})\quad . \tag{B.5}$$

Indeed, using (B.2) *we get*

$$|\langle M_\varepsilon \alpha, \alpha\rangle_{\varepsilon,\ell^2}| \;\le\; \sum_{x\in\varepsilon\mathbb{Z}^n}\sum_{\gamma\in\mathbb{Z}^n} \|R_{\varepsilon,\gamma}(x)\|\;\|\alpha(x+\varepsilon\gamma)\|\;\|\alpha(x)\| \;=$$

$$= \sum_{x\in\varepsilon\mathbb{Z}^n}\sum_{\gamma\in\mathbb{Z}^n} \sqrt{\|R^t_{\varepsilon,-\gamma}(x+\varepsilon\gamma)\|}\;\|\alpha(x+\varepsilon\gamma)\|\;\sqrt{\|R_{\varepsilon,\gamma}(x)\|}\;\|\alpha(x)\| \;\le$$

$$\le \sum_{\gamma\in\mathbb{Z}^n} \sqrt{\sum_{x\in\varepsilon\mathbb{Z}^n} \|R^t_{\varepsilon,-\gamma}(x+\varepsilon\gamma)\|\;\|\alpha(x+\varepsilon\gamma)\|^2}\;\sqrt{\sum_{x\in\varepsilon\mathbb{Z}^n}\|R_{\varepsilon,\gamma}(x)\|\;\|\alpha(x)\|^2} \;=$$

$$= \sum_{\gamma\in\mathbb{Z}^n} \sqrt{\sum_{x\in\varepsilon\mathbb{Z}^n} \|R_{\varepsilon,-\gamma}(x)\|\;\|\alpha(x)\|^2}\;\sqrt{\sum_{x\in\varepsilon\mathbb{Z}^n}\|R_{\varepsilon,\gamma}(x)\|\;\|\alpha(x)\|^2} \;.$$

The inequality (B.4) *thus gives for a suitable* $\tilde{C} > 0$

$$|\langle M_\varepsilon \alpha, \alpha\rangle_{\varepsilon,\ell^2}| \;\le\; \tilde{C} \sum_{x\in\varepsilon\mathbb{Z}^n} (1+V(x))\;\|\alpha(x)\|^2 \;\;,$$

which is the same as (B.5).

Proposition B.2. *$H_{\varepsilon,0}$ is semibounded from below and essentially selfadjoint for $\varepsilon > 0$ sufficiently small.*

Proof. The inequality (B.5) and the condition $V \ge 0$, together with

$$\langle -L_\varepsilon \alpha, \alpha\rangle_{\varepsilon,\ell^2} \;\ge\; 0 \;\;, \tag{B.6}$$

valid for $\varepsilon > 0$ and every $\alpha \in \ell^2(\varepsilon\mathbb{Z}^n;\mathbb{R}^m)$, imply that $H_{\varepsilon,0}$ is semibounded from below for sufficiently small ε.

In order to prove essential selfadjointness we may assume without loss of generality (by possibly adding a constant to V) that

$$\langle H_{\varepsilon,0}\alpha, \alpha\rangle_{\varepsilon,\ell^2} \;\ge\; \|\alpha\|^2_{\varepsilon,\ell^2} \tag{B.7}$$

for every $\varepsilon > 0$ smaller than some $\varepsilon_0 > 0$ and every $\alpha \in C_c(\varepsilon\mathbb{Z}^n;\mathbb{R}^m)$.

Fix $\varepsilon \in (0,\varepsilon_0)$. By general principles it is enough to show that $H_{\varepsilon,0}$ has dense range. This is equivalent to show that the only function $f \in \ell^2(\varepsilon\mathbb{Z}^n;\mathbb{R}^m)$ satisfying

$$\langle f, H_{\varepsilon,0}\alpha\rangle_{\varepsilon,\ell^2} \;=\; 0 \qquad \forall \alpha \in C_c(\varepsilon\mathbb{Z}^n;\mathbb{R}^m) \tag{B.8}$$

is the function $f \equiv 0$.

For $k \in \mathbb{N}_*$ let χ_k be the indicator function of the closed ball in $\mathbb{R}^n$ of radius k and centered at 0. Then for every $f \in \ell^2(\varepsilon\mathbb{Z}^n;\mathbb{R}^m)$

$$\|f\|^2_{\varepsilon,\ell^2} \;=\; \lim_{k\to\infty} \|\chi_k f\|^2_{\varepsilon,\ell^2} \;\leq\; \liminf_{k\to\infty} \langle H_{\varepsilon,0}(\chi_k f), \chi_k f\rangle_{\varepsilon,\ell^2} \quad ,$$

where for the last inequality we used (B.7). Moreover, if f satisfies (B.8), one gets by taking $\alpha = \chi_k f$ in (B.8) and by (B.1)

$$\begin{aligned} \langle H_{\varepsilon,0}(\chi_k f), \chi_k f\rangle_{\varepsilon,\ell^2} \;&=\; \langle H_{\varepsilon,0}(\chi_k f), \chi_k f - f\rangle_{\varepsilon,\ell^2} \;= \\ =\; \langle -L_\varepsilon(\chi_k f), (\chi_k - 1)f\rangle_{\varepsilon,\ell^2} \;&+\; \langle V\chi_k f, (\chi_k - 1)f\rangle_{\varepsilon,\ell^2} \;+ \\ &+\; \langle \varepsilon\; M_\varepsilon(\chi_k f), (\chi_k - 1)f\rangle_{\varepsilon,\ell^2} \quad . \end{aligned} \tag{B.9}$$

The boundedness of L_ε and $\lim_{k\to\infty} \|(\chi_k - 1)f\|_{\varepsilon,\ell^2} = 0$ imply that the first summand in (B.9) converges to 0 for $k \to \infty$. The fact that χ_k and $\chi_k - 1$ have disjoint support implies that the second term vanishes for every k. $\square$

We shall consider henceforth the unique selfadjoint extension of $H_{\varepsilon,0}$, which we denote by $H_{\varepsilon,\mathbb{Z}^n}$. It follows again from Assumption IV.1 that the essential spectrum of the latter is bounded away from zero:

Proposition B.3. *There exists a constant $C > 0$ such that for $\varepsilon > 0$ sufficiently small*

$$\mathrm{Spec}_{\mathrm{ess}}\left(H_{\varepsilon,\mathbb{Z}^n}\right) \;\subset\; [C, \infty) \quad .$$

Proof. Let $\chi \in C_c(\mathbb{R}^n;\mathbb{R})$ and note that seen as a multiplication operator in $\ell^2(\varepsilon\mathbb{Z}^n;\mathbb{R}^m)$, χ is finite rank (in particular compact) for every $\varepsilon > 0$. It follows from Weyl's theorem that

$$\inf\; \mathrm{Spec}_{\mathrm{ess}}\left(H_{\varepsilon,\mathbb{Z}^n}\right) \;=\; \inf\; \mathrm{Spec}_{\mathrm{ess}}\left(H_{\varepsilon,\mathbb{Z}^n} \;+\; \chi\,\right) \quad . \tag{B.10}$$

Moreover

$$\begin{aligned} \inf\; \mathrm{Spec}_{\mathrm{ess}}\left(H_{\varepsilon,\mathbb{Z}^n} \;+\; \chi\,\right) \;&\geq\; \inf\; \mathrm{Spec}\left(H_{\varepsilon,\mathbb{Z}^n} \;+\; \chi\,\right) \;= \\ &=\; \inf_{\substack{\alpha\in C_c(\varepsilon\mathbb{Z}^n;\mathbb{R}^m)\\ \alpha\neq 0}} \frac{\langle (H_{\varepsilon,0} + \chi)\alpha, \alpha\rangle_{\varepsilon,\ell^2}}{\langle \alpha, \alpha\rangle_{\varepsilon,\ell^2}} \quad , \end{aligned} \tag{B.11}$$

where for the last equality we used that $C_c(\varepsilon\mathbb{Z}^n;\mathbb{R}^m)$ is a core for $H_{\varepsilon,\mathbb{Z}^n}$.

Now take χ such that for some constant $R > 0$ the inequality $\frac{1}{2}V(x) + \chi(x) \geq R$ holds for every $x \in \mathbb{R}^n$ (this is possible thanks to Assumption IV.1 (i)). It follows using also (B.6) and (B.5) that for some constant

$C > 0$, $\varepsilon > 0$ sufficiently small and every $\alpha \in C_c(\varepsilon\mathbb{Z}^n;\mathbb{R}^m)$

$$\langle (H_{\varepsilon,0} + \chi)\alpha, \alpha\rangle_{\varepsilon,\ell^2} \ \geq\ \langle (V + \chi)\alpha, \alpha\rangle_{\varepsilon,\ell^2} \ -\ \varepsilon\, C\ \big(\ \langle \alpha, \alpha\rangle_{\varepsilon,\ell^2} \ +\ \langle V\alpha, \alpha\rangle_{\varepsilon,\ell^2}\ \big) \ \geq$$
$$\geq\ \langle (\frac{1}{2}V + \chi)\alpha, \alpha\rangle_{\varepsilon,\ell^2} \ - \varepsilon\, C\ \langle \alpha, \alpha\rangle_{\varepsilon,\ell^2} \ \geq\ \frac{1}{2}R\langle \alpha, \alpha\rangle_{\varepsilon,\ell^2} \quad ,$$

which together with (B.10) and (B.11) gives the desired result. □

We are interested in the asymptotic behaviour as $\varepsilon \to 0$ of the eigenvalues of $H_{\varepsilon,\mathbb{Z}^n}$. The so-called harmonic approximation is obtained by comparison with a direct sum of suitable harmonic oscillators located at the global minima of V, provided that these are non degenerate. Indeed we shall also assume the following. Recall that we assume throughout $V \geq 0$.

Assumption IV.2. *There are exactly N points $\bar{x}^{(1)}, \ldots, \bar{x}^{(N)}$ such that $V(\bar{x}^{(k)}) = 0$. Moreover the matrix*

$$D^2V(\bar{x}^{(k)}) \ :=\ \Big(\ \frac{\partial^2 V}{\partial x_i \partial x_j}(\bar{x}^{(k)})\ \Big)_{i,j}$$

is striclty positive definite for every $k = 1, \ldots, N$.

The approximating harmonic oscillators are defined as follows. Let for $i, j = 1, \ldots, n$

$$a_{i,j} \ :=\ \frac{1}{2}\sum_{\gamma\in\mathbb{Z}^n} a_\gamma\ \gamma_i\gamma_j \qquad ,$$

and let for $x, \xi \in \mathbb{R}^n$

$$\hat{M}(x,\xi) \ :=\ \sum_{\gamma\in\mathbb{Z}^n} R_\gamma(x)\ e^{-\mathrm{i}\langle\gamma,\xi\rangle}$$

be the leading semiclassical symbol of M_ε. Note that for every $x \in \mathbb{R}^n$ we have that $\hat{M}(x,0) = \sum_{\gamma\in\mathbb{Z}^n} R_\gamma(x)$ is in $\mathcal{M}_m(\mathbb{R})$ and satisfies $\big(\hat{M}(x,0)\big)^t = \hat{M}(x,0)$ thanks to the assumptions (B.2) and (B.3).

Then, recalling that V has N global minima, define for every $k = 1, \ldots, N$ the formal operators

$$H_k^{\mathrm{osc}} \ :=\ -\sum_{i,j=1}^{n} a_{i,j}\ \partial^2_{x_i,x_j} \ +\ \frac{1}{2}\langle D^2V(\bar{x}^{(k)})x, x\rangle \ +\ \hat{M}(\bar{x}^{(k)},0)$$

and denote by $H^{\mathrm{osc}}_{k;\mathbb{R}^n}$ the Friedrichs extension in $L^2(\mathbb{R}^n, dx;\mathbb{R}^m)$ of the restriction of H_k^{osc} to $C_c^\infty(\mathbb{R}^n;\mathbb{R}^m)$. Finally let

$$H^{\mathrm{osc}}_{\mathbb{R}^n} \ :=\ \oplus_{k=1}^{N}\ H^{\mathrm{osc}}_{k;\mathbb{R}^n} \quad .$$

Remark B.4. *Observe that $H^{\mathrm{osc}}_{k;\mathbb{R}^n}$ is not exactly a harmonic oscillator in the classical sense, since $a := (a_{i,j})_{i,j}$ is not the identity matrix and since there is an additional constant given by the matrix $\hat{M}(\bar{x}^{(k)}, 0)$. But one can still explicitly compute the full spectrum of $H^{\mathrm{osc}}_{\mathbb{R}^n}$. Indeed, observe first that $H^{\mathrm{osc}}_{k;\mathbb{R}^n}$ has the same spectrum as $\tilde{H}^{\mathrm{osc}}_{k;\mathbb{R}^n}$, the latter being obtained as Friedrichs extension of*

$$\tilde{H}^{\mathrm{osc}}_k \;:=\; -\sum_{i,j=1}^{n} \partial^2_{x_i,x_j} \;+\; \frac{1}{2}\langle a D^2 V(\bar{x}^{(k)}) x, x\rangle \;+\; \hat{M}(\bar{x}^{(k)}, 0) \qquad ,$$

since $\tilde{H}^{\mathrm{osc}}_{k;\mathbb{R}^n} = \Phi\, H^{\mathrm{osc}}_{k;\mathbb{R}^n} \Phi^{-1}$ with Φ the linear transformation on $L^2(\mathbb{R}^n, dx; \mathbb{R}^m)$ given by $\Phi\alpha(x) := \alpha(\sqrt{a}x)$. Now let for every $k = 1, \ldots, N$ be $\omega^{(k)}_1, \ldots, \omega^{(k)}_n$ the square roots of the positive symmetric matrix $\frac{1}{2} a D^2 V(\bar{x}^{(k)})$ and let $\mu^{(k)}_1, \ldots, \mu^{(k)}_m$ be the eigenvalues of the symmetric matrix $\hat{M}(\bar{x}^{(k)}, 0)$. Then the spectrum of $\tilde{H}^{\mathrm{osc}}_{k;\mathbb{R}^n}$ is given by

$$\mathrm{Spec}\left(\tilde{H}^{\mathrm{osc}}_{k;\mathbb{R}^n}\right) \;=\; \Big\{ \;\sum_{i=1}^{n} \omega^{(k)}_i \;(2r_i + 1) \;+\; \mu^{(k)}_j \;\Big\}_{\substack{r_1,\ldots,r_n \in \mathbb{N}_0 \\ j=1,\ldots,m}} \quad .$$

Finally, the spectrum of $H^{\mathrm{osc}}_{\mathbb{R}^n}$ is given by the union $\bigcup_{k=1}^{N} \mathrm{Spec}\left(\tilde{H}^{\mathrm{osc}}_{k;\mathbb{R}^n}\right)$.

The relation between the spectrum of $H_{\varepsilon,\mathbb{Z}^n}$ and $H^{\mathrm{osc}}_{\mathbb{R}^n}$ is quantified by the following fundamental result. We omit the proof which can be done by slightly modifying the arguments in [65], where only the case $m = 1$ is treated. Reference [65] is based on classical results on harmonic approximation of Schrödinger operators in $\mathbb{R}^n$ (see [89, 21, 27, 43]).

Theorem B.5.

The operator $H_{\varepsilon,\mathbb{Z}^n}$ has for any fixed $j_0 \in \mathbb{N}_*$ and $\varepsilon > 0$ sufficiently small at least j_0 eigenvalues.

Moreover, denoting by $\nu_{j,\varepsilon}$ the j'th eigenvalue of $H_{\varepsilon,\mathbb{Z}^n}$ and by ν^{osc}_j the j'th eigenvalue of $H^{\mathrm{osc}}_{\mathbb{R}^n}$ (by increasing order and counting multiplicity in both cases) we have

$$\nu_{j,\varepsilon} \;=\; \varepsilon\, \nu^{\mathrm{osc}}_j \;+\; \mathcal{O}(\varepsilon^{6/5}) \quad .$$

Appendix C. Asymptotics of sums

The main tool to compute asymptotics of integrals with respect to rescaled lattice measures is the following simple application of the Poisson summation formula.

Proposition C.1.

Let $f_h \in C_c^\infty(\mathbb{R}^n;\mathbb{R})$ for $h > 0$ [42] *and assume that there exists an $N_0 \in \mathbb{N}_0$ with the following property: for every multiindex α of length $|\alpha| \geq N_0$ there exists an h-independent constant $C_\alpha > 0$ such that*

$$\int_{\mathbb{R}^n} |\partial^\alpha f_h\ (x)|\ dx\ \leq C_\alpha \quad . \tag{C.1}$$

Then

$$h^n \sum_{x\in h\mathbb{Z}^n} f_h(x)\ -\ \int_{\mathbb{R}^n} f_h(x)\ dx\ =\ \mathcal{O}(h^\infty) \quad . \tag{C.2}$$

Proof. The Poisson summation formula gives for $h > 0$

$$\sum_{x\in\mathbb{Z}^n} f_h(hx)\ =\ h^{-n} \sum_{x\in\mathbb{Z}^n} \hat{f}_h(x/h) \quad , \tag{C.3}$$

where $\hat{f}_h : \mathbb{R}^n \to \mathbb{R}$ is the Fourier transform of f_h, defined as

$$\hat{f}_h(x) := \int_{\mathbb{R}^n} f_h(y)\ e^{-2\pi \mathrm{i} x\cdot y}\ dy \quad .$$

Rewrite the identity (C.3) as

$$h^n \sum_{x\in h\mathbb{Z}^n} f_h(x)\ =\ \hat{f}_h(0)\ +\ \sum_{x\in\mathbb{Z}^n\setminus\{0\}} \hat{f}_h(x/h) \tag{C.4}$$

and observe that

$$\hat{f}_h(0) = \int_{\mathbb{R}^n} f_h(x)\ dx \quad .$$

The remainder $\sum_{x\in\mathbb{Z}^n\setminus\{0\}} \hat{f}_h(x/h)$ appearing on the right hand side of (C.4) is estimated using standard decay properties of the Fourier transform. To be precise, observe that for $h > 0$, every multiindex α and every $x \in \mathbb{R}^n$

$$|(x/h)^\alpha\ \hat{f}_h(x/h)|\ =\ \frac{1}{(2\pi)^\alpha}\ |\widehat{\partial^\alpha f_h}\ (x/h)| \quad .$$

This last identity together with the estimate

$$|\widehat{\partial^\alpha f_h}\ (x/h)|\ \leq\ \int_{\mathbb{R}^n} |\partial^\alpha f_h\ (y)|\ dy \quad ,$$

[42] We stress that here (as elsewhere) $f_h \in C_c^\infty(\mathbb{R}^n;\mathbb{R})$ is a condition given on f_h for every fixed h. In particular the supprot of f_h is allowed to grow to infinity with $h \to 0$.

again valid for $h > 0$, every multiindex α and every $x \in \mathbb{R}^n$ gives for the remainder

$$\Big| \sum_{x \in \mathbb{Z}^n \setminus \{0\}} \hat{f}_h(x/h) \Big| \leq h^{|\alpha|} \int_{\mathbb{R}^n} |\partial^\alpha f_h\ (y)|\ dy \sum_{x \in \mathbb{Z}^n \setminus \{0\}} \frac{1}{|x^\alpha|} \quad .$$

The claim (C.2) follows now immediatley from the assumption (C.1). $\square$

Corollary C.2 (Laplace asymptotics)**.**

Let $a \in C_c^\infty(\mathbb{R}^n;\mathbb{R})$ and $\varphi \in C^\infty(\mathbb{R}^n;\mathbb{R})$. Assume that there exists an $x_0 \in \mathbb{R}^n$ such that

$$\varphi(x_0) = 0 \quad , \quad \operatorname{Hess} \varphi(x_0) > 0 \quad , \quad \varphi(x) > 0 \ \textit{ for every } \ x \in \operatorname{supp} a \setminus \{x_0\} \quad . \tag{C.5}$$

Then there exists a sequence $(I_k)_{k \in \mathbb{N}_0}$ in $\mathbb{R}$ with

$$I_0 \ = \ \frac{(2\pi)^{n/2}\ a(x_0)}{\sqrt{\det \operatorname{Hess} \varphi(x_0)}} \tag{C.6}$$

such that

$$\varepsilon^{n/2} \sum_{x \in \varepsilon\mathbb{Z}^n} a(x)\ e^{-\varphi(x)/\varepsilon} \ \sim \ \sum_{k=0}^\infty \varepsilon^k\ I_k \quad .$$

Proof. With $h := \sqrt{\varepsilon}$ and $f_h(x) \ := \ a(hx)\ e^{-\varphi(hx)/h^2}$ we have

$$\varepsilon^{n/2} \sum_{x \in \varepsilon\mathbb{Z}^n} a(x)\ e^{-\varphi(x)/\varepsilon} \ = \ h^n \sum_{x \in h\mathbb{Z}^n} f_h(x) \quad .$$

Observe that the classical Laplace asymptotics (see for example [41, Theorem 4.2.1]) gives

$$\int_{\mathbb{R}^n} f_h(x)\ dx \ = \ h^{-n} \int_{\mathbb{R}^n} a(x)\ e^{-\varphi(x)/h^2} \ \sim \sum_{k=0}^\infty h^{2k}\ I_k \quad ,$$

with the sequence $(I_k)_{k \in \mathbb{N}_0}$ in $\mathbb{R}$ and I_0 as in (C.6).

Thus, to finish the proof, it is sufficient to show that f_h satisfies the assumption (C.1) of Proposition C.1. To this end, observe that for every multiindex α

$$|\partial^\alpha f_h| \ = g_{h,\alpha}\ e^{-\varphi_h} \quad , \tag{C.7}$$

where $\varphi_h(x) := \frac{\varphi(hx)}{h^2}$ and $g_{h,\alpha}$ can be expressed as a sum of products with factors of the type $|\partial^{\alpha'}\varphi_h(x)|$ and $|\partial^{\alpha''}a_h(x)|$, with $a_h(x) := a(hx)$.

Moreover, observe that

(i) For every multiindex α there exists a constant $C_\alpha > 0$ (independent of h and x) such that

a)

$$|\partial^\alpha a_h(x)| \le C_\alpha \quad \text{for} \quad h > 0 \quad \text{and every} \quad x \in \mathbb{R}^n \quad .$$

b) denoting by $B_1(0)$ the unit ball centered at the origin

$$|\partial^\alpha \varphi_h(x)| \le C_\alpha \quad \text{for} \quad h > 0 \quad \text{and every } x \in B_1(0)$$

and

$$|\partial^\alpha \varphi_h(x)| \le C_\alpha |x|^2 \quad \text{for} \quad h > 0 \quad \text{and every } x \in B_1^c(0) \cap \operatorname{supp} a_h \quad .$$

The estimate $a)$ follows from the assumption that a has compact support. The estimates in $b)$ can be easily obtained from the Taylor expansion

$$\partial^\alpha \varphi_h(x) \ = \ h^{|\alpha|-2} \partial^\alpha \varphi(hx) \ =$$

$$= \ h^{|\alpha|-2} \partial^\alpha \varphi(0) \ + \ h^{|\alpha|-1} \langle \nabla \partial^\alpha \varphi(0), x \rangle \ + \ h^{|\alpha|} \int_0^1 \frac{(1-t)^2}{2} \langle \operatorname{Hess} \partial^\alpha \varphi(htx)x, x \rangle \, dt$$

using that htx varies in a (h-independent) compact set when $x \in \operatorname{supp} a_h$, $t \in [0,1]$ and using, in the cases $|\alpha| = 0, 1$, that $\varphi(0) = \nabla \varphi(0) = 0$.

(ii) From (C.5) it follows that there exists a $\gamma > 0$ (independent of h) such that

$$\varphi(x) \ \ge \ \gamma |x|^2 \quad \text{for every} \quad x \in \operatorname{supp} a$$

or, equivalently, for $h > 0$

$$\varphi_h(x) \ \ge \ \gamma |x|^2 \quad \text{for every} \quad x \in \operatorname{supp} a_h \quad .$$

Using (C.7) and the estimates (i) and (ii) above (in fact from (i) b) we need only the case $|\alpha| > 0$) we can conclude that for $h > 0$ and every multiindex α there exist $k \in \mathbb{N}_0$ and $\gamma > 0$ such that

$$\int_{\mathbb{R}^n} |\partial^\alpha f_h \ (x)| \ dx \ = \int_{\operatorname{supp} a_h} |\partial^\alpha f_h \ (x)| \ dx \ \le$$

$$\le \ \text{Const} \int_{B_1(0)} e^{-\gamma |x|^2} \ dx \ + \ \text{Const} \int_{\operatorname{supp} a_h} |x|^k \ e^{-\gamma |x|^2} \ dx \ \le \ \text{Const} \quad .$$

□

Appendix D. Asymptotics of the spectrum of a matrix

Let $m_0, m_1 \in \mathbb{N}_*$ and let, for $\varepsilon > 0$, B_ε be a $m_1 \times m_0$ real matrix. We shall consider for $\varepsilon > 0$ the $m_0 \times m_0$ matrix

$$A_\varepsilon \;:=\; B_\varepsilon^t \; B_\varepsilon \quad ,$$

with B_ε^t denoting the transposed of B_ε. Observe that A_ε is symmetric and nonnegative, i.e. for every $x \in \mathbb{R}^{m_0}$

$$\langle A_\varepsilon x, x\rangle \;=\; \langle x, A_\varepsilon x\rangle \;\geq\; 0 \quad .$$

Here and in the sequel $\langle\cdot,\cdot\rangle$ stands for the standard scalar product in coordinate space.

We shall denote for $\varepsilon > 0$ by $(\lambda_{i,\varepsilon})_{i=1,\ldots,m_0}$ the set of eigenvalues of A_ε ordered such that

$$\lambda_{1,\varepsilon} \;\geq\; \ldots \;\geq\; \lambda_{m_0,\varepsilon} \;\geq 0 \quad .$$

The following theorem is a slight modification of a result proven in [71]. For completeness we shall give here a selfcontained proof.

Theorem D.1.

For $\varepsilon > 0$ let $(e_{i,\varepsilon})_{i=1,\ldots,m_0}$ be a basis of $\mathbb{R}^{m_0}$ and $(f_{i,\varepsilon})_{i=1,\ldots,m_1}$ a basis of $\mathbb{R}^{m_1}$. Assume that $m_1 \geq m_0 - 1$ and that

(i) *for $i, j = 1\ldots, m_0$*

$$\langle e_{i,\varepsilon}, e_{j,\varepsilon}\rangle \;=\; 1_{i,j} \;+\; \mathcal{O}(\varepsilon^\infty)$$

and for $i, j = 1, \ldots, m_1$

$$\langle f_{i,\varepsilon}, f_{j,\varepsilon}\rangle \;=\; 1_{i,j} \;+\; \mathcal{O}(\varepsilon^\infty) \quad .$$

(ii) *$B_\varepsilon\, e_{m_0,\varepsilon} = 0$ and there exists a strictly increasing sequence $(b_i)_{i=1,\ldots,m_0-1}$ in $\mathbb{R}$ such that for $i = 1, \ldots, m_0 - 1$*

a) *there exists an $N \in \mathbb{N}_0$ such that for $\varepsilon > 0$ sufficiently small*

$$\varepsilon^N \; e^{-b_i/\varepsilon} \;\leq\; |\langle f_{i,\varepsilon}, B_\varepsilon\; e_{i,\varepsilon}\rangle| \;\leq\; \varepsilon^{-N} \; e^{-b_i/\varepsilon}$$

b) *for $j = 1, \cdots, m_1$ with $j \neq i$*

$$|\langle f_{j,\varepsilon}, B_\varepsilon\; e_{i,\varepsilon}\rangle| \;\leq\; \mathcal{O}(\varepsilon^\infty)\; e^{-b_i/\varepsilon} \quad .$$

Then $\lambda_{m_0,\varepsilon} = 0$ and for every $i = 1, \ldots, m_0 - 1$

$$\lambda_{i,\varepsilon} \;=\; |\langle f_{i,\varepsilon}, B_\varepsilon\; e_{i,\varepsilon}\rangle|^2 \;\; \big(\, 1 + \mathcal{O}(\varepsilon^\infty)\; \big) \quad . \tag{D.1}$$

Remark D.2. *Observe that from Theorem D.1 it follows that under the assumptions made therein*

$$\lambda_{1,\varepsilon} \; > \; \ldots \; > \lambda_{m_0,\varepsilon} \; = \; 0 \qquad \text{for } \varepsilon \text{ small enough.}$$

This is the situation we are interested in, but observe that analogous versions of Theorem D.1 hold mutatis mutandis in the case that for some $\bar{m} \in \{1, \ldots, m_0\}$

$$\lambda_{1,\varepsilon} \; > \; \ldots \; > \lambda_{\bar{m},\varepsilon} \; = \lambda_{\bar{m}+1,\varepsilon} \; = \; \ldots \; = \lambda_{m_0,\varepsilon} \; = \; 0$$

or in the case

$$\lambda_{1,\varepsilon} \; > \; \ldots \; > \lambda_{m_0,\varepsilon} \; > \; 0 \quad .$$

Before giving the proof of Theorem D.1 we fix some notation and terminology.

Given an $m \times n$ matrix C we denote by $\|C\|$ its operator norm and by $\mu_1(C) \geq \cdots \geq \mu_n \geq 0$ its singular values. Recall that by definition $\mu_i(C)$ equals the square root of the i-th eigenvalue (according to a decreasing ordering) of the $n \times n$ symmetric and nonnegative matrix C^tC. Note that C and C^t have the same non-zero singular values. [43] As a consequence, if for another $m \times n$ matrix C' and $i = 1, \ldots, m$ we have $\mu_i(C'^t) \leq \mu_i(C^t)$, then also $\mu_i(C') \leq \mu_i(C)$ for $i = 1, \ldots, n$.

We shall call an ε-dependent square matrix S_ε quasi-orthogonal if there exists an orthogonal matrix S such that

$$S_\varepsilon \; = \; S + \mathcal{O}(\varepsilon^\infty) \quad .$$

Remark D.3. *The transposed of a quasi-orthogonal matrix and the product of two quasi-orthogonal matrices are again quasi-orthogonal. Moreover every quasi-orthogonal matrix is invertible for* ε *sufficiently small, with quasi-orthogonal inverse. Note also that*

$$\|C_\varepsilon\| \; \leq \; 1 + \mathcal{O}(\varepsilon^\infty) \tag{D.2}$$

if C_ε *is quasi-orthogonal.*

[43] Indeed, if u is an eigenvector of C^tC, then Cu is eigenvector of CC^t with same eigenvalue, provided that $Cu \neq 0$, and an analogous statement holds for an eigenvector v of CC^t. That C and C^t have the same non-zero singular values follows also immediately from the singular value decomposition.

We say that two ε-dependent $m \times n$ matrices C_ε, C'_ε are quasi-equivalent if there exists an $m \times m$ quasi-orthogonal matrix S_ε and an $n \times n$ quasi-orthogonal matrix R_ε such that

$$C'_\varepsilon \; = \; S_\varepsilon \; C_\varepsilon \; R_\varepsilon \quad .$$

By Remark D.3 this is an equivalence relation.

The proof of Theorem D.1 is based on the following simple lemma.

Lemma D.4. *Let C_ε, C'_ε be $m \times n$ quasi-equivalent matrices. Then*

$$\mu_i(C'_\varepsilon) \; = \; \mu_i(C_\varepsilon) \quad \big(\, 1 + \mathcal{O}(\varepsilon^\infty) \, \big) \quad . \tag{D.3}$$

Proof. Let S and C be respectively an $n \times n$ and an $n \times m$ matrix. From the inequality $\|SCx\|^2 \leq \|S\|^2 \|Cx\|^2$, valid for every $x \in \mathbb{R}^n$, and from the min-max theorem for symmetric matrices one gets for every $i = 1, \ldots, n$

$$\mu_i(SC) \; \leq \; \|S\| \; \mu_i(C) \quad . \tag{D.4}$$

Similarly, if R is an $m \times m$ matrix, using $\|R^t\| = \|R\|$, one gets for every $i = 1, \ldots, m$

$$\mu_i((CR)^t) \; = \; \mu_i(R^t C^t) \; \leq \; \|R\| \; \mu_i(C^t) \quad ,$$

implying for $i = 1, \ldots, n$

$$\mu_i(CR) \quad \leq \; \|R\| \; \mu_i(C) \quad . \tag{D.5}$$

The inequalities (D.4),(D.5) together with (D.2) give (D.3), using that by assumption there exist quasi-orthogonal matrices S_ε and R_ε such that $C'_\varepsilon \; = \; S_\varepsilon \; C_\varepsilon \; R_\varepsilon$ and using that $C_\varepsilon = S_\varepsilon^{-1} \; C'_\varepsilon \; R_\varepsilon^{-1}$.

□

Proof of Theorem D.1. We will show that B_ε is quasi-equivalent to a diagonal $m_1 \times m_0$ matrix $D_\varepsilon = (D_{i,j,\varepsilon})_{i,j}$, satisfying for $i = 1, \ldots, m_0 - 1$

$$D_{i,i,\varepsilon} \; = \; \langle f_{i,\varepsilon}, B_\varepsilon \; e_{i,\varepsilon} \rangle \quad \big(\, 1 + \mathcal{O}(\varepsilon^\infty) \, \big)$$

and $D_{m_0,m_0,\varepsilon} = 0$. Observe that this implies (D.1) by Lemma D.4, since $[\mu_i(B_\varepsilon)]^2 \; = \; \lambda_{i,\varepsilon}$.

Step 1

Define the $m_1 \times m_0$ matrix $B^{(1)}_\varepsilon := (B^{(1)}_{i,j,\varepsilon})_{i,j}$ as

$$B^{(1)}_{i,j,\varepsilon} \ := \ \langle f_{i,\varepsilon}, B_\varepsilon \ e_{j,\varepsilon} \rangle$$

and observe that, writing the $e_{i,\varepsilon}$'s and $f_{j,\varepsilon}$'s as column vectors, and letting $E_\varepsilon = (e_{1,\varepsilon}, \ldots, e_{m_0,\varepsilon})$ and $F_\varepsilon = (f_{2,\varepsilon}, \ldots, f_{m_1+1,\varepsilon})$ we have

$$B^{(1)}_\varepsilon \ = \ F^t_\varepsilon \ B_\varepsilon \ E_\varepsilon \quad .$$

From assumption (i) it follows that F^t_ε and E_ε are quasi-orthogonal, and therefore $B^{(1)}_\varepsilon$ and B_ε are quasi-equivalent. Note that the m_0-th column of $B^{(1)}$ is zero. If $B^{(1)}$ happens to be diagonal the proof is thus completed. Otherwise one can proceed with a Gaussian-type elimination to diagonalize $B^{(1)}$, as explained in Step 2.

Step 2

For $k, l = 1, \ldots, m_1$ and $\alpha \in \mathbb{R}$ define the left elementary matrix

$$S(k,l;\alpha) \ := \ \mathrm{Id} \ + \alpha E(k,l) \quad ,$$

where Id denotes the $m_1 \times m_1$ identity matrix and $E_{k,l}$ is the $m_1 \times m_1$ matrix with (k,l)-th entry equal to 1 and all other entries equal to zero. Observe that multiplying $S(k,l;\alpha)$ on the left of an $m_1 \times m_0$ matrix C has the effect of adding to the k-th row of C α times the l-th row of C.

Similarly one defines for $k, l = 1, \ldots, m_0$ and $\alpha \in \mathbb{R}$ an $m_0 \times m_0$ right elementary matrix $R(k,l;\alpha)$ which by multiplcation on the right operates analogously on columns of an $m_1 \times m_0$ matrix.

Note that $\alpha_\varepsilon = \mathcal{O}(\varepsilon^\infty)$ implies that $S_{k,l;\alpha_\varepsilon}$ and $R_{k,l;\alpha_\varepsilon}$ are quasi-orthogonal.

If $B^{(1)}_\varepsilon$ has non-vanishing offdiagonal entry on the first column, say at row $k = 2, \ldots, m_1$, we let

$$B^{(2)}_\varepsilon \ := \ S(k,1;\langle f_{1,\varepsilon}, B_\varepsilon e_{1,\varepsilon} \rangle) \ B^{(1)}_\varepsilon \quad .$$

We have now $B^{(2)}_{k,1,\varepsilon} = 0$. Moreover, using assumption (ii),

$$B^{(2)}_{k,k,\varepsilon} \ = \ \langle f_{k,\varepsilon}, B_\varepsilon \ e_{k,\varepsilon} \rangle \ \ \big(\ 1 + \mathcal{O}(\varepsilon^\infty) \ \big) \quad , \tag{D.6}$$

while for $k' \neq k, 1$

$$B^{(2)}_{k,k',\varepsilon} \ = \ \mathcal{O}(\varepsilon^\infty) \ \langle f_{k',\varepsilon}, B_\varepsilon \ e_{k',\varepsilon} \rangle \quad . \tag{D.7}$$

Repeating this procedure at most $m_1 - 2$ times, one eliminates all the non-zero off-diagonal entries of the first column, obtaining a matrix $B^{(3)}_\varepsilon$, still quasi-equivalent to B_ε and satisfying (D.6) and (D.7) for every $k = 2, \ldots, m_1$.

Similarly, using the right elementary matrix, one eliminates all the non-zero off-diagonal entries of the first row, obtaining a matrix $B_\varepsilon^{(4)}$, still quasi-equivalent to B_ε and satisfying (D.6) and (D.7) for every $k = 2, \ldots, m_1$.

The procedure can be repeated for the second column and second row, and continuing this way one obtains in the end a diagonal matrix D_ε with the properties announced at the beginning of the proof. $\square$

Notation for asymptotic expansions.

We use in this work the following standard notation. If $N \in \mathbb{N}_0$ and $\nu_\varepsilon \in \mathbb{R}$ for $\varepsilon > 0$,

$$\nu_\varepsilon = \mathcal{O}(\varepsilon^N)$$

means that there exist constants $C_1, C_2 > 0$ such that $|\nu_\varepsilon| \le C_1\ \varepsilon^N$ for $\varepsilon \in (0, C_2)$. If there exists a sequence $\{\hat{\nu}_k\}_{k\in\mathbb{N}_0} \subset \mathbb{R}$ such that for every $N \in \mathbb{N}_0$

$$\nu_\varepsilon - \sum_{k=0}^{N} \varepsilon^k\ \hat{\nu}_k = \mathcal{O}(\varepsilon^{N+1})$$

we write for short

$$\nu_\varepsilon \sim \sum_{k=0}^{\infty}\ \varepsilon^k\ \hat{\nu}_k \quad .$$

More generally, if instead of ν_ε we deal with smooth ε-dependent functions, we use the $\mathcal{O}$ and $\sim$ notation as follows: let $\Omega \subset M$ be open and for $\varepsilon > 0$ let $\alpha_\varepsilon \in C^\infty(\Omega; \mathbb{R}_a^{V^p,\mu})$ for some $p \in \mathbb{N}_0$. Assume there exists an $N \in \mathbb{N}_0$ such that for every $j \in \mathbb{N}_0$, every compact $K \subset \Omega$ and every $\mathbf{v} \in V^j$ there exist constants $C_1, C_2 > 0$ satisfying

$$\left\| \ \nabla^j_{\mathbf{v}}\ \alpha_\varepsilon(\zeta)\ \right\|_\mu \le C_1\ \varepsilon^N \quad \text{for } \varepsilon \in (0, C_2) \ \text{ and for every } \ \zeta \in K \quad .$$

In this case we write

$$\alpha_\varepsilon = \mathcal{O}(\varepsilon^N) \quad .$$

If there exists a sequence $\{\hat{\alpha}_k\}_{k\in\mathbb{N}_0}$ contained in $C^\infty(\Omega; \mathbb{R}_a^{V^p,\mu})$ such that for every $N \in \mathbb{N}_0$

$$\alpha_\varepsilon - \sum_{k=0}^{N}\ \varepsilon^k \quad \hat{\alpha}_k = \mathcal{O}(\varepsilon^{N+1})$$

we shall write for short

$$\alpha_\varepsilon \sim \sum_{k=0}^{\infty}\ \varepsilon^k \quad \hat{\alpha}_k \quad .$$

In particular $\alpha_\varepsilon \sim 0$ means that $\alpha_\varepsilon = \mathcal{O}(\varepsilon^N)$ for every $N \in \mathbb{N}_0$. In this case we write also $\alpha_\varepsilon = \mathcal{O}(\varepsilon^\infty)$.

Remark E.1. *Let $\Omega \subset M$ be open and $\alpha \in C^\infty(\Omega;\mathbb{R}_a^{V^p,\mu})$. Recall the definition of the scaled shift operator:*

$$(\tau_{\varepsilon *}\alpha)_{\mathbf{v}}(\zeta) = \alpha_{\mathbf{v}}(\zeta + \varepsilon\mathbf{v}/2)$$

appearing in the definition of the scalar product in $L^2(M\times V^p,\Lambda_{\varepsilon,\mu})$ given in (9.1)*. It can be easily seen that the property $\alpha_\varepsilon = \mathcal{O}(\varepsilon^N)$ for some $N\in\mathbb{N}_0$ is equivalent to the following:*

For every $j\in\mathbb{N}_0$, every compact $K\subset\Omega$ and every $\mathbf{v}\in V^j$ there exist constants $C_1, C_2 > 0$ satisfying

$$\Big\| \ \nabla^j_{\mathbf{v}}\ \tau_{\varepsilon *}\alpha_\varepsilon(\zeta)\ \Big\|_\mu \le C_1\ \varepsilon^N \quad \textit{for } \varepsilon\in(0,C_2) \ \ \textit{and for every} \ \ \zeta\in K \quad .$$

In fact this is the property one uses when estimating L^2 norms where the shift appears. Observe that, due to the fact that μ has finite support, $\tau_{\varepsilon *}\alpha_\varepsilon(\zeta)$ is well-defined for every $\varepsilon\in(0,C_2)$ and $\zeta\in K$ as long as C_2 is chosen sufficiently small.

Complements to Section 9.

Lemma E.2. *For $w_1, w_2\in V$ and $(\zeta,\xi)\in V\times V^*$*

$$\mathring{\mathfrak{m}}_{f;w_1,w_2}(\zeta,\xi) \ := \ \frac{1}{4}\sum_{\mathbf{s}\in\{-1,1\}^2} \operatorname{sign}(\mathbf{s}) \ \ e^{\frac{1}{2}\nabla_{s_1w_1-s_2w_2}f(\zeta)} \ \ \nabla^2_{s_1w_1,s_2w_2}f(\zeta)\ e^{-\frac{1}{2}i\xi_{s_1w_1+s_2w_2}} \ = \tag{E.1}$$

$$= \ \nabla^2_{w_1,w_2}f(\zeta)\ \cosh\frac{\nabla_{w_1}f - i\xi_{w_1}}{2} \ \cosh\frac{\nabla_{w_2}f + i\xi_{w_2}}{2} \quad .$$

In particular

$$\mathring{\mathfrak{m}}_{f;w,w}(\zeta,\xi) \ = \ \nabla^2_w f(\zeta)\ \Big(\ -\sin^2\frac{\xi_w}{2} + \cosh^2\frac{\nabla_w f(\zeta)}{2} \ \Big) \quad . \tag{E.2}$$

Proof. We have

$$\mathring{\mathfrak{m}}_{f;w_1,w_2}(\zeta,\xi) \ = \ \frac{1}{4}\sum_{\mathbf{s}\in\{-1,1\}^2} \ \nabla^2_{w_1,w_2}f(\zeta)\ e^{\frac{1}{2}\nabla_{s_1w_1-s_2w_2}f(\zeta)\ -\ \frac{1}{2}\mathrm{i}\xi_{s_1w_1+s_2w_2}} \ =$$

$$= \ \frac{1}{2}\ \ \nabla^2_{w_1,w_2}f(\zeta)\ \Big\{ \ \cosh\Big(\frac{1}{2}(\nabla_{w_1}f(\zeta) - \mathrm{i}\xi_{w_1}) \ - \ \frac{1}{2}(\nabla_{w_2}f(\zeta) + \mathrm{i}\xi_{w_2})\Big) \ +$$

$$+ \ \cosh\Big(\frac{1}{2}(\nabla_{w_1}f(\zeta) - \mathrm{i}\xi_{w_1}) \ + \ \frac{1}{2}(\nabla_{w_2}f(\zeta) + \mathrm{i}\xi_{w_2})\Big) \ \Big\} \quad .$$

Statement (E.1) follows now by using with $x = \frac{1}{2}(\nabla_{w_1} f(\zeta) - \mathrm{i}\xi_{w_1})$ and $y = \frac{1}{2}(\nabla_{w_2} f(\zeta) + \mathrm{i}\xi_{w_2}$ the identity $\cosh(x+y) = \cosh x \cosh y + \sinh x \sinh y$, implying $\cosh(x+y) + \cosh(x-y) = \cosh x \cosh y$.

Statement (E.2) follows by using the identity $\cosh(a+b)\cosh(a-b) = \sinh^2 a + \cosh^2 b$ with $a = \frac{1}{2}(\nabla_w f(\zeta)$ and $b = \mathrm{i}\xi_w$.

□

Lemma E.3.

(1) *As an operator in* $L^2(\varepsilon\mathbb{Z}^n;\mathbb{R})$

$$\tilde{\mathcal{H}}^{(0)}_{\rho_\varepsilon,\Lambda_{\varepsilon,\mu}} \;=\; \sum_{\gamma\in\mathbb{Z}^n} b_{\varepsilon,\gamma}\;\tau_{\varepsilon\gamma} \quad , \tag{E.3}$$

where $b_{\varepsilon,\gamma} : \mathbb{R}^n \to \mathbb{R}$ *for every* $\gamma \in \mathbb{R}^n$, $\varepsilon > 0$ *and*

$$b_{\varepsilon,\gamma} \;:=\; \begin{cases} \mu(\{\gamma\})\; \mathfrak{b}_{\rho_\varepsilon;\varepsilon\gamma,\varepsilon\gamma} & \text{if } \gamma = \pm(e^k_1)_k,\dots,\pm(e^k_N)_k \\ -\;\sum_{k=1}^N \mu_k\;\big(\;\mathfrak{b}_{\rho_\varepsilon;\varepsilon e_k,-\varepsilon e_k} \;+\; \mathfrak{b}_{\rho_\varepsilon;-e_k,e_k}\;\big) & \text{if } \gamma = 0 \\ 0 & \text{otherwise} \end{cases} \quad . \tag{E.4}$$

(2) *As an operator in* $L^2(\varepsilon\mathbb{Z}^n;\mathbb{R}^N,\mu)$

$$\tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\Lambda_{\varepsilon,\mu}} \;=\; \sum_{\gamma\in\mathbb{Z}^n} \big[\; B^d_{\varepsilon,\gamma} \;+\; B_{\varepsilon,\gamma}\;\big]\;\tau_{\varepsilon\gamma} \quad , \tag{E.5}$$

where $B^d_{\varepsilon,\gamma} = (B^d_{\varepsilon,\gamma;i,j})_{i,j=1,\dots,N}$, $B_{\varepsilon,\gamma} = (B_{\varepsilon,\gamma;i,j})_{i,j=1,\dots,N}$ *with* $B^d_{\varepsilon,\gamma;i,j}, B_{\varepsilon,\gamma;i,j} : \mathbb{R}^n \to \mathbb{R}$ *for every* $\gamma \in \mathbb{R}^n$, $\varepsilon > 0$, $i,j = 1,\dots,N$, *given by the following:* $B^d_{\varepsilon,\gamma;i,j} = 0$ *if* $i \neq j$ *and for* $i = 1\dots,N$

$$B^d_{\varepsilon,\gamma;i,i} \;:=\; \begin{cases} \mu(\{\gamma\})\; \mathcal{T}_{\varepsilon e_i}\;\mathfrak{b}_{\rho_\varepsilon;\varepsilon\gamma,\varepsilon\gamma} & \text{if } \gamma = \pm(e^k_1)_k,\dots,\pm(e^k_N)_k \\ -\;\sum_{k=1}^N \mu_k\big(\;\mathcal{T}_{\varepsilon e_i}\;\mathfrak{b}_{\rho_\varepsilon;\varepsilon e_k,-\varepsilon e_k} \;+\; \mathcal{T}_{\varepsilon e_i}\;\mathfrak{b}_{\rho_\varepsilon;-\varepsilon e_k,\varepsilon e_k}\;\big) & \text{if } \gamma = 0 \\ 0 & \text{otherwise} \end{cases} \quad . \tag{E.6}$$

Moreover for $i,j = 1,\dots,N$

$$B_{\varepsilon,\gamma;i,j} \;:=\; \begin{cases} 1_{\gamma,e_i}\;\mu_j\;\mathcal{T}_{\varepsilon e_i}\;\bar{\mathfrak{b}}_{\rho_\varepsilon;\varepsilon e_i,\varepsilon e_j} \;+\; 1_{\gamma,-e_j}\;\mu_j\;\mathcal{T}_{\varepsilon e_i}\;\bar{\mathfrak{b}}_{\rho_\varepsilon;-\varepsilon e_i,-\varepsilon e_j} & \text{if } \gamma = \pm(e^k_1)_k,\dots,\pm(e^k_N)_k \\ -\;\mu_j\;\mathcal{T}_{\varepsilon e_i}\;\bar{\mathfrak{b}}_{\rho_\varepsilon;-\varepsilon e_i,\varepsilon e_j} & \text{if } \gamma = 0 \\ -\;\mu_j\;\mathcal{T}_{\varepsilon e_i}\;\bar{\mathfrak{b}}_{\rho_\varepsilon;\varepsilon e_i,-\varepsilon e_j} & \text{if } \gamma = (e^k_i)_k - (e^k_j)_k \\ 0 & \text{otherwise} \end{cases} \quad . \tag{E.7}$$

Remark E.4. *For convenience we recall here the definitions of* $\mathfrak{b}_\rho$ *and* $\bar{\mathfrak{b}}_\rho$ *given in Remark 8.8:*

$$\mathfrak{b}_{\rho;w_1,w_2} \;:=\; -\; \frac{1}{\sqrt{\rho}}\; \mathcal{T}_{w_1}\; \rho\; \mathcal{T}_{w_2}\; \frac{1}{\sqrt{\rho}}$$

and

$$\bar{\mathfrak{b}}_{\rho;v_1,v_2} \;:=\; \mathfrak{b}_{\frac{1}{\rho};v_1,v_2} \;-\; \mathfrak{b}_{\rho;v_2,v_1} \quad .$$

Note that in particular

$$\mathfrak{b}_{\rho_\varepsilon;\varepsilon e_i,\varepsilon e_j}(x) \;=\; -\; \exp\frac{1}{\varepsilon}\Big[\; -2f(x+\varepsilon\frac{e_i}{2}) \;+\; f(x) \;+\; f(x+\varepsilon\frac{e_i+e_j}{2})\;\Big]$$

$$\mathcal{T}_{\varepsilon e_k}\; \mathfrak{b}_{\rho_\varepsilon;\varepsilon e_i,\varepsilon e_j}(x) \;=\; -\; \exp\frac{1}{\varepsilon}\Big[-2f(x+\varepsilon\frac{e_i+e_k}{2}) + f(x+\varepsilon\frac{e_k}{2}) + f(x+\varepsilon\frac{e_i+e_j+e_k}{2})\Big]$$

$$\begin{aligned}\mathcal{T}_{\varepsilon e_k}\; \bar{\mathfrak{b}}_{\rho_\varepsilon;\varepsilon e_i,\varepsilon e_j}(x) \;=\; -\; &\exp\frac{1}{\varepsilon}\Big[\; 2f(x+\varepsilon\frac{e_i+e_k}{2}) \;-\; f(x+\varepsilon\frac{e_k}{2}) \;-\; f(x+\varepsilon\frac{e_i+e_j+e_k}{2})\;\Big] \;+\\ &+\; \exp\frac{1}{\varepsilon}\Big[\; -2f(x+\varepsilon\frac{e_j+e_k}{2}) \;+\; f(x+\varepsilon\frac{e_k}{2}) \;+\; f(x+\varepsilon\frac{e_i+e_j+e_k}{2})\;\Big] \quad .\end{aligned}$$

Remark E.5. *One can check for every* $\gamma, x \in \mathbb{R}^n$*,* $i,j = 1\ldots,N$ *the relations* $b_{\varepsilon,\gamma}(x) = b_{\varepsilon,-\gamma}(x+\varepsilon\gamma)$*,* $\mu_j B^d_{\varepsilon,\gamma;i,j}(x) = \mu_i B^d_{\varepsilon,-\gamma;j,i}(x+\varepsilon\gamma)$ *and* $\mu_j B_{\varepsilon,\gamma;i,j}(x) = \mu_i B_{\varepsilon,-\gamma;j,i}(x+\varepsilon\gamma)$ *which express the symmetry of* $\tilde{\mathcal{H}}^{(0)}_{\rho_\varepsilon,\Lambda_{\varepsilon,\mu}}$ *with respect to the scalar product of* $L^2(\varepsilon\mathbb{Z}^n;\mathbb{R})$ *and of* $\tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\Lambda_{\varepsilon,\mu}}$ *with respect to the scalar product of* $L^2(\varepsilon\mathbb{Z}^n;\mathbb{R}^{N,\mu})$.

Proof of Lemma E.3.

(i) (case $p=0$):

(Note that for $p=0$, $\tilde{\mathcal{H}}^{(0)}_{\rho_\varepsilon,\Lambda_{\varepsilon,\mu}}$ and $\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}}$ are defined by the same formula).

From Remark 8.8 it follows that

$$\mathcal{H}^{(0)}_{\rho_\varepsilon,\Lambda_{\mu_\varepsilon}} \;=\; \sum_{\mathbf{s}\in\{-1,1\}^2} \mathrm{sign}(\mathbf{s}) \sum_{j=1}^{N} \mu_j \left(\, \mathfrak{b}_{\rho_\varepsilon;\varepsilon s_1 e_j,\varepsilon s_2 e_j}\; \tau_{\frac{1}{2}\varepsilon(s_1+s_2)e_j} + \mathfrak{b}_{\rho_\varepsilon;-\varepsilon s_1 e_j,-\varepsilon s_2 e_j}\; \tau_{-\frac{1}{2}\varepsilon(s_1+s_2)e_j}\,\right) \;.$$

Considering the different signs case by case gives (E.3).

(ii) (case $p = 1$):

From Remark 8.8 it follows that

$$(\tilde{\mathcal{H}}^{(1)}_{\rho_\varepsilon,\Lambda_{\varepsilon,\mu}} \ \alpha \ )_i \quad = \sum_{\mathbf{s}\in\{-1,1\}^2} \mathrm{sign}(\mathbf{s}) \ \frac{1}{2} \sum_{j=1}^{N} \ \mu_j \ \Big\{$$

$$(\mathcal{T}_{\varepsilon e_i} \ \mathfrak{b}_{\rho_\varepsilon;\varepsilon s_1 e_j,\varepsilon s_2 e_j}) \ \tau_{\frac{1}{2}\varepsilon(s_1+s_2)e_j} \ \alpha_i \ + \ (\mathcal{T}_{\varepsilon e_i} \ \mathfrak{b}_{\rho_\varepsilon;-\varepsilon s_1 e_j,-\varepsilon s_2 e_j}) \ \tau_{-\frac{1}{2}\varepsilon(s_1+s_2)e_j} \ \alpha_i \ +$$

$$+ \ (\mathcal{T}_{\varepsilon e_i} \ \bar{\mathfrak{b}}_{\rho_\varepsilon;\varepsilon s_1 e_i,\varepsilon s_2 e_j}) \ \ \tau_{\frac{1}{2}\varepsilon(s_1+1)e_i+\frac{1}{2}\varepsilon(s_2-1)e_j} \ \alpha_j \ \ - \ \ (\mathcal{T}_{\varepsilon e_i} \ \bar{\mathfrak{b}}_{\rho_\varepsilon;\varepsilon s_1 e_i,-\varepsilon s_2 e_j}) \ \ \tau_{\frac{1}{2}\varepsilon(s_1+1)e_i+\frac{1}{2}\varepsilon(-s_2-1)e_j} \ \alpha_j \ \Big\}$$

Again considering the different signs case by case gives (E.5).

□

For the next Lemma recall that q_γ, D_γ and G_γ were defined in (E.6), (9.14) and (9.15) as follows:

$$q_\gamma \ := \begin{cases} - \ \frac{1}{4} \ \mu(\{\gamma\}) \ \nabla^2_\gamma f & \text{if } \gamma = \pm(e^k_1)_k, \ldots, \pm(e^k_N)_k \\ - \ \frac{1}{2} \ \sum_{j=1}^N \mu_j \ \nabla^2_{e_j} f \ \cosh \nabla_{e_j} f & \text{if } \gamma = 0 \\ 0 & \text{otherwise} \end{cases} ,$$

$$D_{\gamma;i,i} \ := \begin{cases} q_\gamma & \text{if } \gamma = \pm(e^k_1)_k, \ldots, \pm(e^k_N)_k \\ q_\gamma \ + \ \sum_{k=1}^N \mu_k \ \nabla^2_{e_k,e_i} f \ \sinh \nabla_{e_k} f & \text{if } \gamma = 0 \\ 0 & \text{otherwise} \end{cases} ,$$

$$G_{\gamma;i,j} \ := \begin{cases} \frac{1}{2}\mu_j \ \nabla^2_{e_i,e_j} f \ \big(\ 1_{\gamma,e_i} \ e^{\frac{1}{2}\nabla_{e_i-e_j} f} \ + \ 1_{\gamma,-e_j} \ e^{-\frac{1}{2}\nabla_{e_i-e_j} f} \ \big) & \text{if } \gamma = \pm(e^k_1)_k, \ldots, \pm(e^k_N)_k \\ \frac{1}{2}\mu_j \ \nabla^2_{e_i,e_j} f \ e^{-\frac{1}{2}\nabla_{e_i+e_j} f} + \frac{1}{8}\mu_j \big(\ \nabla^2_{e_i} f + \nabla^2_{e_j} f \ \big) \sinh \frac{1}{2}\nabla_{e_i+e_j} f & \text{if } \gamma = 0 \\ \frac{1}{2}\mu_j \ \nabla^2_{e_i,e_j} f \ e^{\frac{1}{2}\nabla_{e_i+e_j} f} & \text{if } \gamma = (e^k_i)_k - (e^k_j)_k \\ 0 & \text{otherwise} \end{cases}$$

Recall also that

$$V(x) \ := \ \sum_{j=1}^N 4\mu_j \ \sinh^2 \frac{\nabla_{e_j} f(x)}{2} \ = \ \sum_{j=1}^N 2\mu_j \ [\cosh \nabla_{e_j} f(x) \ - \ 1] \ .$$

Lemma E.6.

Let $b_{\varepsilon,\gamma}$, $B^d_{\varepsilon,\gamma}$ *and* $B_{\varepsilon,\gamma}$ *as defined in* (E.4), (E.6) *and* (E.7). *Then there exist for* $\varepsilon > 0$, *every* $\gamma \in \mathbb{R}^n$ *and* $i, j = 1, \ldots, N$ *functions* $\tilde{b}_{\varepsilon,\gamma}, \tilde{B}^d_{\varepsilon,\gamma;i,j}, \tilde{B}_{\varepsilon,\gamma;i,j} \in C^\infty(\mathbb{R}^n; \mathbb{R})$ *such that with* $\tilde{B}^d_{\varepsilon,\gamma} = (\tilde{B}^d_{\varepsilon,\gamma;i,j})_{i,j}$ *and* $\tilde{B}_{\varepsilon,\gamma} = (\tilde{B}_{\varepsilon,\gamma;i,j})$

$$\tilde{b}_{\varepsilon,\gamma} \;=\; \mathcal{O}(1) \quad , \quad \tilde{B}^d_{\varepsilon,\gamma} \;=\; \mathcal{O}(1) \quad , \tilde{B}_{\varepsilon,\gamma} \;=\; \mathcal{O}(1)$$

and

$$b_{\varepsilon,\gamma} \;=\; \begin{cases} -\mu(\{\gamma\}) \;+\; \varepsilon\,[q_\gamma \;+\; \varepsilon\;\tilde{b}_{\varepsilon,\gamma}\;] & \textit{if } \gamma = \pm(e^k_1)_k, \ldots, \pm(e^k_N)_k \\ 2N \;+\; V \;+\; \varepsilon\,[q_\gamma \;+\; \varepsilon\;\tilde{b}_{\varepsilon,\gamma}\;] & \textit{if } \gamma = 0 \\ 0 & \textit{otherwise} \end{cases} \quad ,$$

$$B^d_{\varepsilon,\gamma} \;=\; \begin{cases} -\mu(\{\gamma\}) \;+\; \varepsilon\,[D_\gamma \;+\; \varepsilon\;\tilde{B}^d_{\varepsilon,\gamma}\;] & \textit{if } \gamma = \pm(e^k_1)_k, \ldots, \pm(e^k_N)_k \\ 2N \;+\; V \;+\; \varepsilon\,[D_\gamma \;+\; \varepsilon\;\tilde{B}^d_{\varepsilon,\gamma}\;] & \textit{if } \gamma = 0 \\ 0 & \textit{otherwise} \end{cases} \quad ,$$

$$B_{\varepsilon,\gamma} \;=\varepsilon\,[G_\gamma \;+\; \varepsilon\;\tilde{B}_{\varepsilon,\gamma}\;] \quad .$$

Proof. Recall Remark E.4.

Case I: $b_{\varepsilon,\gamma}$

We have by Taylor expansion of f

$$\mathfrak{b}_{\rho_\varepsilon;\varepsilon e_i,\varepsilon e_j}(x) \;:=\; -\;\exp\frac{1}{\varepsilon}\Big[\; -2f(x+\varepsilon\frac{e_i}{2}) \;+\; f(x) \;+\; f(x+\varepsilon\frac{e_i+e_j}{2})\;\Big] \;=$$
$$=\; -\;\exp\Big[\; -\frac{1}{2}\nabla_{e_i-e_j}f(x)\Big] \;\;\exp\Big[\;\varepsilon\frac{1}{4}\big(-\frac{1}{2}\nabla^2_{e_i}f(x)+\frac{1}{2}\nabla^2_{e_j}f(x)+\nabla^2_{e_i,e_j}f(x)+\mathcal{O}(\varepsilon)\big)\Big] \quad .$$

Case Ia: $b_{\varepsilon,\gamma}$ with $\gamma = \pm e_1, \ldots, \pm e_N$. Then

$$b_{\varepsilon,\gamma} \;:=\; \mu(\{\gamma\})\;\mathfrak{b}_{\rho_\varepsilon;\varepsilon\gamma,\varepsilon\gamma} \;=\; -\mu(\{\gamma\}) \;\;\exp\Big[\;\varepsilon\frac{1}{4}\big(\nabla^2_{\gamma,\gamma}f+\mathcal{O}(\varepsilon)\big)\Big] \quad .$$

Case Ib: $b_{\varepsilon,\gamma}$ with $\gamma = 0$. Then

$$b_{\varepsilon,\gamma} \;:=\; -\;\sum_{k=1}^{N}\mu_k\;\Big(\;\mathfrak{b}_{\rho_\varepsilon;\varepsilon e_k,-\varepsilon e_k} \;+\; \mathfrak{b}_{\rho_\varepsilon;-\varepsilon e_k,\varepsilon e_k}\;\Big) \;=$$

$$= \sum_{k=1}^{N} \mu_k \Big(\ \exp\big[-\nabla_{e_k} f\big] \ \exp\big[\varepsilon\frac{1}{4}\big(-\nabla^2_{e_k} f + \mathcal{O}(\varepsilon)\big)\big] +$$

$$+ \ \exp\big[\nabla_{e_k} f\big] \ \exp\big[\varepsilon\frac{1}{4}\big(-\nabla^2_{e_k} f + \mathcal{O}(\varepsilon)\big)\big] \ \Big) \ .$$

Case II: $B^d_{\varepsilon,\gamma}$

Taylor expanding f we get

$$\mathcal{T}_{\varepsilon e_k} \ \mathfrak{b}_{\rho_\varepsilon;\varepsilon e_i,\varepsilon e_j} \ = \ - \ \exp\big[-\frac{1}{2}\nabla_{e_i-e_j} f\big] \ \times$$

$$\times \ \exp\big[\varepsilon\frac{1}{4}\big(-\frac{1}{2}\nabla^2_{e_i} f + \frac{1}{2}\nabla^2_{e_j} f + \nabla^2_{e_i,e_j} f - \nabla^2_{e_i,e_k} f + \nabla^2_{e_j,e_k} f + \mathcal{O}(\varepsilon)\big)\big] \ .$$

Case IIa: $B^d_{\varepsilon,\gamma;i,i}$ with $\gamma = \pm e_1, \ldots, \pm e_N$. Then

$$B^d_{\varepsilon,\gamma;i,i} \ := \ \mu(\{\gamma\}) \ \mathcal{T}_{\varepsilon e_i} \ \mathfrak{b}_{\rho_\varepsilon;\varepsilon\gamma,\varepsilon\gamma} \ = \ -\mu(\{\gamma\}) \ \exp\big[\varepsilon\frac{1}{4}\big(\nabla^2_{\gamma,\gamma} f + \mathcal{O}(\varepsilon)\big)\big] \ .$$

Case IIb: $B^d_{\varepsilon,\gamma;i,i}$ with $\gamma = 0$. Then

$$B^d_{\varepsilon,\gamma;i,i} \ := \ - \sum_{k=1}^{N} \mu_k \ \big(\ \mathcal{T}_{\varepsilon e_i} \ \mathfrak{b}_{\rho_\varepsilon;\varepsilon e_k,-\varepsilon e_k} \ + \ \mathcal{T}_{\varepsilon e_i} \ \mathfrak{b}_{\rho_\varepsilon;-\varepsilon e_k,\varepsilon e_k} \ \big) \ =$$

$$= \sum_{k=1}^{N} \mu_k \Big(\ \exp\big[-\nabla_{e_k} f\big] \ \exp\big[\varepsilon\frac{1}{4}\big(-\nabla^2_{e_k} f - 2\nabla^2_{e_k,e_i} f + \mathcal{O}(\varepsilon)\big)\big] +$$

$$+ \ \exp\big[\nabla_{e_k} f\big] \ \exp\big[\varepsilon\frac{1}{4}\big(-\nabla^2_{e_k} f + 2\nabla^2_{e_k,e_i} f + \mathcal{O}(\varepsilon)\big)\big] \ \Big) \ .$$

Case III: $B_{\varepsilon,\gamma}$

Taylor expanding f we get

$$\mathcal{T}_{\varepsilon e_k} \ \bar{\mathfrak{b}}_{\rho_\varepsilon;\varepsilon e_i,\varepsilon e_j} \ := \mathcal{T}_{\varepsilon e_k} \ \mathfrak{b}_{\frac{1}{\rho_\varepsilon};\varepsilon e_i,\varepsilon e_j} \ - \ \mathcal{T}_{\varepsilon e_k} \ \mathfrak{b}_{\rho_\varepsilon;\varepsilon e_j,\varepsilon e_i} \ =$$

$$= \ - \ \exp\big[\frac{1}{2}\nabla_{e_i-e_j} f\big] \ \times$$

$$\times \ \exp\big[\varepsilon\frac{1}{4}\big(\frac{1}{2}\nabla^2_{e_i} f - \frac{1}{2}\nabla^2_{e_j} f - \nabla^2_{e_i,e_j} f + \nabla^2_{e_i,e_k} f - \nabla^2_{e_j,e_k} f + \mathcal{O}(\varepsilon)\big)\big] \ +$$

$$+ \ \exp\big[\frac{1}{2}\nabla_{e_i-e_j} f\big] \ \times$$

$$\times \ \exp\big[\varepsilon\frac{1}{4}\big(-\frac{1}{2}\nabla^2_{e_j} f + \frac{1}{2}\nabla^2_{e_i} f + \nabla^2_{e_i,e_j} f - \nabla^2_{e_j,e_k} f + \nabla^2_{e_i,e_k} f + \mathcal{O}(\varepsilon)\big)\big] \ .$$

Case IIIa': $B_{\varepsilon,\gamma;i,j}$ with $\gamma = e_i$ Then

$$\begin{aligned} B_{\varepsilon,\gamma;i,j} \; &:= \; \mu_j \; \mathcal{T}_{\varepsilon e_i} \; \bar{\mathfrak{b}}_{\rho_\varepsilon;\varepsilon e_i,\varepsilon e_j} \; = \\ &= \; - \, \mu_j \; \exp\big[\; \frac{1}{2}\nabla_{e_i - e_j} f \big] \; \times \\ &\times \; \exp\big[\; \varepsilon \frac{1}{4}\big(\frac{1}{2}\nabla^2_{e_i} f - \frac{1}{2}\nabla^2_{e_j} f - 2\nabla^2_{e_i,e_j} f + \nabla^2_{e_i,e_i} f + \mathcal{O}(\varepsilon)\big)\big] \; + \\ &+ \mu_j \; \exp\big[\; \frac{1}{2}\nabla_{e_i - e_j} f \big] \; \times \\ &\times \; \exp\big[\; \varepsilon \frac{1}{4}\big(- \frac{1}{2}\nabla^2_{e_j} f + \frac{1}{2}\nabla^2_{e_i} f + \nabla^2_{e_i,e_i} f + \mathcal{O}(\varepsilon)\big)\big] \quad . \end{aligned}$$

Case IIIa": $B_{\varepsilon,\gamma;i,j}$ with $\gamma = -e_1, \ldots, -e_N$. Then

$$\begin{aligned} B_{\varepsilon,\gamma;i,j} \; &:= \; \mu_j \; \mathcal{T}_{\varepsilon e_i} \; \bar{\mathfrak{b}}_{\rho_\varepsilon;-\varepsilon e_i,-\varepsilon e_j} \; = \\ &= \; - \, \mu_j \; \exp\big[\; - \frac{1}{2}\nabla_{e_i - e_j} f \big] \; \times \\ &\times \; \exp\big[\; \varepsilon \frac{1}{4}\big(\frac{1}{2}\nabla^2_{e_i} f - \frac{1}{2}\nabla^2_{e_j} f - \nabla^2_{e_i} f + \mathcal{O}(\varepsilon)\big)\big] \; + \\ &+ \mu_j \; \exp\big[\; - \frac{1}{2}\nabla_{e_i - e_j} f \big] \; \times \\ &\times \; \exp\big[\; \varepsilon \frac{1}{4}\big(- \frac{1}{2}\nabla^2_{e_j} f + \frac{1}{2}\nabla^2_{e_i} f + 2\nabla^2_{e_i,e_j} f - \nabla^2_{e_i} f + \mathcal{O}(\varepsilon)\big)\big] \quad . \end{aligned}$$

Case IIIb: $B_{\varepsilon,\gamma;i,j}$ with $\gamma = 0$. Then

$$\begin{aligned} B_{\varepsilon,\gamma;i,j} \; &= \; -\mu_j \; \mathcal{T}_{\varepsilon e_i} \; \bar{\mathfrak{b}}_{\rho_\varepsilon;-\varepsilon e_i,\varepsilon e_j} \; = \\ &= \; \mu_j \; \exp\big[\; - \frac{1}{2}\nabla_{e_i + e_j} f \big] \; \times \\ &\times \; \exp\big[\; \varepsilon \frac{1}{4}\big(\frac{1}{2}\nabla^2_{e_i} f - \frac{1}{2}\nabla^2_{e_j} f - \nabla^2_{e_i} f + \mathcal{O}(\varepsilon)\big)\big] \; + \\ &- \mu_j \; \exp\big[\; - \frac{1}{2}\nabla_{e_i + e_j} f \big] \; \times \\ &\times \; \exp\big[\; \varepsilon \frac{1}{4}\big(- \frac{1}{2}\nabla^2_{e_j} f + \frac{1}{2}\nabla^2_{e_i} f - 2\nabla^2_{e_i,e_j} f - \nabla^2_{e_i} f + \mathcal{O}(\varepsilon)\big)\big] \quad . \end{aligned}$$

Case IIIc: $B_{\varepsilon,\gamma;i,j}$ with $\gamma = e_i - e_j$. Then

$$
\begin{aligned}
B_{\varepsilon,\gamma;i,j} \;&=\; -\mu_j \;\mathcal{T}_{\varepsilon e_i}\;\bar{\mathfrak{b}}_{\rho_\varepsilon;\varepsilon e_i,-\varepsilon e_j} \;=\\
&=\; \mu_j \exp\big[\,\frac{1}{2}\nabla_{e_i+e_j} f\big]\;\times\\
\times\;\exp\big[\,\varepsilon\frac{1}{4}\big(\frac{1}{2}\nabla^2_{e_i} f &- \frac{1}{2}\nabla^2_{e_j} f + 2\nabla^2_{e_i,e_j} f + \nabla^2_{e_i} f + \mathcal{O}(\varepsilon)\big)\big] \;+\\
&-\;\mu_j\;\exp\big[\,\frac{1}{2}\nabla_{e_i+e_j} f\big]\;\times\\
\times\;\exp\big[\,\varepsilon\frac{1}{4}\big(&-\frac{1}{2}\nabla^2_{e_j} f + \frac{1}{2}\nabla^2_{e_i} f + \nabla^2_{e_i} f + \mathcal{O}(\varepsilon)\big)\big]\quad .
\end{aligned}
$$

The result follows then by expanding in each case the exponential depending on ε. $\square$

Lemma E.7.

With the notation as in Lemma E.6 and with $q_{\varepsilon,\gamma} := q_\gamma + \varepsilon\tilde{b}_{\varepsilon,\gamma}$, $Q_{\varepsilon,\gamma} := D_\gamma + G_\gamma + \varepsilon[\tilde{B}^d_{\varepsilon,\gamma} + \tilde{B}_{\varepsilon,\gamma}]$ *the following holds: there exists a constant* $C > 0$ *and a compact* $K \subset \mathbb{R}^n$ *such that for* $x \in \mathbb{R}^n \setminus K$

$$\sum_{\gamma\in\mathbb{Z}^n} \big(\;|q_{\varepsilon,\gamma}(x)| \;+\; \|Q_{\varepsilon,\gamma}(x)\|\;\big) \;\le\; C\;V(x) \quad .$$

Proof. Due to Assumption II.2(ii) (implying that the Taylor expansion of f stops at the second order term) we have for fixed ε and large $|x|$

$$\sum_{\gamma\in\mathbb{Z}^n} |q_{\varepsilon,\gamma}(x)| \;\le$$

$$\le\;\sum_{k=1}^{N} 2\;\mu\{k\}\;\Big\{\;\cosh\nabla_{e_k} f(x)\;\;\frac{\big|e^{-\varepsilon\frac{1}{4}\nabla^2_{e_k} f(x)} - 1\big|}{\varepsilon}\;\;+\;\;\frac{\big|e^{\varepsilon\frac{1}{4}\nabla^2_{e_k} f(x)} - 1\big|}{\varepsilon}\;\Big\}\quad .$$

We conclude by observing that the fractions are uniformly bounded in x and ε due to the boundedness of the second derivatives of f.

The case of $\|Q_{\varepsilon,\gamma}(x)\|$ can be treated similarly by using the inequalities

$$e^{\frac{1}{2}|\nabla_{e_i} f|}\;e^{\frac{1}{2}|\nabla_{e_j} f|}\;\le\;\frac{1}{2}\big(\;e^{|\nabla_{e_i} f|}\;+\;e^{|\nabla_{e_j} f|}\;\big)\;\le\;\cosh\nabla_{e_i} f\;+\;\cosh\nabla_{e_j} f\quad .$$

$\square$

Complements to the proof of Theorem 11.1.

The following lemma deals with asymptotic expansions in powers of ε of certain coefficients appearing with the WKB-Ansatz of Lemma 11.8. In order to prove the mentioned asymptotic expansions it is convenient to express exponentials of sums as series involving Bell-polynomials. Recall that for $k \in \mathbb{N}_*$ the k-th complete Bell polynomial $\mathbb{B}_k : \mathbb{R}^k \to \mathbb{R}$ is defined via

$$\mathbb{B}_k\big[\ (x_j)_{j=1,\dots,k}\ \big] := \sum_{q=1}^{k} \sum_{\substack{(q_j)\in\mathbb{N}_0^{k-q+1} \\ \sum_j q_j = q \\ \sum_j j\ q_j = k}} k! \prod_{j=1}^{k-q+1} \frac{1}{q_j!}\Big(\frac{x_j}{j!}\Big)^{q_j} \quad .$$

For convenience we set $\mathbb{B}_0 := 1$. Observe that $\mathbb{B}_1\big[\ x\ \big] = x$ and $\mathbb{B}_2\big[\ (x_1,x_2)\ \big] = x_1^2 - x_2$. Given a sequence $(x_k)_{k\in\mathbb{N}_0}$ in $\mathbb{R}$ and an $N \in \mathbb{N}_0$ we shall denote by $(x_k^{(N)})_{k\in\mathbb{N}_0}$ the sequence truncated at N, defined by setting $x_k^{(N)} = x_k$ for $k \le N$ and $x_k^{(N)} = 0$ for $k \ge 0$. The utility of Bell-polynomials for our purposes stems from the fact that for every sequence $(x_k)_{k\in\mathbb{N}_0}$ in $\mathbb{R}$ and $N \in \mathbb{N}_0$ we have the identity

$$\exp\big[\ \sum_{k=1}^{N} \varepsilon^k\ \frac{x_k}{k!}\ \big] = \sum_{k=0}^{\infty} \varepsilon^k\ \ \frac{1}{k!}\mathbb{B}_k\big[\ (x_j^N)_{j=1,\dots,k}\ \ ,\ \big] \tag{E.8}$$

as can be easily checked by writing the exponential series, using the multinomial theorem for the power of sums and suitably rearranging terms in the series.

Lemma E.8.

Let $f, \varphi \in C^\infty(M;\mathbb{R})$ and define for every $w_1, w_2 \in V$ the function $\mathfrak{c}_{\varepsilon;w_1,w_2} \in C^\infty(M;\mathbb{R})$ by

$$\mathfrak{c}_{\varepsilon;w_1,w_2} := \mathfrak{c}_{f,\varepsilon;w_1,w_2} := e^{\frac{f+\varphi}{\varepsilon}}\ \ \mathcal{T}_{\varepsilon w_1}\ e^{\frac{-2f}{\varepsilon}}\ \ \mathcal{T}_{\varepsilon w_2}\ e^{\frac{f-\varphi}{\varepsilon}} \quad .$$

Then for every $N \in \mathbb{N}_0$

$$\mathfrak{c}_\varepsilon\ =\ \sum_{k=0}^{N}\ \varepsilon^k\ \ \hat{\mathfrak{c}}_k\ +\ \varepsilon^{N+1}\ \ r_{\mathfrak{c},\varepsilon}^{(N+1)} \quad ,$$

with

$$\hat{\mathfrak{c}}_{k;w_1,w_2} := \hat{\mathfrak{c}}_{f,k;w_1,w_2}\ := $$

$$:=\ e^{\frac{\nabla_{w_2}(f-\varphi)-\nabla_{w_1}(f+\varphi)}{2}}\ \ \frac{1}{k!}\mathbb{B}_k\Big[\ \Big(\ \frac{-2\nabla_{w_1}^j f + \nabla_{w_1+w_2}^j(f-\varphi)}{j2^j}\ \Big)_{j=2,\dots,k+1}\ \Big] \tag{E.9}$$

and $r^{(N+1)}_{\mathfrak{c},\varepsilon;w_1,w_2}$ *in* $C^\infty(M;\mathbb{R})$ *satisfying* $r^{(N+1)}_{\mathfrak{c},\varepsilon;w_1,w_2} = \mathcal{O}(1)$.

Proof. We have

$$\mathfrak{c}_{\varepsilon;w_1,w_2} \; = \; \exp \varepsilon^{-1} \big[\; \varphi + f - 2\mathcal{T}_{\varepsilon w_1} f + \mathcal{T}_{\varepsilon w_1} \mathcal{T}_{\varepsilon w_2} (f - \varphi) \; \big] \quad .$$

A Taylor expansion gives for every $N \in \mathbb{N}_0$

$$\varepsilon^{-1} \big[\; \varphi + f - 2\mathcal{T}_{\varepsilon w_1} f + \mathcal{T}_{\varepsilon w_1} \mathcal{T}_{\varepsilon w_2} (f - \varphi) \; \big] \; = \tag{E.10}$$

$$= \; \frac{\nabla_{w_2}(f-\varphi) - \nabla_{w_1}(f+\varphi)}{2} \quad + \quad \sum_{k=1}^{N} \varepsilon^k \; \frac{-2\nabla_{w_1}^{k+1} f \; + \; \nabla_{w_1+w_2}^{k+1}(f-\varphi)}{2^{k+1}(k+1)!} \quad +$$

$$+ \;\; \varepsilon^{N+1} \;\; \tilde{r}^{(N+1)}_{\mathfrak{c},\varepsilon;w_1,w_2} \quad ,$$

with

$$\tilde{r}^{(N+1)}_{\mathfrak{c},\varepsilon;w_1,w_2} \; := \; \int_0^1 dt \; \frac{(1-t)^{N+1}}{(N+1)!} \; \frac{-2\mathcal{T}_{\varepsilon t v_1} \;\; \nabla_{w_1}^{N+2} f + \mathcal{T}_{\varepsilon t (w_1+w_2)} \nabla_{w_1+w_2}^{N+2}(f-\varphi)}{2^{N+2}} \; = \; \mathcal{O}(1) \quad .$$

It follows from (E.10) using (E.8) that

$$\mathfrak{c}_\varepsilon \; = \; \sum_{k=0}^{N} \varepsilon^k \;\; \hat{\mathfrak{c}}_k \; + \; \varepsilon^{N+1} \;\; r^{(N+1)}_{\mathfrak{c},\varepsilon}$$

with the $\mathfrak{c}_k$'s as in (E.9) and with

$$\varepsilon^{N+1} \, r^{(N+1)}_{\mathfrak{c},\varepsilon} \; := \; \sum_{k=1}^{N} \varepsilon^k \;\; \hat{\mathfrak{c}}_k \; \big(\; \exp[\, \varepsilon^{N+1} \, \tilde{r}^{(N+1)}_{\mathfrak{c},\varepsilon} \,] - 1 \, \big) + \sum_{k=N+1}^{\infty} \varepsilon^k \;\; \hat{\mathfrak{c}}^{(N+1)}_k \; \exp[\, \varepsilon^{N+1} \, \tilde{r}^{(N+1)}_{\mathfrak{c},\varepsilon} \,]$$

and

$$\hat{\mathfrak{c}}^{(N+1)}_{k;w_1,w_2} \; :=$$

$$= \; e^{\frac{\nabla_{w_2}(f-\varphi) - \nabla_{w_1}(f+\varphi)}{2}} \;\; \frac{1}{k!} \mathbb{B}_k \Big[\; \Big(\; (\; \frac{-2\nabla_{w_1}^{j} f + \nabla_{w_1+w_2}^{j}(f-\varphi)}{j 2^j} \;\;)^{(N+1)} \; \Big)_{j=2,\ldots,k+1} \; \Big] \quad .$$

In particular, $r^{(N+1)}_{\mathfrak{c},\varepsilon} = \mathcal{O}(1)$ for every $N \in \mathbb{N}_0$ as claimed. $\square$

Remark E.9. *[Computation of* $\hat{\mathfrak{c}}_0$ *and* $\hat{\hat{\mathfrak{c}}}_0$*]*

We compute here more explicit formulas for the leading coefficients $\hat{\mathfrak{c}}_0$ *and* $\hat{\hat{\mathfrak{c}}}_0$*, the latter being defined as*

$$\hat{\hat{\mathfrak{c}}}_{0;w_1,w_2} \;\; := \;\; \hat{\hat{\mathfrak{c}}}_{f,0;w_1,w_2} \;\; := \;\; \hat{\mathfrak{c}}_{f,0;w_2,w_1} - \hat{\mathfrak{c}}_{-f,0;w_1,w_2} \quad .$$

Since by definition

$$\hat{\mathfrak{c}}_{f,k;w_1,w_2} =$$
$$= \ e^{\frac{\nabla_{w_2}(f-\varphi)-\nabla_{w_1}(f+\varphi)}{2}} \ \frac{1}{k!}\mathbb{B}_k\Big[\ \Big(\ \frac{-2\nabla^j_{v_1} f + \nabla^j_{v_1+v_2}(f-\varphi)}{j2^j} \ \Big)_{j=2,\ldots,k+1} \ \Big] \ \ ,$$

using $\mathbb{B}_0 = 1$*, we get for* $k = 0$

$$\hat{\mathfrak{c}}_{f,0;w_1,w_2} \ = e^{\frac{\nabla_{w_2}(f-\varphi)-\nabla_{w_1}(f+\varphi)}{2}} \quad . \tag{E.11}$$

In particular

$$\hat{\mathfrak{c}}_{f,0;w,w} = e^{-\nabla_w\varphi} \quad , \quad \hat{\mathfrak{c}}_{f,0;-w,-w} = e^{\nabla_w\varphi} \tag{E.12}$$

and

$$\hat{\mathfrak{c}}_{f,0;-w,w} = e^{\nabla_w f} \quad , \quad \hat{\mathfrak{c}}_{f,0;w,-w} = e^{-\nabla_w f} \quad .$$

It follows that

$$\sum_{\mathbf{s}\in\{-1,1\}^2} \mathrm{sign}(\mathbf{s}) \ \hat{\mathfrak{c}}_{f,0;s_1 w,s_2 w} = 2\cosh\nabla_w\varphi - 2\cosh\nabla_w f \quad . \tag{E.13}$$

To compute $\hat{\hat{\mathfrak{c}}}_{0;w_1,w_2}$ *observe that*

$$\hat{\mathfrak{c}}_{-f,0;w_1,w_2} = \exp\frac{1}{2}\Big[\ -\nabla_{w_2}(f+\varphi) - \nabla_{w_1}(\varphi - f) \ \Big] \quad . \tag{E.14}$$

Using (E.14) *together with* (E.11) *gives*

$$\hat{\hat{\mathfrak{c}}}_{0;w_1,w_2} \ = \hat{\mathfrak{c}}_{f,0;w_2,w_1} - \hat{\mathfrak{c}}_{-f,0;w_1,w_2} \ =$$
$$= \ \exp\frac{1}{2}\Big[\ \nabla_{w_1}(f-\varphi) - \nabla_{w_2}(f+\varphi) \ \Big] - \exp\frac{1}{2}\Big[\ -\nabla_{w_2}(f+\varphi) - \nabla_{w_1}(\varphi - f) \ \Big] \ =$$
$$= \ 0 \quad . \tag{E.15}$$

Remark E.10. *[Computation of* $\hat{\mathfrak{c}}_1$ *and* $\hat{\hat{\mathfrak{c}}}_1$*]*

We compute here more explicit formulas for the subleading coefficients $\hat{\mathfrak{c}}_1$ *and* $\hat{\hat{\mathfrak{c}}}_1$*, the latter being defined as*

$$\hat{\hat{\mathfrak{c}}}_{1;w_1,w_2} \ := \ \hat{\hat{\mathfrak{c}}}_{f,1;w_1,w_2} \ := \ \hat{\mathfrak{c}}_{f,1;w_2,w_1} - \hat{\mathfrak{c}}_{-f,1;w_1,w_2} \quad .$$

Since by definition

$$\hat{\mathfrak{c}}_{f,k;w_1,w_2} =$$
$$= \ e^{\frac{\nabla_{w_2}(f-\varphi)-\nabla_{w_1}(f+\varphi)}{2}} \ \frac{1}{k!}\mathbb{B}_k\Big[\ \Big(\ \frac{-2\nabla^j_{v_1} f + \nabla^j_{v_1+v_2}(f-\varphi)}{j2^j} \ \Big)_{j=2,\ldots,k+1} \ \Big] \ \ ,$$

using $\mathbb{B}_1(x) = x$*, we get*

$$\hat{\mathfrak{c}}_{f,1;w_1,w_2} = e^{\frac{\nabla_{w_2}(f-\varphi)-\nabla_{w_1}(f+\varphi)}{2}} \ \Big(\ \frac{-2\nabla^2_{w_1} f + \nabla^2_{w_1+w_2}(f-\varphi)}{8} \ \Big) \quad . \tag{E.16}$$

In particular

$$\hat{\mathfrak{c}}_{f,1;w,w} = \left(\frac{1}{4}\nabla^2_w f - \frac{1}{2}\nabla^2_w \varphi \right) e^{-\nabla_w \varphi} \quad , \quad \hat{\mathfrak{c}}_{f,1;-w,-w} = \left(\frac{1}{4}\nabla^2_w f - \frac{1}{2}\nabla^2_w \varphi \right) e^{\nabla_w \varphi}$$

and

$$\hat{\mathfrak{c}}_{f,1;-w,w} = -\frac{1}{4}\nabla^2_w f \ e^{\nabla_w f} \quad , \quad \hat{\mathfrak{c}}_{f,1;w,-w} = -\frac{1}{4}\nabla^2_w f \ e^{-\nabla_w f} \quad .$$

It follows that

$$\sum_{\mathbf{s}\in\{-1,1\}^2} \mathrm{sign}(\mathbf{s}) \ \hat{\mathfrak{c}}_{1;s_1 w, s_2 w} \ =$$

$$= \ \left(\frac{1}{2}\nabla^2_w f - \nabla^2_w \varphi \right) \ \cosh \nabla_w \varphi \ + \ \frac{1}{2}\nabla^2_w f \ \cosh \nabla_w f \quad .$$

Using the identities

$$\frac{1}{2}\cosh \nabla_w \varphi = \sinh^2 \frac{\nabla_w \varphi}{2} + \frac{1}{2} \quad \textit{and} \quad \frac{1}{2}\cosh \nabla_w f = \cosh^2 \frac{\nabla_w f}{2} - \frac{1}{2}$$

we also get

$$\sum_{\mathbf{s}\in\{-1,1\}^2} \mathrm{sign}(\mathbf{s}) \ \hat{\mathfrak{c}}_{1;s_1 w, s_2 w} \ =$$

$$= \ -\nabla^2_w \varphi \ \cosh \nabla_w \varphi \ + \ \nabla^2_w f \ \left(\ \sinh^2 \frac{\nabla_w \varphi}{2} + \cosh^2 \frac{\nabla_w f}{2} \ \right) \quad . \qquad \text{(E.17)}$$

Finally we notice that the identity $\cosh x = \cosh^2 \frac{x}{2} + \sinh^2 \frac{x}{2}$ *gives*

$$\sum_{\mathbf{s}\in\{-1,1\}^2} \mathrm{sign}(\mathbf{s}) \ \hat{\mathfrak{c}}_{f,\varphi,1;s_1 w, s_2 w} \ =$$

$$= \ -\nabla^2_w \varphi \ \left(\ \cosh^2 \frac{\nabla_w \varphi}{2} + \sinh^2 \frac{\nabla_w \varphi}{2} \ \right) \ + \ \nabla^2_w f \ \left(\ \sinh^2 \frac{\nabla_w \varphi}{2} + \cosh^2 \frac{\nabla_w f}{2} \ \right) \ =$$

$$= -\nabla^2_w \varphi \ \cosh \nabla_w \varphi + \nabla^2_w f \ \cosh \nabla_w f \ + \ \nabla^2_w f \ \left(\ \sinh^2 \frac{\nabla_w \varphi}{2} - \sinh^2 \frac{\nabla_w f}{2} \ \right) \quad .$$

To compute $\hat{\hat{\mathfrak{c}}}_1$ *observe that*

$$\hat{\mathfrak{c}}_{-f,1;w_1,w_2} = e^{\frac{-\nabla_{w_2}(f+\varphi) - \nabla_{w_1}(\varphi - f)}{2}} \ \left(\ \frac{2\nabla^2_{w_1} f - \nabla^2_{w_1+w_2}(f+\varphi)}{8} \ \right) \quad . \qquad \text{(E.18)}$$

Using (E.18) *together with* (E.16) *gives*

$$\hat{\hat{\mathfrak{c}}}_{1;w_1,w_2} \ = \ \hat{\mathfrak{c}}_{f,1;w_2,w_1} - \hat{\mathfrak{c}}_{-f,1;w_1,w_2} \ =$$

$$= \ \left(\ \frac{-2\nabla^2_{w_1} f + \nabla^2_{w_1+w_2}(f-\varphi) - 2\nabla^2_{w_2} f + \nabla^2_{w_1+w_2}(f+\varphi)}{8} \ \right) \times$$

$$\times \ \exp \frac{1}{2}\Big[\ \nabla_{w_1}(f-\varphi) - \nabla_{w_2}(f+\varphi) \ \Big] \quad .$$

Applying the identity

$$\nabla^2_{w_1+w_2} = \nabla^2_{w_1} + 2\nabla_{w_1}\nabla_{w_2} + \nabla^2_{w_2}$$

we get

$$\hat{\hat{\mathfrak{c}}}_{1;w_1,w_2} = \frac{1}{2}\nabla_{w_1}\nabla_{w_2}f \;\; \exp\frac{1}{2}\Big[\; \nabla_{w_1}(f-\varphi) - \nabla_{w_2}(f+\varphi)\;\Big] \quad .$$

It follows that

$$\sum_{\mathbf{s}\in\{-1,1\}^2} \mathrm{sign}(\mathbf{s})\; \hat{\hat{\mathfrak{c}}}_{1;s_1w_1,s_2w_2} \;\; =$$

$$= 2\nabla_{w_1}\nabla_{w_2}f \;\; \cosh\frac{\nabla_{w_1}(f-\varphi)}{2}\cosh\frac{\nabla_{w_2}(f+\varphi)}{2} \quad . \qquad \text{(E.19)}$$

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