Some Problems of Control of Semiclassical States for the Schrödinger Equation

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Introduction. We consider some statements of control problems for systems described by partial differential equation with a small parameter multiplying the higher-order derivatives (or, equivalently, a large parameter multiplying lower-order terms). It is widely known that the asymptotic behavior of solutions to such equations is described by the WKB approximation or the global analog, the Maslov canonical operator. In this framework, it is nature to consider the same class of asymptotic solutions for controlled systems closed by some choice of control provided that one deals with a feedback of a special form (see below).

The approach described in the present paper formally applies to two large classes of problems, namely, quantum-mechanical and wave propagation problems. Quantum-mechanical problems are a subtler application in that a feedback control normally relies

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on measurement whilst quantum measurement cannot usually be precise and often destroys the pre-existing state of the system. Hence a fully developed control theory of quantum systems (even an asymptotic one) should incorporate quantum measurement theory. However, here we do not touch these issues and consider a simplified statement in which the description of the measurement procedure itself is this paper we give some motivation as to why this simplified scheme still applies to quantum-mechanical problems. As to wave propagation problems, our statement applies in full generality. The solution of the problems stated in this paper will be considered elsewhere. At the end of this preprint, we have placed the transparencies of the talk given at the workshop “Partial Differential Equations” at Potsdam University in November, 2001.

Controlled Quantum Systems. We consider the system described by a differential equation of the form[1]

$$-ih\frac{\partial\psi}{\partial t} + H(u, \overset{2}{x}, \overset{1}{\widehat{p}})\psi = 0. \tag{1}$$

Here h is a small parameter ($h = k^{-1}$ in wave propagation problems, where k is the wave number), $\widehat{p} = -ih\ \partial/\partial x$, and

$$H : \mathcal{M} \times \mathbb{R}^{2n} \to \mathbb{R}$$

is a Hamilton function depending on a control parameter $u \in \mathcal{M}$ that range in some metric linear space $\mathcal{M}$. When considering program controls $u = u(t)$ as well as realizations of feedback controls, we assume that they depend on h regularly:

$$u(t) = u_0(t) + hu_1(t) + \dots .$$

Thus, the closed system with a given program control has the form

$$-ih\frac{\partial\psi}{\partial t} + H\big(u(t), \overset{2}{x}, \overset{1}{\widehat{p}}\big)\psi = 0 \tag{2}$$

and is just the Schrödinger equation (or the wave equation) with Hamilton function regularly depending on time. It is well known (e.g., see [2, 6]) that the asymptotic solutions of Eq. (2) as $h \to 0$ are described by Maslov's canonical operator. Hence for Eqs. (1) and (2) it is natural to consider special *semiclassical states* given by the canonical operator. Every semiclassical state corresponds to a quantized Lagrangian manifold Λ, a quantized measure $d\mu$ on that manifold, and an amplitude function φ on Λ satisfying the (physical) normalization condition

$$\int\limits_{\Lambda} |\varphi|^2 d\mu = 1.$$

[1]We use the notation of noncommutative analysis [3, 8]

The state itself has the form

$$\psi = K_{\Lambda,d\mu}\varphi,$$

where $K_{\Lambda,d\mu}$ is Maslov's canonical operator on Λ corresponding to the measure $d\mu$ and acting by the formula

$$K_{\Lambda,d\mu}\varphi = \sum_I K_I e_I \varphi,$$

where the K_I are local canonical operators in canonical charts $U_I, I \subset [n]$, and e_I is the partition of unity corresponding to the cover of Λ by the charts U_I. Details of the construction can be found, e.g., in [6].

The Asymptotic Controllability Problem. For semiclassical states of Eq. (1), we can state the following controllability problem.

> Given two states $\psi_1 = K_{\Lambda_1,d\mu_1}\varphi_1$ and $\psi_2 = K_{\Lambda_2,d\mu_2}\varphi_2$, does there exist a program control $h(t)$ regularly depending on h and such that the solution of Eq. (2) with the initial condition
>
> $$\psi|_{t=0} = \psi_1$$
>
> satisfies the condition
>
> $$\psi|_{t=T} = \psi_2 + O(h^N),$$
>
> where $T > 0$ is some number (given or not given in advance) and $N \geq 1$?

The canonical operator theory says that if the initial state in the Cauchy problem corresponds to some Lagrangian manifold, then the solution at time t corresponds to the shift of this manifold along the trajectories of the Hamiltonian system

$$\begin{cases} \dot{q} = H_p\big(u(t), q, p\big), \\ \dot{p} = H_q\big(u(t), q, p\big). \end{cases} \tag{3}$$

Furthermore, the measure is also shifted along the trajectories, while the amplitude function φ can be found from the transport equation along the same trajectories. Hence the canonical operator theory reduces the asymptotic controllability problems for the Schrödinger equation (1) to a hierarchic sequence of three controllability problems for the corresponding classical objects. Here the following control problem for the Hamiltonian system (3) is the main problem.

> Given two Lagrangian manifolds Λ_1 and Λ_2 in the phase space $\mathbb{R}^{2n}$, does there exist a control $u(t)$ such that the phase flow of system (3) closed by this control takes Λ_1 to Λ_2 in some time T?

Statements in which the control $u(t)$ is compactly supported on the interval $[0, T]$ seem to be most meaningful from the viewpoint of physics. In this case, the controllability problem is essentially a special case of a nonstationary inverse scattering problem. There is a vast literature concerning control of Hamiltonian systems as well as the inverse scattering problem, and here we do not dwell on the solution of the classical problems corresponding to a given quantum problem.

One can also consider a different asymptotic controllability problem for semiclassical states, which is in a sense *elementary* (the class of states related to this problem plays a fundamental role in quantum mechanics). Specifically, consider the semiclassical states given by Gaussian wave packets (see, e.g., [7])

$$G(q,p,A)(x,h) = \frac{1}{(2\pi h \det A)^{3n/4}} \exp\left\{\frac{i}{h}\Big[xp + \frac{i}{2}\langle x-q, A(x-q)\rangle\Big]\right\}, \tag{4}$$

where $\langle\ ,\ \rangle$ is the usual bilinear pairing and $A = A^* = A_1 + iA_2$ is a symmetric matrix with strictly positive imaginary part.

A system in the state (4) is localized in a neighborhood of the point (q, p) of the phase space, and the matrix A (more precisely, its imaginary part) describes the so-called "scattering ellipsoid."

The asymptotic controllability problem for wave packets is as follows.

> Given two Gaussian wave packets $G(q_1, p_1, A_1)$ and $G(q_2, p_2, A_2)$, is there a program control $u(t)$ regularly depending on h such that the solution of the Cauchy problem for Eq. (2) with the initial conditions
>
> $$\psi_{t=0} = G(q_1, p_1, A_1)$$
>
> satisfies the condition
>
> $$\psi|_{t=T} = G(q_2, p_2, A_2) + O(h^N),$$
>
> where $N \geq 1$ and $T > 0$ is some number (given or not given in advance)?

The semiclassical evolution of the Gaussian wave packet (4) under the Schrödinger equation (2) is as follows: the point (q, p) moves along a trajectory of the Hamiltonian system (3), while the shape factor A satisfies some matrix Riccati equation (too cumbersome to be presented here). A detailed exposition can be found, e.g., in [5].

Thus, the solution of the asymptotic controllability problem for Gaussian packets can be reduced to the pointwise controllability problem for the Hamiltonian system and the analysis of the above-mentioned Riccati equation.

The Stabilization Problem. Let us now dwell on the stabilization problem. Here one must choose the control u as a functional of the solution ψ so as to ensure that a given state ψ_0 be stable in the closed system. Thus, what form of feedback [1] is appropriate in asymptotic control problems? The feedback must satisfy the following conditions:

- it must be natural from the physical viewpoint;
- the closed system must be tractable by some known methods (or, otherwise, one has to develop some new methods).

In that connection, it seems natural to take the feedback in the form of a function of a sesquilinear functional of the solution. In particular, this guarantees that the implementations of controls regularly depend on h. In quantum mechanics, the interpretation of this is as follows: *the feedback is a function of the mean values of quantum-mechanical variables.* In the simplest case, the feedback has the form

$$u = \left(\psi, \vec{A}(\overset{2}{x}, \overset{1}{\widehat{p}})\psi\right)_{L^2(\mathbb{R}^n)} \tag{5}$$

where $\vec{A}(q,p)$ is a symbol ranging in the linear space $\mathcal{M}$ and numbers over operators indicate the order in which these operators act (e.g., see [3, 8]). Then the closed equation

$$-ih\frac{\partial\psi}{\partial t} + H\left[\left(\psi, \vec{A}(\overset{2}{x}, \overset{1}{\widehat{p}})\psi\right)_{L^2(\mathbb{R}^n)}, \overset{2}{x}, \overset{1}{\widehat{p}}\right]\psi = 0 \tag{6}$$

is a nonlinear Schrödinger equation (more precisely, a unitarily nonlinear equation). The word "unitarily" refers to the special form in which ψ occurs in the coefficients of the equation (the inner product). The stabilization problem can be stated in the framework of controls of this form as follows:

> For a semiclassical state $\psi = K_{(\Lambda,d\mu)}$ given by Maslov's canonical operator, find a feedback (5) such that this state will be a stable equilibrium of the closed system (6).

This problem, just as the previous ones, will be reduced to the corresponding classical problems by the methods for constructing semiclassical asymptotics for unitarily nonlinear equations.

Unitarily Nonlinear Equations. Let us briefly describe the above-mentioned methods. They were introduced in [4], where one can find a detailed exposition.

First, we give some definitions.

Definition 1. The space $S^{\infty}(\mathbb{R}^k)$ consists of functions $u(x) \in C^{\infty}(\mathbb{R}^k)$ such that

$$\exists\, m\, \forall\, l \quad \sup_{\mathbb{R}^k} (1+|x|)^{-m} \left| u^{(l)}(x) \right| < \infty \tag{7}$$

The convergence in this space is determined by the family of seminorms given by the suprema in (7). The space $S^{-\infty}(\mathbb{R}^k)$ is the (topological) dual space of $S^{\infty}(\mathbb{R}^k)$. Next, $G(\mathbb{R}^k)$ is the space of maps $f : \mathbb{R}^k \longrightarrow \mathbb{R}^k$ such that

$$\sup \frac{|f(x)|}{1+|x|} < \infty \quad \text{and} \quad \sup |f^{\alpha}(x)| < \infty$$

for every α.

Let us also introduce some notation concerning the symplectic structure. The variables in the symplectic space $\mathbb{R}^{2n}$ will be denoted by $z = (q, p)$. Then the symplectic form is

$$\omega^2 = \frac{1}{2} J\, dz \wedge dz,$$

where

$$J = \begin{pmatrix} 0 & E \\ -E & 0 \end{pmatrix}$$

is the matrix of the symplectic structure (the Darboux matrix).

Now we can introduce the notion of a classical Hamiltonian.

Definition 2. A *Hamiltonian* is a smooth map

$$\begin{aligned} H : S^{-\infty}(\mathbb{R}^{2n}) \times G(\mathbb{R}^{2n}) &\longrightarrow S^{\infty}(\mathbb{R}^{2n}), \\ (f, v) &\longmapsto H[f, v], \end{aligned}$$

such that

$$H[\gamma^* f, v \circ \gamma](z) \equiv H[f, \gamma](z)$$

for every canonical transformation $\gamma \in G(\mathbb{R}^{2n})$.

An example of a classical Hamiltonian is given by the formula

$$H[f, v](z) = H_0(z) + \int V(z, v(z')) f(z')\, dz',$$

where

$$dz' = \frac{(\omega^2)^{\wedge n}}{n!}.$$

Here $H_0(z)$ is the "nonperturbed" Hamiltonian, and the integral term describes the self-consistent particle interaction. Such Hamiltonians occur, e.g., in the classical Vlasov equations as well as the quantum Hartree and Hartree–Fock equations.

In the back of an integral term, we arrive at the ordinary Hamilton function. Thus, the new notion includes the old one. Associated with a given Hamilton function H are two important equations, namely, the Vlasov–Liouville equation and the Vlasov–Hamilton equation. They are analogs of the Liouille and Hamilton equations, respectively, of the ordinary classical mechanics.

The Vlasov–Liouville equation has the form

$$\frac{\partial F}{\partial t} + \{H[F, \mathrm{id}], F\} = 0, \tag{8}$$

where id is the identity map, $F \in S^{-\infty}(\mathbb{R}^{2n})$ is a given distribution (the *classical density function*), and

$$\{f, g\} = \left\langle J\frac{\partial f}{\partial z}, \frac{\partial g}{\partial z}\right\rangle$$

is the usual Poisson bracket.

The Vlasov–Hamilton equation has the form

$$\dot{Z} = V_{H[F_0, Z]}, \tag{9}$$

where

$$V_f = \left\langle J\frac{\partial f}{\partial z}, \frac{\partial}{\partial z}\right\rangle$$

is the Hamilton vector field and $Z \in G(\mathbb{R}^{2n})$ is the unknown map to be found. We equip this equation with the initial condition

$$Z|_{t=0} = \mathrm{id}\,. \tag{10}$$

In turns out that under some (rather weak) conditions on the Hamiltonian and the initial density function F_0, both the Vlasov–Hamilton and the Vlasov–Liouville equations are uniquely solvable, and their solutions are related by a simple, important formula.

Theorem 1. *Suppose that the classical Hamiltonian H and the initial function F_0 satisfy the following conditions:*

1) *The map*

$$\begin{aligned} G(\mathbb{R}^{2n}) &\longrightarrow S^{\infty}(\mathbb{R}^{2n}) \\ v &\longmapsto \frac{\partial H}{\partial z}[F_0, v] \end{aligned}$$

extends to be a Lipschitz continuous map in the L^2 topology;

2) *the derivative*

$$\frac{\partial^\alpha H}{\partial z^\alpha}[F_0, v]$$

is uniformly bounded for each $\alpha \geq 2$.

Then the Vlasov–Hamilton equation (9) *with the initial conditions* (10) *has a unique solution for all* t, *and moreover,*

1) $Z(t) \in G(\mathbb{R}^{2n})$ *for all* t;

2) $Z(t)$ *is a canonical transformation* [2] *for all* t;

3) (*corollary*) *if* Λ_0 *is a Lagrangian manifold, then* $\Lambda(t) = Z(t)\Lambda_0$ *is also a Lagrangian manifold for all* t;

4) *the Vlasov–Liouville equation* (8) *with the initial condition*

$$F|_{t=0} = F_0;$$

is uniquely solvable for all t, *and the solution has the form*

$$F(t) = (Z(t))^{-1} F_0.$$

The last assertion of the theorem is more or less trivial. The most difficult result concerning the existence of solutions of the Hamilton–Vlasov system can be proved essentially in the same way as the existence and uniqueness theorem for ordinary differential equations, that is, by Picard's method.

Now we introduce some objects related to the construction of the canonical operator on the Lagrangian manifolds obtained from the initial manifold by the Hamilton–Vlasov flow. The trajectories of the Hamilton–Vlasov equation are given by the formula

$$\begin{pmatrix} q(q_0, t) \\ p(p_0, t) \end{pmatrix} \stackrel{\text{def}}{=} Z(t) \begin{pmatrix} q_0 \\ p_0 \end{pmatrix}.$$

Consider a quantized Lagrangian manifold Λ_0 equipped with an action function Λ_0 and a quantized measure $d\mu_0$. For an arbitrary function $\varphi \in S^\infty(\mathbb{R}^{2n})$, we set

$$\langle F_0, \varphi \rangle = \int\limits_{\Lambda_0} \varphi|_{\Lambda_0} \, d\mu_0. \tag{11}$$

[2]Since the equation is nonlinear, these transformations fail to form a one-parameter group, except for the case in which the initial distribution is trajectory invariant.

Thus we have defined a classical density function F_0. Let $Z(t)$ be the corresponding solution of the Hamilton–Vlasov system, and let $\Lambda_t = Z(t)\Lambda_0$ be the corresponding family of Lagrangian manifolds. The action function on Λ_t is given by the formula

$$S_t = \big(Z(t)^{-1}\big)^* \Big\{ S_0 + \int_0^t [p\dot{q} - H[F_0, Z(t)](q,p)]\, d\tau \Big\}. \tag{12}$$

The Quantum Problem. Now we can describe the construction of semiclassical asymptotics for the closed equation (6). Suppose that the classical Hamiltonian occurring in the equation has the form

$$\mathcal{H}[\rho] = H[\rho, \mathrm{id}].$$

In other words, it is included in a family parametrized by canonical transformations.

In this case, to construct the asymptotics, one can use the above-mentioned machinery of classical mechanics for the Hamilton–Liouville equation. Thus, consider the unitarily nonlinear Schrödinger equation

$$-ih\frac{\partial\psi}{\partial t} + \widehat{\mathcal{H}}\psi = 0$$

with the initial conditions

$$\psi|_{t=0} = \psi_0(x) = K_{\Lambda_{0,d\mu}}\varphi(x),$$

where $K_{\Lambda_{0,d\mu}}$ is Maslov's canonical operator on the Lagrangian manifold Λ_0 equipped with the measure $d\mu$. To find the asymptotics of the solution, we first construct the asymptotics of the quantum density function

$$\rho_\psi(q,p) = \left(\frac{1}{2\pi h}\right)^{n/2} \psi(q)\overline{\widetilde{\psi}(p)} e^{-\frac{i}{h}qp}. \tag{13}$$

The equation for ρ_ψ (the Vlasov–Wigner equation) and the initial conditions have the form

$$\begin{cases} \dfrac{\partial\rho_\psi}{\partial t} + \frac{i}{h}\Big\{ H[\rho_\psi, \mathrm{id}]\Big(q^2, p - ih\overset{1}{\dfrac{\partial}{\partial q}}\Big) - H[\rho_\psi, \mathrm{id}]\Big(q - ih\overset{1}{\dfrac{\partial}{\partial p}}, \overset{2}{p}\Big)\Big\}\rho_\psi = 0 \\ \rho_\psi|_{t=0} = \rho_{\psi_0} \end{cases}. \tag{14}$$

For $t = 0$, the initial density function has the asymptotics

$$F|_{t=0} = |\varphi|^2 \delta_{\Lambda, d\mu} + O(h^2), \tag{15}$$

which can readily be verified with the help of the stationary phase method. Here $\delta_{\Lambda,d\mu}$ is the delta function on the initial Lagrangian manifold with the measure $d\mu$. We seek the density function in the form

$$\rho_\psi \simeq F + \sum_{k=0}^{\infty} (-ih)^k F^k. \tag{16}$$

Then for the leading term F of the density function we obtain the Liouville–Vlasov equation with the initial condition (15). The subsequent terms of the expansion are given by regular perturbation theory. Once we find the asymptotics of the density function, we can substitute it into the Hamiltonian, and then Eq. (13) becomes a *linear* equation for the function ψ, which can already be solved by the standard canonical operator method.

One can verify that the solution thus obtained just results in the density function that has been found by solving the Vlasov–Wigner equation.

The Stabilization Problem for the Schrödinger Equation with a Unitarily Nonlinear Control. We see that if the feedback has the form (5), then the unitarily nonlinear Schrödinger equation (6) can be solved by semiclassical asymptotic method.

Now let us state the semiclassical stabilization problem.

> For given system (1) and a semiclassical state $\psi_0 = K_{\Lambda,d\mu}\varphi$ given by Maslov's canonical operator on a quantized Lagrangian manifold with a measure $d\mu$ and an amplitude function φ, find a unitarily nonlinear feedback (5) such that the solution of the closed equation (6) with this feedback and the initial data ψ_0 satisfies the condition[3]
>
> $$\psi(t) = e^{\frac{i}{h}\lambda t}\psi + O(h^N) \tag{17}$$
>
> on the time interval $[0, T/h]$, where $N > 0$, $\lambda \in \mathbb{R}$, and $T > 0$ is independent of h.

Thus, one actually specks of finding a feedback such that the state ψ is a metastable state of the closed system. The number λ (which is independent of h or depends on h regularly) is naturally interpreted as the *energy* of this metastable state.

The construction of asymptotics of unitarily nonlinear equations (see the preceding section) reduces this stabilization problem to the study of invariant Lagrangian manifolds of the Hamilton–Vlasov and invariant solutions of the corresponding transport equation.

In closing, let us note that the choice of the control in the form (5) apparently permits one to sidestep issues related to the measurement procedure provided that this procedure is not separated from the substitution of the "measured" mean value into the equation (in other words, the control process itself is quantum rather than classical).

[3]This definition of asymptotic eigenfunctions is due to Maslov.

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