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Dedicated to the memory of Mark Iosifovich Vishik

On quantum averaging, quantum KAM, and quantum diffusion

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Abstract. For non-autonomous Hamiltonian systems and their quantizations this paper discusses properties of the quantized systems whose classical analogues constitute the subject of KAM theory and related areas: KAM theory proper, averaging theory, Nekhoroshev stability, and diffusion.

Bibliography: 31 titles.

Keywords: infinite-dimensional KAM theory, quantum diffusion, quantum adiabatic theorem.

Contents

1. Introduction

Consider a classical non-autonomous Hamiltonian system on the phase space $T^*\mathbb{T}^d = \mathbb{R}^d \times \mathbb{T}^d = \{(p,q)\}$ or $T^*\mathbb{R}^d = \mathbb{R}^d \times \mathbb{R}^d$ with Hamiltonian $H(p,q,t)$:

$$\dot p = -\nabla_q H, \qquad \dot q = \nabla_p H. \tag{1}$$

The corresponding quantum Hamiltonian operator is obtained from $H(p,q,t)$ by replacing the variable q_j, $j = 1,\dots,d$, by the operator which acts on

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complex functions $u(x)$ as multiplication by x_j, and replacing each p_j by the operator $(\hbar/i)(\partial/\partial x_j)$, where $\hbar$ is the Planck constant.[1] The Hamiltonian operator $\mathscr{H} = H((\hbar/i)\nabla_x, x, t)$ defines a quantum system. A classical problem from the very beginning of quantum mechanics has been to study the (spectral) properties of the operator $\mathscr{H}$ and the properties of the corresponding evolution equation

$$i\hbar\dot{u}(t,x) = \mathscr{H}u(t,x) \tag{2}$$

in their relation to those of the classical system (1).

For example, if

$$H(p,q,t) = |p|^2 + V(t,q), \tag{3}$$

then

$$\mathscr{H} = \mathscr{H}_t = -\hbar^2\Delta + V(t,x), \tag{4}$$

that is, $\mathscr{H}$ is the Schrödinger operator with potential V.

In this paper we discuss properties of the Hamiltonian operator $\mathscr{H}$ corresponding to properties of the system (1) described by the KAM (Kolmogorov–Arnold–Moser) theory and related theories, namely, by KAM theory proper, averaging, Nekhoroshev stability, and diffusion (this list is by no means canonical but reflects the authors' taste). We discuss results for quantum systems (2) which we regard as parallel to the indicated classical theories, restricting ourselves mostly to the case of periodic boundary conditions $x \in \mathbb{T}^d$ and assuming that $\hbar = \text{const}$. By rescaling x and t in the dynamical equations (2), (4) we can set $\hbar = 1$. But there is a discussion in § 6 concerning the semiclassical limit $\hbar \to 0$ when it is not appropriate to scale $\hbar$ to 1. There we consider the equations in the whole space $x \in \mathbb{R}^d$, since for periodic boundary conditions the corresponding results are less well developed.

All quantum results we discuss involve non-autonomous equations (2), (4), so their classical analogues are 'KAM related' results for the theory of non-autonomous Hamiltonian systems (3). We do not touch upon the very interesting, important, and complicated problem of constructing eigenfunctions of nearly integrable Hamiltonian operators by quantizing KAM tori of the corresponding autonomous Hamiltonian systems (see [23]).

Let $u(t)$ be a solution of (2), (4). Multiplying the equation by $\bar{u}$ and integrating over $\mathbb{T}^d$, we get that $\|u(t)\|^2_{L^2} = \text{const}$. We write $u(t,x) = \sum_s u_s(t)\varphi_s(x)$, where $\{\varphi_s\}$ are eigenfunctions of the 'unperturbed' Hamiltonian operator. Then $\sum_s |u_s(t)|^2 \equiv \text{const}$. What happens to the quantities $|u_s(t)|^2$ as t grows, that is, how is the total probability $\sum_s |u_s(t)|^2$ distributed among the states $s \in \mathbb{Z}^d$ when t is large? This is the question which is addressed by the theorems we discuss.

2. Quantum averaging

2.1. Averaging and adiabatic invariance. Suppose that a classical Hamiltonian (3) has the form

$$H(p,q,\varepsilon t) = H_\varepsilon = |p|^2 + V(\varepsilon t, q), \tag{5}$$

[1] This quantization rule is the most common, but it is far from the only one. More generally, one may replace q_j and p_j by any operators Q_j and P_j such that $[Q_j, P_k] = i\hbar\delta_{j,k}$, for all j and k.

where the unperturbed Hamiltonian $|p|^2+V(\tau,q)$, $\tau=\text{const}$, is integrable for any τ. Let I_j, $1\leqslant j\leqslant d$, be the corresponding actions. The classical averaging principle (see, for instance, [3], [25]) implies that each action is an adiabatic invariant, namely, if $u_\varepsilon(t)$ is a solution of the perturbed equation $(1)_{H=H_\varepsilon}$, then $I_j(u_\varepsilon(t))$ stays almost constant on time intervals of order ε^{-1}. The averaging principle is a heuristic statement, and it does not always lead to correct results. The adiabatic invariance for classical systems is discussed in more detail in § 6.

We now consider the corresponding quantum system

$$\dot u=-i(-\Delta u+V(\varepsilon t,x)u),\qquad x\in\mathbb{T}^d. \tag{6}$$

Assume that the function $V(\tau,x)$ is C^2-smooth and bounded, and denote by A_τ the linear operator in (6):

$$A_\tau=-\Delta+V(\tau,x).$$

Let $\{\varphi_s(\tau),\ s\in\mathbb{Z}^d\}$ and $\{\lambda_s(\tau)\}$ be the eigenvectors and eigenvalues of A_τ, where each $\lambda_s(\tau)$ is continuous in τ. Let $u(t,x)$ be a solution of (6) equal at $t=0$ to a pure state

$$u(0,x)=\varphi_{s_0}(0) \tag{7}$$

such that for each εt the number $\lambda_{s_0}(\varepsilon t)$ is an isolated eigenvalue of $A_{\varepsilon t}$ with constant multiplicity. We consider the series expansion of $u(t,x)$ with respect to the basis $\{\varphi_s(\tau),\ s\in\mathbb{Z}^d\}$:

$$u(t,x)=\sum_s u_s(t)\varphi_s(\varepsilon t).$$

The quantum adiabatic theorem says that $u(t,x)$ stays close to the eigenspace corresponding to $\lambda_{s_0}(\varepsilon t)$:

Theorem 2.1 (Born, Fock [8], and Kato [20]).

$$\sup_{0\leqslant t\leqslant\varepsilon^{-1}}\sum_{s:\ \lambda_s(\varepsilon t)\neq\lambda_{s_0}(\varepsilon t)}|u_s(t)|^2\to 0\quad as\quad \varepsilon\to 0. \tag{8}$$

This is a very general result which remains true for systems in the whole space (when $x\in\mathbb{R}^d$) if the operators $A_{\varepsilon t}$ have mixed spectrum but $\lambda_{s_0}(\varepsilon t)$ is always an isolated eigenvalue with constant multiplicity (see [25]). The case when this eigenvalue can be approached by other eigenvalues is considered in [4].

For both classical and quantum systems, adiabatic theorems are often considered on the infinite time interval $-\infty<t<\infty$ under the condition that the dependence of the potential V on the time disappears sufficiently fast as $t\to\pm\infty$ and the system is sufficiently smooth. For classical Hamiltonians with $d=1$ the difference between the values of the action on the trajectory for $t\to\pm\infty$ tends to 0 much faster than ε as $\varepsilon\to 0$ in this case; in the analytic case this difference is $O(\exp(-\text{const}/\varepsilon))$ (see [22] and references in [3], § 6.4.5). For quantum systems if all the probability is concentrated in states corresponding to the eigenvalue $\lambda_{s_0}(\tau)$ for $\tau\to-\infty$, then all but a very small remnant of the probability will be absorbed by these same states as $\tau\to+\infty$. In the analytic case this remnant is $O(\exp(-\text{const}/\varepsilon))$ [18], [29] (this result also follows from the calculus developed in [30]).

We will return to quantum adiabaticity in § 6. We note that there are also adiabatic theorems for systems where the Hamiltonian depends slowly not only on the time, but also on a part of the space variables (for example, see [3], § 6.4.1 for classical systems and [6] for quantum systems).

2.2. About Nekhoroshev's Theorem. Let us start with classical systems. Let $H_\varepsilon(p,q) = h_0(p) + \varepsilon h_1(p,q)$, where the function h_0 is analytic and steep (for instance, strictly convex; for the definition of steep functions see [28] and [25], [3]). Let $(p(t), q(t))$ be a solution of (1). Then there are $a, b > 0$ such that

$$|p(t) - p(0)| \leqslant \varepsilon^a \qquad \forall |t| \leqslant e^{\varepsilon^{-b}} \tag{9}$$

(see [28], [25], [3]). There are many related results. For example, let

$$H_\varepsilon(p,q,t) = h_0(p) + \varepsilon h_1(\omega t; p, q), \qquad \omega \in \mathbb{R}^N,$$

where h_1 is an analytic function on $\mathbb{T}^N \times \mathbb{R}^d \times \mathbb{T}^d$, $N \geqslant 1$. Then for a typical ω the estimate (9) holds. In particular, let us take

$$H_\varepsilon(p,q,t) = |p|^2 + \varepsilon V(\omega t, q).$$

The corresponding quantized Hamiltonian is the operator $-\Delta + \varepsilon V(\omega t, x)$, and the evolution equation is

$$\dot u = -i(-\Delta u + \varepsilon V(\omega t, x) u). \tag{10}$$

Is there an analogue of the Nekhoroshev estimate (9) for solutions of (10)? In other words, is it true that actions of the unperturbed system, evaluated along solutions of the perturbed equation (10), do not change much over an exponentially long time? It turns out that a weaker form of this assertion holds, even when $\varepsilon = 1$! Let us consider the equation

$$\dot u = -i(-\Delta u + V(t,x) u) \tag{11}$$

and the square of the rth Sobolev norm of u:

$$\|u\|_r^2 = \sum_{s \in \mathbb{Z}^d} |u_s|^2 (1 + |s|^2)^r, \qquad r \in \mathbb{R}.$$

This is a linear combination of the actions for the unperturbed system with $V = 0$.

Theorem 2.2 [10]. *Let $V(t,x) = \widetilde V(\omega t, x)$, where $\omega \in \mathbb{R}^N$ is a Diophantine vector and $\widetilde V$ is a smooth function on $\mathbb{T}^N \times \mathbb{T}^d$. Then for each $r \geqslant 1$ there exists a number $c(r)$ such that any solution $u(t)$ of (11) satisfies*

$$\|u(t)\|_r \leqslant \text{const} \cdot (\log t)^{c(r)} \|u_0\|_r \qquad \forall t \geqslant 2. \tag{12}$$

Thus, if u_0 is smooth, then the higher states u_s stay almost non-excited for a very long time. We do not have a result which would imply that the quantity in (8), calculated for solutions of (11), (7), stays small for a long time.

It is surprising that a weaker version of this result holds for potentials V that are not time quasi-periodic.

Theorem 2.3 [11]. *Let V be smooth and C^k-bounded uniformly with respect to (t,x) for each k. Then for each $r \geqslant 1$ and $a > 0$ there exists a constant C_a such that*

$$\|u(t)\|_r \leqslant C_a t^a \|u_0\|_r \qquad \forall t \geqslant 2.$$

Also see [12]. If the potential $V(t,x)$ is analytic, then the norm $\|u(t)\|_r$ satisfies (12) (see [31]). We are not aware of any classical analogues of these results.

3. Quantum KAM theory

Let $(p,q) \in \mathbb{R}^d \times \mathbb{T}^d$. We consider the integrable Hamiltonian $h_0(p) = |p|^2$ and a time quasi-periodic perturbation of it $H_\varepsilon(p,q) = h_0(p) + \varepsilon V(\omega t, q)$, $\omega \in \mathbb{R}^n$, where V is analytic. For the corresponding Hamiltonian equation we have a KAM theorem: *For a typical initial condition $(p(0),q(0))$ and a typical ω the solution $(p(t),q(t))$ is time quasi-periodic.*

The quantized Hamiltonian defines the dynamical equation (10). We regard the vector ω as a parameter of the problem: $\omega \in U \Subset \mathbb{R}^n$. Let us use the abbreviated notation $L^2 = L^2(\mathbb{T}^d, \mathbb{C})$ and provide this space with the basis of exponentials

$$\{e^{is\cdot x},\ s \in \mathbb{Z}^d\}$$

($\cdot$ denotes the Euclidean scalar product). For any linear operator $B\colon L^2 \to L^2$ let $(B_{ab},\ a,b \in \mathbb{Z}^d)$ be its matrix in this basis.

The theorem below may be regarded as a quantum analogue of the KAM theorem above. For $d = 1$ it is proved in [5], and for $n \geqslant 2$ in [16]. We do not know how to pass in this result to the semiclassical limit.

Theorem 3.1. *If $\varepsilon \ll 1$, then for most ω there exist a φ-dependent complex-linear isomorphism $\Psi(\varphi) = \Psi_{\varepsilon,\omega}(\varphi)$, $\varphi \in \mathbb{T}^N$,*

$$\Psi(\varphi)\colon L^2 \to L^2, \qquad u(x) \mapsto \Psi(\varphi)u(x),$$

and a bounded Hermitian operator $Q = Q^{\varepsilon,\omega}$ such that a curve $u(t) \in L^2$ solves equation (10) if and only if $v(t) = \Psi(t\omega)u(t)$ satisfies

$$\dot v = i(\Delta v - \varepsilon Q v).$$

The matrix (Q_{ab}) is block-diagonal, that is, $Q_{ab} = 0$ if $|a| \neq |b|$, and it satisfies

$$Q_{ab} = (2\pi)^{-n-d} \int_{\mathbb{T}^n} \int_{\mathbb{T}^d} V(\varphi,x) e^{i(a-b)\cdot x}\, dx\, d\varphi + O(\varepsilon^\gamma), \qquad \gamma > 0.$$

Moreover, $\|Q\|_{H^p,H^p} \leqslant C_1$ and $\|\Psi(\varphi) - \mathrm{id}\,\|_{H^p,H^p} \leqslant \varepsilon C_2$ for any $p \in \mathbb{N}$.

Here 'for most' means 'for all $\omega \in U_\varepsilon \subset U$, where $\mathrm{meas}(U \setminus U_\varepsilon) \leqslant \varepsilon^\kappa$ for some $\kappa > 0$'. In particular, for any such ω all solutions of equation (10) are almost periodic functions of the time. Their Sobolev norms are almost constant, namely, we have the following result.

Corollary 3.2. *For ω as in the theorem and for any p all solutions of (10) satisfy*

$$(1 - C\varepsilon)\|u(0)\|_p \leqslant \|u(t)\|_p \leqslant (1 + C\varepsilon)\|u(0)\|_p \qquad \forall t \geqslant 0.$$

This property is called the *dynamical localization*.

Proof. Since Q is block diagonal, we have $\|v(t)\|_p = \text{const}$. The estimate follows from the facts that $v(t) = \Psi(t)u(t)$ and $\|\Psi - \mathrm{id}\,\|_{H^p,H^p} \leqslant \varepsilon C_2$.

Remarks. 1) Let $n = 0$. Then (10) becomes the equation $\dot u = -i(\Delta u + \varepsilon V(x)u$. The theorem states that this equation can be reduced to a block-diagonal equation $\dot u = -iAu$, where $A_{ab} = 0$ if $|a| \neq |b|$. This is a well known fact.

2) For $n = 1$ the theorem's assertion is the Floquet theorem for the time periodic equation (10). In contrast to the finite-dimensional case, this is a perturbative result, valid only for 'typical' frequencies $\omega \in \mathbb{R}$ and small ε.

Proof of Theorem 3.1. Equation (10) is a non-autonomous linear Hamiltonian system in L^2:

$$\dot u = -i\,\frac{\delta}{\delta \bar u} H_\varepsilon(u), \qquad H_\varepsilon(u) = \frac{1}{2}\langle \nabla u, \nabla \bar u\rangle + \frac{1}{2}\varepsilon\langle V(\varphi_0 + t\omega, x)u, \bar u\rangle.$$

Consider the extended phase space $L^2 \times \mathbb{T}^n \times \mathbb{R}^n = \{(u, \varphi, r)\}$. There the equation above can be written as the autonomous Hamiltonian system

$$\begin{aligned} \dot u &= -i\frac{\delta}{\delta \bar u} h_\varepsilon(u, \varphi, r),\\ \dot\varphi &= \nabla_r h_\varepsilon = \omega,\\ \dot r &= -\nabla_\varphi h_\varepsilon, \end{aligned}$$

where $h_\varepsilon(u, \varphi, r, \varepsilon) = \omega \cdot r + \langle \nabla u, \nabla \bar u\rangle/2 + \varepsilon\langle V(\varphi, x)u, \bar u\rangle/2$. Thus, h_ε is a small perturbation of the integrable quadratic Hamiltonian $h_0 = \omega \cdot r + \langle \nabla u, \nabla \bar u\rangle/2$. The KAM theorem in [16] is applicable to perturbations of h_0. To show how this implies Theorem 3.1 let us write h_ε as

$$h_\varepsilon(u, \varphi, r, \varepsilon) = \omega \cdot r + \frac{1}{2}\langle \nabla u, \nabla \bar u\rangle + \varepsilon f(u, \varphi, r).$$

In our case $f = \langle V(\varphi, x)u, \bar u\rangle/2$. The theorem below is the main result of [16].

Theorem 3.3. *There exist a domain $\mathscr{O} = \{\|u\| < \delta\} \times \mathbb{T}^n \times \{|r| < \delta\}$ and a symplectic transformation $\Phi\colon \mathscr{O} \to L^2 \times \mathbb{T}^n \times \mathbb{R}^n$ which takes h_ε to*

$$h_0 = \omega' \cdot r + \frac{1}{2}\langle \nabla u, \nabla \bar u\rangle + \varepsilon\langle Qu, \bar u\rangle + f'(u, \varphi, r),$$

where $f' = O(|u|^3) + O(|r|^2)$.

The torus $T_0 = \{0\} \times \mathbb{T}^n \times \{0\}$ is invariant for the transformed system, so $\Phi(T_0)$ is invariant for the original equation. This is the usual KAM statement. Here it is trivial, since it simply states that $u(t) \equiv 0$ is a solution on the original equation.

But the KAM theorem above tells us more. A simple analysis of the proof (see a remark in [16]) shows that if the perturbation εf is quadratic in u and independent of r, then the KAM transformations are linear in u and do not change ω. Therefore, the transformed Hamiltonians stay quadratic in u, and hence the Hamiltonian h_0 is such that $f' = 0$. That is,

$$h_0 = \omega' \cdot r + \frac{1}{2}\langle \nabla u, \nabla \bar u\rangle + \varepsilon\langle Qu, \bar u\rangle.$$

This proves Theorem 3.1.

4. Quantum diffusion

Let $(p,q) \in \mathbb{R}^d \times \mathbb{T}^d$, and consider the Hamiltonian $H_\varepsilon(p,q) = |p|^2 + \varepsilon V(\omega t, q)$, where $\omega \in \mathbb{R}^N$ and V is analytic. Then:

i) by KAM, for a typical ω and typical initial data (p_0, q_0) the solution with $(p(0), q(0)) = (p_0, q_0)$ is time quasi-periodic;

ii) for exceptional ω and (p_0, q_0) we 'should' have Arnold diffusion, with the action $p(t)$ of a corresponding solution slowly 'diffusing away' from p_0.

As before, the quantized Hamiltonian defines the dynamical equation (10).

Claim 4.1. *Let $d = 1$ and $N \geqslant 2$, and suppose that V is non-degenerate in a suitable sense. Then there exist a smooth function $u(0,x)$ and a vector $\omega \in \mathbb{R}^N$ such that*

$$\limsup_{t\to\infty} \|u(t)\|_s = \infty \tag{13}$$

for some $s \geqslant 1$.

An *example* of a time periodic potential V satisfying (13) is given in [10]. It is conjectured by Eliasson that the above claim can be established for a *typical* potential by the methods in his paper [14]. A proof of this will be given in a paper under preparation.

5. Perturbed harmonic and anharmonic oscillators.

In §§ 3 and 4 we dealt with the Schrödinger evolution equation under periodic boundary conditions. Some similar results are known for equations in the whole space with growing potentials:

• Consider the Schrödinger equation

$$\dot{u} = -i(-u_{xx} + (x^2 + \mu x^{2m})u + \varepsilon V(t\omega, x)u)$$

in $\mathbb{R}^1$, where $\mu > 0$, $m \in \mathbb{N}$, $m \geqslant 2$, and $V(\varphi, x)$ is C^2-smooth with respect to φ and x, analytic with respect to φ, and uniformly bounded with respect to φ, x. Then an analogue of Theorem 3.1 holds. See § 2.5 in [21] for the needed KAM theorem.

• According to to Bambusi and Graffi [5], the same result holds for non-integers m, that is, for equations

$$\dot{u} = -i(-u_{xx} + Q(x)u + \varepsilon V(\varphi_0 + t\omega, x)u)$$

with $Q(x) \sim |x|^\alpha$ for some $\alpha > 2$ as $|x| \to \infty$. The potential V can grow to infinity as $|x| \to \infty$.

• Liu and Yuan [24] allow faster growth of $V(x)$ with respect to x. Their result can be used to prove an analogue of Theorem 3.1 for the *quantum Duffing oscillator*

$$\dot{u} = -i(-u_{xx} + x^4 u + \varepsilon x V(\varphi_0 + t\omega, x)u).$$

• According to Grébert and Thomann [17], the assertion holds for the perturbed harmonic oscillator

$$\dot{u} = -i(-u_{xx} + x^2 u + \varepsilon V(\varphi_0 + t\omega, x)u).$$

What happens in higher dimensions $d \geqslant 2$ remains completely unknown.

6. Quantum adiabatic theorem in the semiclassical limit

In this section we consider the classical system on $T^*\mathbb{R}^d = \mathbb{R}^d \times \mathbb{R}^d$ with Hamiltonian

$$H(p,q,\tau) = |p|^2 + V(\tau,q), \qquad \tau = \varepsilon t, \tag{14}$$

and the corresponding quantum system

$$i\hbar\dot{u} = -\hbar^2\Delta u + V(\tau,x)u = \mathscr{H}_\tau u, \qquad \tau = \varepsilon t \tag{15}$$

(see (4)). We assume that for each τ the potential $V(\tau,x)$ grows to infinity with $|x|$, so that the operator $\mathscr{H}_\tau$ has a discrete spectrum.

We fix an ε small enough that we can say some things about the dynamics of the classical system, and then we pass to the limit as $\hbar \to 0$. This limiting dynamics may be quite different from that in § 2.1 when $\hbar$ is fixed and $\varepsilon \to 0$, as was demonstrated by Berry [7] in the following striking example. Let $d = 1$ and assume that for $\tau = \text{const}$ the potential V has two (non-symmetric) potential wells. Generically, for $\tau = \text{const}$ and small enough $\hbar$ each well supports a family of pure quantum states localized mainly in this well. Consider a solution $u(t,x)$ of equation (15) with initial condition which is a pure quantum state in the left well. For arbitrarily small ε there exists a number $\hbar_0 = \hbar_0(\varepsilon) > 0$ such that if $0 < \hbar < \hbar_0$, then for each $t \in [0, 1/\varepsilon]$ the function $u(t,\cdot)$ is also localized in the left well. On the other hand, under some rather general assumptions, for arbitrarily small $\hbar$ there exist a number $\varepsilon_0 = \varepsilon_0(\hbar)$ and positive constants $a_1 < a_2$ such that if $0 < \varepsilon < \varepsilon_0$, then the function $u(t,\cdot)$ is localized in the right well for $a_1\hbar/\varepsilon \leqslant t \leqslant a_2\hbar/\varepsilon$.

The case $\varepsilon \sim \hbar$ is discussed in [19]. In what follows, ε_0, c, and c_i denote positive constants.

6.1. Systems with one degree of freedom. Assume first that the classical Hamiltonian (14) has one degree of freedom. We suppose that V is C^∞-smooth and that for each $\tau = \text{const}$ the phase plane of the Hamiltonian system (14) contains a domain filled by closed trajectories. In this domain we introduce the action-angle variables $I = I(p,q,\tau)$, $\chi = \chi(p,q,\tau) \mod 2\pi$ (that is, $\chi \in \mathbb{T}^1$). We invert these relations: $p = p(I,\chi,\tau)$, $q = q(I,\chi,\tau)$. Suppose that there is an interval $[a_1,b_1]$, $0 < a_1 < b_1$, such that the map $(I,\chi,\tau) \mapsto (p,q,\tau)$ is smooth for $I \in [a_1,b_1]$, $\chi \in \mathbb{T}^1$, $\tau \in [0,1]$. We express the Hamiltonian (14) in terms of the action variable and the slow time: $H(p,q,\tau) = E(I,\tau)$.

For $\varepsilon > 0$ let $p(t)$, $q(t)$ be a solution of the perturbed system with the Hamiltonian $H(p,q,\varepsilon t)$.

Theorem 6.1 (see, for instance, [2]). *There exist ε_0 and c_1 such that if $0 < \varepsilon < \varepsilon_0$, then*

$$|I(p(t),q(t),\varepsilon t) - I(p(0),q(0),0)| < c_1\varepsilon \quad \textit{for} \quad 0 \leqslant t \leqslant \frac{1}{\varepsilon}.$$

Now assume that for each $\tau = \text{const} \in [0,1]$ and each $I_* \in (a_1,b_1)$ the Hamiltonian H (14) has a unique trajectory with the action $I = I_*$. Consider the corresponding quantum system (15). The operator $\mathscr{H}_\tau$ has a series of eigenfunctions $\varphi_s(\tau) = \varphi_s(\tau,x)$ such that

$$\|\varphi_s(\tau)\| = 1, \qquad \varphi_s(\tau,x) \to 0 \quad \text{as} \quad x \to \infty, \tag{16}$$

and the corresponding eigenvalues are $\lambda_s(\tau) = E(I_s, \tau) + O(\hbar^2)$, where $I_s = \hbar(s + 1/2) \in [a_1, b_1]$ (this is the Bohr–Sommerfeld quantization rule; see [26]). We assume that V is such that the convergence to zero in (16) is faster than $|x|$ raised to any negative power. Let $u(t, x)$ be a solution of the non-stationary equation (15) with a pure-state initial condition $u(0, x) = \varphi_{s_0}(0)$. Denote by $\mathbb{P}^{\tau}_{(\alpha,\beta)}$ the orthogonal projection from $L^2(\mathbb{R})$ onto the linear span of the vectors $\varphi_s(\tau)$ with $I_s \in (\alpha, \beta)$. The approach in [9] leads to the following conjecture.

Conjecture 6.2. *There exist ε_0 and c_1 such that if $0 < \varepsilon < \varepsilon_0$ and $0 < \hbar \leqslant \varepsilon$, then for any $m \geqslant 1$ and a suitable $c_2(m) > 0$*

$$\sup_{0 \leqslant t \leqslant \varepsilon^{-1}} \left\| u - \mathbb{P}^{\varepsilon t}_{(I_{s_0} - c_1\varepsilon, I_{s_0} + c_1\varepsilon)} u \right\| < c_2(m) \left(\frac{\hbar}{\varepsilon} \right)^m. \tag{17}$$

Thus, $u(t, \cdot\,)$ stays close to the eigenspace that corresponds to eigenvalues in an $O(\varepsilon)$-neighbourhood of $E(I_{s_0}, \varepsilon t)$.

6.2. Systems with several degrees of freedom. Now let the classical Hamiltonian (14) have $d > 1$ degrees of freedom. As before, we assume that $V \in C^\infty$. For each $\tau = \text{const}$ let the corresponding Hamiltonian system be completely integrable and assume that its phase space contains a domain filled by invariant tori. In this domain we introduce the action-angle variables $I = I(p, q, \tau)$, $\chi = \chi(p, q, \tau) \in \mathbb{T}^d$. We invert these relations: $p = p(I, \chi, \tau)$, $q = q(I, \chi, \tau)$. Suppose that there is a compact domain $\mathscr{A} \Subset \mathbb{R}^d_+$ such that the map $(I, \chi, \tau) \mapsto (p, q, \tau)$ is smooth for $I \in \mathscr{A}$, $\chi \in \mathbb{T}^d$, and $\tau \in [0, 1]$. We express the Hamiltonian (14) in terms of the action variables and the slow time, $H(p, q, \tau) = E(I, \tau)$, and we denote by $\omega(I, \tau) = \partial E / \partial I$ the frequency vector of the unperturbed motion. Assume that the system is non-degenerate or iso-energetically non-degenerate (see the definition in [2], Appendix 8). The dynamics of the variables $(I, \chi)(t) = (I, \chi)(p(t), q(t), \varepsilon t)$ is described by a Hamiltonian of the form (see [2], § 52F)

$$\mathscr{H}(I, \chi, \tau, \varepsilon) = E(I, \tau) + \varepsilon H_1(I, \chi, \tau), \tag{18}$$

where H_1 is a smooth function on $\mathscr{A} \times \mathbb{T}^d \times [0, 1]$.

Let K_0 be a compact set in $\mathbb{R}^{2d}$. For $(p_0, q_0) \in K_0$ denote by $(p, q)(t) = (p, q)(t, p_0, q_0)$ a solution of the perturbed system with initial condition $(p, q)(0) = (p_0, q_0)$.

Theorem 6.3 (see, for instance, [3], [25]). *If $0 < \varepsilon < \varepsilon_0$, then*

$$\int_{K_0} \sup_{0 \leqslant t \leqslant \varepsilon^{-1}} |I(p(t), q(t), \varepsilon t) - I(p(0), q(0), 0)| \, dp_0 \, dq_0 < c_1 \sqrt{\varepsilon}.$$

In systems with $d > 1$ degrees of freedom the value of the action vector as a function of the time can change considerably for some initial conditions due to the effect of resonance between unperturbed frequencies, that is, components of the vector $\omega(I, \tau)$. We say that there is a resonance for some (I, τ) if $(k \cdot \omega)(I, \tau) = 0$ for a suitable vector $k \in \mathbb{Z}^d \setminus \{0\}$ (here $\cdot$ denotes the Euclidean scalar product).

Now consider the corresponding quantum system (15). Under some conditions the operator $\mathscr{H}_\tau$ has a series of eigenfunctions $\varphi_m(\tau) = \varphi_m(\tau, x)$ satisfying (16) and

with eigenvalues $\lambda_m(\tau) = E(I_m, \tau) + O(\hbar^2)$, where $I_m = \hbar(m + \frac{1}{4}\kappa) \in \mathscr{A}$, $m \in \mathbb{Z}^d_+$, and $\kappa \in \mathbb{Z}^d$ is the vector of Maslov–Arnold indices [26] (the Bohr–Sommerfeld quantization rule). Consider the solution $u(t,x)$ of the non-stationary equation (15) with a pure-state initial condition $u(0,x) = \varphi_{m_0}(0)$. If we fix some small $\hbar$ and pass to the limit as $\varepsilon \to 0$, then Theorem 2.1 would apply. However, now we are interested in a different limit: when a small ε is fixed and $\hbar \to 0$. Not much is known about the corresponding limiting dynamics. Therefore, we will formulate natural *hypotheses* about the limiting quantum dynamics as $\hbar \to 0$ and use them together with known results about the dynamics for the classical Hamiltonian (14) with small ε.

For Theorem 2.1 to hold it is important that $\lambda_{m_0}(\tau)$ be an isolated eigenvalue for all τ. Consider the distance between $\lambda_m(\tau)$ and $\lambda_{m_0}(\tau)$, where $m, m_0 \in \mathbb{Z}^d$ are such that $m \neq m_0$ and $|m - m_0| \sim 1$:

$$\begin{aligned}\lambda_m(\tau) - \lambda_{m_0}(\tau) &= E(I_m, \tau) - E(I_{m_0}, \tau) + O(\hbar^2)\\ &= (I_m - I_{m_0}) \cdot \omega(I_{m_0}, \tau) + O((I_m - I_{m_0})^2) + O(\hbar^2)\\ &= \hbar(m - m_0) \cdot \omega(I_{m_0}, \tau) + O(\hbar^2).\end{aligned}$$

Thus if there is no resonance at (I_{m_0}, τ), then the distance between $\lambda_{m_0}(\tau)$ and nearby eigenvalues is $\sim \hbar$. However, if there is a resonance $k \cdot \omega(I_{m_0}, \tau) = 0$, then $\lambda_{m_0+\nu k}(\tau) - \lambda_{m_0}(\tau) = O(\hbar^2)$ for integer $\nu \sim 1$. Hence, classical resonances correspond to almost multiple points of the spectrum of the quantum problem, and therefore it seems that they should also appear in questions of quantum adiabaticity.

For the Hamiltonian (14) there is quite detailed information about the dynamics in the two-frequency case $d = 2$. We now use this information together with the Bohr–Sommerfeld quantization rule to state some conjectures about dynamics for the two-dimensional quantum system (15).

Following Dirac [13], we assume that[2]

$$\omega_2 \frac{\partial \omega_1}{\partial \tau} - \omega_1 \frac{\partial \omega_2}{\partial \tau} - \left(\omega_2 \frac{\partial \omega_1}{\partial I} - \omega_1 \frac{\partial \omega_2}{\partial I}\right) \frac{\partial H_1}{\partial \chi} > c^{-1} \tag{19}$$

for all I, φ. General results of Arnold about averaging in two-frequency systems [1], [3] imply that in this case

$$|I(p(t), q(t), \varepsilon t) - I(p(0), q(0), 0)| < c_1\sqrt{\varepsilon} \quad \text{for} \quad 0 \leqslant t \leqslant \frac{1}{\varepsilon}. \tag{20}$$

On the basis of the Bohr–Sommerfeld quantization rule and by analogy with Conjecture 6.2 it is natural to conjecture that for $0 \leqslant t \leqslant 1/\varepsilon$ the total probability $|u(t)|^2_{L_2}$ is mostly concentrated in the states corresponding to actions in the $C\sqrt{\varepsilon}$-neighbourhood of the original action I_{s_0}.

Now assume that instead of (19) the following condition is satisfied (cf. footnote 2):

$$\omega_2 \frac{\partial \omega_1}{\partial \tau} - \omega_1 \frac{\partial \omega_2}{\partial \tau} > c^{-1}. \tag{21}$$

[2]The condition (19) just means that the ratio of the frequencies changes at a non-zero rate along solutions of the system with Hamiltonian (18): $\omega_2^2\,(d/dt)(\omega_1/\omega_2) > c^{-1}\varepsilon$. Similarly, the condition (21) means that ratio of the frequencies changes at a non-zero rate in the adiabatic dynamics: $\omega_2^2\,(d/dt)(\omega_1/\omega_2)_{I=\text{const}} > c^{-1}\varepsilon$.

This is a particular case of a condition introduced by Arnold in [1]. If, in addition to (21), a certain general position condition is satisfied (see details in [3]), then the estimate (20) with $\sqrt{\varepsilon}$ replaced by $\sqrt{\varepsilon}|\log\varepsilon|$ holds for all initial data outside a set of measure $O(\sqrt{\varepsilon})$ ([3], § 6.1.8). The latter set consists mostly of initial data for trajectories with *capture into resonance*, and along these trajectories the actions change by quantities of order ~ 1. Since for some initial data $I(0)$, $\chi(0)$ the solution $I(t)$ is not localized in a neighbourhood of $I(0)$, we should not expect for the quantum system (15) any estimate similar to that in Conjecture 6.2, where the amplitudes of the eigenmodes tend to 0 as $\hbar \to 0$ outside some small interval of values of the action.

Consider the classical Hamiltonian (14) under the condition (21). Then capture is only possible for a finite number of resonances, and the dynamics for a capture into resonance $k_1\omega_1 + k_2\omega_2 = 0$ with coprime k_1 and k_2 is as follows [27]. Let $(I,\chi)(t) = (I,\chi)(p(t),q(t),\varepsilon t)$. Suppose that at the initial moment $t = 0$ we have no resonance,

$$k_1\omega_1(I(0),0) + k_2\omega_2(I(0),0) \neq 0,$$

and let $\tau_* \in (0,1)$ be the first moment when resonance occurs:

$$k_1\omega_1(I(0),\tau_*) + k_2\omega_2(I(0),\tau_*) = 0.$$

Then for $0 \leqslant \varepsilon t \leqslant \tau_*$ the values of the actions are approximately conserved:

$$I(t) = I(0) + O(\sqrt{\varepsilon}\log\varepsilon).$$

For $\tau_* \leqslant \varepsilon t \leqslant 1$ the system is captured into resonance, and the evolution of the actions is described by the two relations

$$\begin{aligned} k_1\omega_1(I(t),\varepsilon t) + k_2\omega_2(I(t),\varepsilon t) &= O(\sqrt{\varepsilon}\log\varepsilon),\\ k_2I_1(t) - k_1I_2(t) &= k_2I_1(0) - k_1I_2(0) + O(\sqrt{\varepsilon}\log\varepsilon). \end{aligned}$$

The first of them means that the system stays near the resonance, while the second says that the dynamics has an approximate first integral. The two relations together approximately determine the trajectory $I(t)$ for $\tau_* \leqslant \varepsilon t \leqslant 1$.

Using this description and the Bohr–Sommerfeld quantization rule, we conjecture by analogy with Conjecture 6.2 that for the quantum problem (15) the capture into resonance of the classical system (14) results in transfer of an amount $C\varepsilon$ of the total probability from a neighbourhood of the initially excited pure state corresponding to the action I_{s_0}, to a neighbourhood of a state $s_t \in \mathbb{Z}^2$ such that the lattice vector $I(t) = \hbar(s_t + \frac{1}{4}\kappa)$ satisfies the two relations above. This transfer happens for $t \geqslant \varepsilon^{-1}\tau_*$. When $\hbar \to 0$, this amount $C\varepsilon$ remains positive of order ε.

For the dynamics of phase points captured into resonance there is also a more detailed description [27]. Consider the resonant phase $\gamma = k_1\chi_1 + k_2\chi_2$. It turns out that the behaviour of γ is described by an auxiliary Hamiltonian system with one degree of freedom and a Hamiltonian of the form

$$F = \sqrt{\varepsilon}\left(\frac{\alpha(\tau)p_\gamma^2}{2} + f(\gamma,\tau) + L(\tau)\gamma\right).$$

Here p_γ, γ are canonically conjugate variables, the function f is 2π-periodic with respect to γ, and $\alpha, L \neq 0$. In the phase portrait of the system for frozen τ there are domains of oscillations of γ. The motion in these domains can be approximately represented as the composition of a motion along a trajectory of the Hamiltonian F with frozen τ and a slow evolution of this trajectory due to a change of τ. This evolution follows the adiabatic rule: the area surrounded by the trajectory remains constant. In the original variables p, q this motion is represented as a motion along a slowly evolving torus. The angle variables on the torus are γ and $\psi = l_1\varphi_1 + l_2\varphi_2$, where l_1 and l_2 are integers such that $k_1 l_2 - k_2 l_1 = 1$. The torus itself drifts along the resonant surface $k_1\omega_1 + k_2\omega_2 = 0$ as described above. It is not known what quantum object corresponds to this torus.

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