On quantum averaging, quantum KAM, and quantum diffusion

S.B. Kuksin and A.I. Neishtadt

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: averaging theory, Nekhoroshev stability, and diffusion.

Bibliography: 31 titles.

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

Contents

1. Introduction 335
2. Quantum averaging 336
   2.1. Averaging and adiabatic invariance 336
   2.2. About Nekhoroshev’s Theorem 338
3. Quantum KAM theory 339
4. Quantum diffusion 341
5. Perturbed harmonic and anharmonic oscillators 341
6. Quantum adiabatic theorem in the semiclassical limit 342
   6.1. Systems with one degree of freedom 342
   6.2. Systems with several degrees of freedom 343
Bibliography 346

1. Introduction

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

$$\dot{p} = -\nabla_q H, \quad \dot{q} = \nabla_p H. \quad (1)$$

The corresponding quantum Hamiltonian operator is obtained from $H(p, q, t)$ by replacing the variable $q_j$, $j = 1, \ldots, d$, by the operator which acts on complex functions $u(x)$ as multiplication by $x_j$, and replacing each $p_j$ by
the operator \((h/i)(\partial/\partial x_j)\), where \(h\) is the Planck constant.\(^1\) The Hamiltonian operator \(\mathcal{H} = H((h/i)\nabla_x, x, t)\) defines a quantum system. A classical problem from the very beginning of quantum mechanics has been to study the (spectral) properties of the operator \(\mathcal{H}\) and the properties of the corresponding evolution equation

\[
i\hbar \dot{u}(t, x) = \mathcal{H}u(t, x)
\]

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

For example, if

\[
H(p, q, t) = |p|^2 + V(t, q),
\]

then

\[
\mathcal{H} = \mathcal{H}_t = -\hbar^2 \Delta + V(t, x),
\]

that is, \(\mathcal{H}\) is the Schrödinger operator with potential \(V\).

In this paper we discuss properties of the Hamiltonian operator \(\mathcal{H}\) 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 \(h = \text{const}\). 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 \(\|u(t)\|_L^2 = \text{const}\). 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

\[
H(p, q, \varepsilon t) = H_\varepsilon = |p|^2 + V(\varepsilon t, q),
\]

\(^1\)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 \( \tau \). Let \( I_j, 1 \leq j \leq d \), 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 \( \varepsilon^{-1} \). 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

\[
\dot{u} = -i(-\Delta u + V(\varepsilon t, x)u), \quad x \in T^d.
\]

Assume that the function \( V(\tau, x) \) is \( C^2 \)-smooth and bounded, and denote by \( A_\tau \) 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 \( A_\tau \), where each \( \lambda_s(\tau) \) is continuous in \( \tau \). Let \( u(t, x) \) be a solution of (6) equal at \( t = 0 \) to a pure state

\[
u(0, x) = \varphi_s(0)
\]

such that for each \( \varepsilon t \) 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]).

\[
\sup_{0 \leq t \leq \varepsilon^{-1}} \sum_{s : \lambda_s(\varepsilon t) \neq \lambda_{s_0}(\varepsilon t)} |u_s(t)|^2 \to 0 \quad \text{as} \quad \varepsilon \to 0.
\]

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 \( \varepsilon \) 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 nearly integrable 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

\[
|p(t) - p(0)| \leq \varepsilon^a \quad \forall |t| \leq e^{\varepsilon^{-b}}
\]  

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

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

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

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

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

\[
\dot{u} = -i(-\Delta u + \varepsilon V(\omega t, x)u).
\]

(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

\[
\dot{u} = -i(-\Delta u + V(t, x)u)
\]

(11)

and the square of the \(r\)th Sobolev norm of \(u\):

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

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

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

\[
\|u(t)\|_r \leq \text{const} \cdot (\log t)^{c(r)}\|u_0\|_r \quad \forall t \geq 2.
\]

(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 $r > 1$ and $a > 0$ there exists a constant $C_a$ such that

$$
\|u(t)\|_r \leq C_a t^a \|u_0\|_r \quad \forall t \geq 2.
$$

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 $\omega$ the solution $(p(t), q(t))$ is time quasi-periodic.

The quantized Hamiltonian defines the dynamical equation (10). We regard the vector $\omega$ as a parameter of the problem: $\omega \in U \subseteq \mathbb{R}^n$. 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 $B : L^2 \to L^2$ 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 $n \geq 2$ 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 $\omega$ there exist a $\varphi$-dependent complex-linear isomorphism $\Psi(\varphi) = \Psi_{\varepsilon, \omega}(\varphi), \varphi \in \mathbb{T}^n$,

$$
\Psi(\varphi) : L^2 \to L^2, \quad u(x) \mapsto \Psi(\varphi)u(x),
$$

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

$$
v = i(\Delta v - \varepsilon Qv).
$$

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

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

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

Here ‘for most’ means ‘for all $\omega \in U_\varepsilon \subseteq U$, where $\text{meas}(U \setminus U_\varepsilon) \leq \varepsilon^\kappa$ for some $\kappa > 0$’. In particular, for any such $\omega$ 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 $\omega$ as in the theorem and for any $p$ all solutions of (10) satisfy

$$
(1 - C\varepsilon)\|u(0)\|_p \leq \|u(t)\|_p \leq (1 + C\varepsilon)\|u(0)\|_p \quad \forall t \geq 0.
$$
This property is called the \textit{dynamical localization}.

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

\textbf{Remarks.} 1) Let $n = 0$. Then (10) becomes the equation $\dot{u} = -i(\Delta u + \epsilon V(x)u)$. 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 $\epsilon$.

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

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

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

$$
\begin{align*}
\dot{u} &= -i \frac{\delta}{\delta u} h_\epsilon(u, \varphi, r), \\
\dot{\varphi} &= \nabla_r h_\epsilon = \omega, \\
\dot{r} &= -\nabla_{\varphi} h_\epsilon,
\end{align*}
$$

where $h_\epsilon(u, \varphi, r, \epsilon) = \omega \cdot r + \langle \nabla u, \nabla \bar{u} \rangle/2 + \epsilon \langle V(\varphi, x)u, \bar{u} \rangle/2$. Thus, $h_\epsilon$ 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 $h_\epsilon$ as

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

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

\textbf{Theorem 3.3.} There exist a domain $\mathcal{O} = \{\|u\| < \delta\} \times \mathbb{T}^n \times \{|r| < \delta\}$ and a symplectic transformation $\Phi : \mathcal{O} \to L^2 \times \mathbb{T}^n \times \mathbb{R}^n$ which takes $h_\epsilon$ to

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

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 $\Phi^{-1}(T_0)$ 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 of 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 $\epsilon f$ is quadratic in $u$ and independent of $r$, then the KAM transformations are linear in $u$ and do not change $\omega$. Therefore, the transformed Hamiltonians stay quadratic in $u$, and hence the Hamiltonian $h_0$ is such that $f' = 0$. That is,

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

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 \(\omega\) 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 \(\omega\) 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 \(N \geq 2\), 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

\[
\limsup_{t \to \infty} \|u(t)\|_s = \infty
\]

for some \(s \geq 1\).

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

- According 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

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

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

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

What happens in higher dimensions \(d \geq 2\) 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
\[ H(p, q, \tau) = |p|^2 + V(\tau, q), \quad \tau = \varepsilon t, \tag{14} \]
and the corresponding quantum system
\[ ih\dot{u} = -h^2 \Delta u + V(\tau, x)u = \mathcal{H}_\tau u, \quad \tau = \varepsilon t \tag{15} \]
(see (4)). We assume that for each $\tau$ the potential $V(\tau, x)$ grows to infinity with $|x|$, so that the operator $\mathcal{H}_\tau$ has a discrete spectrum.

We fix an $\varepsilon$ small enough that we can say some things about the dynamics of the classical system, and then we pass to the limit as $h \to 0$. This limiting dynamics may be quite different from that in §2.1 when $h$ 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 $h$ 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 $\varepsilon$ there exists a number $\varepsilon_0 = \varepsilon_0(h)$ 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 $a_1 h/\varepsilon \leq t \leq a_2 h/\varepsilon$.

The case $\varepsilon \sim h$ is discussed in [19]. In what follows, $\varepsilon_0$, $c_1$ and $c_2$ 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 $C^\infty$-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, $\chi \in T^1$). 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 $I \in [a_1, b_1], \chi \in T^1, \tau \in [0, 1]$. 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 $\varepsilon_0$ and $c_1$ such that if $0 < \varepsilon < \varepsilon_0$, then
\[ |I(p(t), q(t), \varepsilon t) - I(p(0), q(0), 0)| < c_1 \varepsilon \quad \text{for} \quad 0 \leq t \leq \frac{1}{\varepsilon}. \]

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 $\mathcal{H}_\tau$ has a series of eigenfunctions $\varphi_s(\tau) = \varphi_s(\tau, x)$ such that
\[ \|\varphi_s(\tau)\| = 1, \quad \varphi_s(\tau, x) \to 0 \quad \text{as} \quad x \to \infty, \tag{16} \]
and the corresponding eigenvalues are \( \lambda_s(\tau) = E(I_s, \tau) + O(h^2) \), where \( I_s = h(s + 1/2) \in [a_1, b_1] \) (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 \( \mathbb{P}_{\lambda}^{\tau} \) the orthogonal projector 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 \( \varepsilon_0 \) and \( c_1 \) such that if \( 0 < \varepsilon < \varepsilon_0 \) and \( 0 < h \leq \varepsilon \), then for any \( m \geq 1 \) and a suitable \( c_2(m) > 0 \)

\[
\sup_{0 \leq t \leq \varepsilon^{-1}} \left\| u - \mathbb{P}_{\lambda}^{\tau}(I_{s_0} - c_1 \varepsilon, I_{s_0} + c_1 \varepsilon) u \right\| < c_2(m) \left( \frac{h}{\varepsilon} \right)^m.
\] (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 \( \mathcal{A} \subseteq \mathbb{R}^d_+ \) such that the map \( (I, \chi, \tau) \mapsto (p, q, \tau) \) is smooth for \( I \in \mathcal{A}, \chi \in \mathbb{T}^d, \) 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)

\[
\mathcal{H}(I, \chi, \varepsilon) = E(I, \tau) + \varepsilon H_1(I, \chi, \tau),
\] (18)

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

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

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

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 \( (I, \tau) \) 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 \( \mathcal{H}_\tau \) has a series of eigenfunctions \( \varphi_m(\tau) = \varphi_m(\tau, x) \) satisfying (16) and...
with eigenvalues $\lambda_m(\tau) = E(I_m, \tau) + O(h^2)$, where $I_m = h(m + \frac{1}{2} \kappa) \in \mathcal{A}$, $m \in \mathbb{Z}_+^d$, 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 $h$ 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 $\varepsilon$ is fixed and $h \to 0$. Not much is known about the corresponding limiting dynamics. Therefore, we will formulate natural hypotheses about the limiting quantum dynamics as $h \to 0$ and use them together with known results about the dynamics for the classical Hamiltonian (14) with small $\varepsilon$.

For Theorem 2.1 to hold it is important that $\lambda_{m_0}(\tau)$ be an isolated eigenvalue for all $\tau$. 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 $|m - m_0| \sim 1$:

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

Thus if there is no resonance at $(I_{m_0}, \tau)$, then the distance between $\lambda_{m_0}(\tau)$ and nearby eigenvalues is $\sim h$. However, if there is a resonance $k \cdot \omega(I_{m_0}, \tau) = 0$, then $\lambda_{m_0 + \nu k}(\tau) - \lambda_{m_0}(\tau) = O(h^2)$ 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 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

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

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

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

On the basis of the Bohr–Sommerfeld quantization rule and by analogy with Conjecture 6.2 it is natural to conjecture that for $0 \leq t \leq 1/\varepsilon$ 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):

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

Footnote 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 $\sim 1$. 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 $h \to 0$ 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 do not
have this 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 this resonance occurs:

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

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

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

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

$$k_1 \omega_1(I(t), \varepsilon t) + k_2 \omega_2(I(t), \varepsilon t) = O(\sqrt{\varepsilon} \log \varepsilon),$$

$$k_2 I_1(t) - k_1 I_2(t) = k_2 I_1(0) - k_1 I_2(0) + O(\sqrt{\varepsilon} \log \varepsilon).$$

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 $\tau_* \leq \varepsilon t \leq 1$.

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 $I(t) = h(s_t + 1/4 \kappa)$ satisfies the two relations above. This transfer happens
for $t \geq \varepsilon^{-1} \tau_*$. When $h \to 0$, this amount $C\varepsilon$ remains positive of order $\varepsilon$.

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 $\gamma$ is described by an auxiliary Hamiltonian system with
one degree of freedom and a Hamiltonian of the form

$$F = \sqrt{\varepsilon} \left( \frac{\alpha(\tau)p_2^2}{2} + f(\gamma, \tau) + L(\tau)\gamma \right).$$
Here $p, \gamma$ are canonically conjugate variables, the function $f$ is $2\pi$-periodic with respect to $\gamma$, and $\alpha, L \neq 0$. In the phase portrait of the system for frozen $\tau$ there are domains of oscillations of $\gamma$. The motion in these domains can be approximately represented as the composition of a motion along a trajectory of the Hamiltonian $F$ with frozen $\tau$ and a slow evolution of this trajectory due to a change of $\tau$. 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 $\gamma$ 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.

The authors are grateful to Sergey Dobrokhotov, Håkan Eliasson, and Johannes Sjöstrand for useful discussions.

Bibliography

[1] В.И. Арнольд, “Условия применимости и оценка погрешности метода усреднения для систем, которые в процессе эволюции проходят через резонансы”, Докл. АН СССР 161:1 (1965), 9–12; English transl., V.I. Arnold, “Conditions for the applicability, and estimate of the error, of an averaging method for systems which pass through states of resonance in the course of their evolution”, Soviet Math. Dokl. 6 (1965), 331–334.

[2] В.И. Арнольд, Математические методы классической механики, Наука, М. 1974, 431 с.; English transl., V.I. Arnold, Mathematical methods of classical mechanics, 2nd ed., Grad. Texts in Math., vol. 60, Springer-Verlag, New York 1989, xvi+508 pp.

[3] В.И. Арнольд, В.В. Козлов, А.И. Нейштадт, Математические аспекты классической и небесной механики, 2-е изд., переработанное и дополненное, УРСС, М. 2002, 414 с.; English transl., V.I. Arnold, V.V. Kozlov, and A.I. Neishtadt, Mathematical aspects of classical and celestial mechanics, 3rd rev. ed., Encyclopaedia Math. Sci., vol. 3, Springer-Verlag, Berlin 2006, xiv+518 pp.

[4] J. E. Avron and A. Elgert, “Adiabatic theorem without a gap condition”, Comm. Math. Phys. 203:2 (1999), 445–463.

[5] D. Bambusi and S. Graffi, “Time quasi-periodic unbounded perturbations of Schrödinger operators and KAM methods”, Comm. Math. Phys. 219:2 (2001), 465–480.

[6] V. V. Belov, S. Yu. Dobrokhotov, and T. Ya. Tudorovskiy, “Operator separation of variables for adiabatic problems in quantum and wave mechanics”, J. Engrg. Math. 55:1-4 (2006), 183–237.

[7] M. V. Berry, “The adiabatic limit and the semiclassical limit”, J. Phys. A: Math. Gen. 17:6 (1984), 1225–1233.

[8] M. Born and V. Fock, “Beweis des Adiabatensatzes”, Z. Phys. 51:3-4 (1928), 165–180.

[9] V. A. Боровиков, Поля в плавно нерегулярных волноводах и задача о вариации аддиабатического инварианта, Препринт № 99, ИПМ АН СССР 1978, 66 с. [V. A. Borovikov, Fields in smoothly irregular waveguides and the problem of the variation of the adiabatic invariant, Preprint № 99, Akad. Nauk SSSR, Institute of Applied Mathematics 1978, 66 pp.]
On quantum averaging

[10] J. Bourgain, “Growth of Sobolev norms in linear Schrödinger equations with quasi-periodic potential”, Comm. Math. Phys. 204:1 (1999), 207–247.

[11] J. Bourgain, “On growth of Sobolev norms in linear Schrödinger equations with smooth time dependent potentials”, J. Anal. Math. 77:1 (1999), 315–348.

[12] J.-M. Delort, “Growth of Sobolev norms of solutions of linear Schrödinger equations on some compact manifolds”, Int. Math. Res. Not. IMRN 2010:12 (2010), 2305–2328.

[13] P.A.M. Dirac, “The adiabatic invariance of the quantum integrals”, Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci. 107 (1925), 725–734.

[14] L.H. Eliasson, “Ergodic skew-systems on $T^d \times SO(3, \mathbb{R})$”, Ergodic Theory Dynam. Systems 22:5 (2002), 1429–1449.

[15] H.L. Eliasson and S.B. Kuksin, “On reducibility of Schrödinger equations with quasiperiodic in time potentials”, Comm. Math. Phys. 286:1 (2009), 125–135.

[16] L.H. Eliasson and S.B. Kuksin, “KAM for the nonlinear Schrödinger equation”, Ann. of Math. (2) 172:1 (2010), 371–435.

[17] B. Grébert and L. Thomann, “KAM for the quantum harmonic oscillator”, Comm. Math. Phys. 307:2 (2011), 383–427.

[18] A. Joye and C.-E. Pfister, “Superadiabatic evolution and adiabatic transition probability between two nondegenerate levels isolated in the spectrum”, J. Math. Phys. 34:2 (1993), 454–479.

[19] М.В. Карасев, “Новые глобальные асимптотики и аномалии в задаче квантования адиабатического инварианта”, Функц. анализ и его прил. 24:2 (1990), 24–36; English transl., M.V. Karasev, “New global asymptotics and anomalies for the problem of quantization of the adiabatic invariant”, Funct. Anal. Appl. 24:2 (1990), 104–114.

[20] T. Kato, “On the adiabatic theorem of quantum mechanics”, J. Phys. Soc. Jpn. 5 (1950), 435–439.

[21] S.B. Kuksin, Nearly integrable infinite-dimensional Hamiltonian systems, Lecture Notes in Math., vol. 1556, Springer-Verlag, Berlin 1993, xxviii+101 pp.

[22] Л.Д. Ландау, Е.М. Лифшиц, Теоретическая физика, т.1: Механика, 4-е изд., Наука, М. 1988, 216 с.; English transl., L.D. Landau and E.M. Lifshitz, Course of theoretical physics, vol. 1: Mechanics, Pergamon Press, Oxford–London–New York–Paris; Addison–Wesley Publishing Co., Inc., Reading, MA 1960, vii+165 pp.

[23] V.F. Lazutkin, KAM theory and semiclassical approximations to eigenfunctions, Ergeb. Math. Grenzgeb. (3), vol. 24, Springer-Verlag, Berlin 1993, x+387 pp.

[24] Jianjun Liu and Xiaoping Yuan, “Spectrum for quantum Duffing oscillator and small-divisor equation with large-variable coefficient”, Comm. Pure Appl. Math. 63:9 (2010), 1145–1172.

[25] P. Lochak and C. Meunier, Multiphase averaging for classical systems. With applications to adiabatic theorems, transl. from the French by H.S. Dumas, Appl. Math. Sci., vol. 72, Springer-Verlag, New York 1988, xii+360 pp.

[26] В.П. Маслов, М.В. Федорюк, Квазиклассическое приближение для уравнений квантовой механики, Наука, М. 1976, 296 с.; English transl., V.P. Maslov and M.V. Fedoryuk, Semi-classical approximation in quantum mechanics, Math. Phys. Appl. Math., vol. 7, D. Reidel Publishing Co., Dordrecht–Boston, MA 1981, ix+301 pp.

[27] А.И. Нейштадт, “Захват в резонанс и рассеяние на резонансах в двухчастотных системах”, Дифференциальные уравнения и динамические системы, Сборник статей, Тр. МИАН, 250, Наука, М. 2005, с. 198–218;
English transl., A. I. Neishtadt, “Capture into resonance and scattering on resonances in two-frequency systems”, Proc. Steklov Inst. Math. 250 (2005), 183–203.

[28] Н. Н. Нехорошев, “Экспоненциальная оценка времени устойчивости гамильтоновых систем, близких к интегрируемым”, УМН 32:6(198) (1977), 5–66; English transl., N. N. Nekhoroshev, “An exponential estimate of the time of stability of nearly-integrable Hamiltonian systems”, Russian Math. Surveys 32:6 (1977), 1–65.

[29] G. Nenciu, “Linear adiabatic theory. Exponential estimates”, Comm. Math. Phys. 152:3 (1993), 479–496.

[30] J. Sjöstrand, “Projecteurs adiabatiques du point de vue pseudodifférentiel”, C. R. Acad. Sci. Paris Sér. I Math. 317:2 (1993), 217–220.

[31] W.-M. Wang, “Logarithmic bounds on Sobolev norms for time dependent linear Schrödinger equations”, Comm. Partial Differential Equations 33:12 (2008), 2164–2179.

S. B. Kuksin
Institut de Mathématiques de Jussieu,
Paris, France;
Steklov Mathematical Institute
of the Russian Academy of Sciences
E-mail: kuksin@gmail.com

A. I. Neishtadt
Loughborough University, UK;
Space Research Institute
of the Russian Academy of Sciences
E-mail: A.Neishtadt@lboro.ac.uk

Received 15/SEP/12