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Quantum averaging, KAM and diffusion.

(based on a joint paper with A. Neishtadt)

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§1. The quantisation.

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

(1) $$\dot p = -\nabla_q H, \qquad \dot q = \nabla_p H.$$

Corresponding quantum hamiltonian operator $\mathcal{H}$ is obtained by replacing in H $q_j \mapsto x_j$, $p_j \mapsto \frac{\hbar}{i}\frac{\partial}{\partial x_j}$:

$$\mathcal{H} = H(\tfrac{\hbar}{i}\nabla_x, x, t).$$

For example, if

$$H(p,q,t) = |p|^2 + V(t,q),$$

then

$$\mathcal{H} = -\hbar^2\Delta + V(t,x).$$

The Plank constant $\hbar$ is very small if we use the usual units SI to measure physical quantities, but it is ~ 1 if we use the atomic units. Both cases $\hbar \ll 1$ and $\hbar \sim 1$ are important.

The *principle of quantisation* tells that some quantitative properties of $\mathcal{H}$ (e.g., some its spectral properties), when $\hbar \to 0$, may be expressed in terms of the classical equation (1) (*the semiclassical limit*). And that some qualitative properties of the quantum systems are parallel to those of the classical equations (1). I will discuss this parallelism for some KAM-related theories.

The evolutionary Schrödinger equations with the non-autonomous Hamiltonian operator $\mathcal{H} = -\hbar^2\Delta + V(t,x)$ is the equation

$$i\hbar\,\dot{u} = -\hbar^2\Delta u + V(t,x)u.$$

Let $\{\varphi_s(x), s \in \mathbb{Z}^d\}$, be some Hilbert basis of $L^2(T^d)$, maybe depending on t. Take any solution $u(t,x)$ and decompose it in this basis: $u(t,x) = \sum_s u_s(t)\varphi_s(x)$. Then $\sum |u_s(t)|^2 \equiv$ Const. I recall that $|u_s|^2$ is the probability that the quantum particle occupies a state s.

What happens to quantities $|u_s(t)|^2$ as t growths, i.e. how the total probability $\sum |u_s(t)|^2$ is distributed between the states $s \in \mathbb{Z}^d$ when $t \gg 1$? This is the question which is addressed by the theorems I will discuss. For most of the talk I will assume that $\hbar = 1$.

§2. Quantum adiabaticity.

Let a classical Hamiltonian H has the form $H = H^\varepsilon = |p|^2 + V(\varepsilon t, q)$.

Then, if $\forall \tau$ the Hamiltonian $H_\tau = |p|^2 + V(\tau, q)$ is integrable, the classical averaging (or "adiabatic") theory applies to the classical system (1) (Laplace, Lagrange, Gauss, ...).

Consider the corresponding quantum Hamiltonian $\mathcal{H}^\varepsilon$ and the (nonautonomous) Schrödinger equation:

$$\dot{u} = -i\mathcal{H}^\varepsilon(u) = -i\big(-\Delta u + V(\varepsilon t, x)u\big). \tag{2}$$

The quantum adiabaticity deals with solutions of (2). It is as old as the quantum mechanics, e.g. see

P. Dirac (1925) "The adiabatic invariance of the quantum integrals".

(Note that Schrödinger published his equation one year later, in 1926.)

What this is about?

Denote $\mathcal{H}_\tau = -\Delta + V(\tau, x)$. Let $\{\varphi_s(\tau) = \varphi_s(\tau; x), s \in \mathbb{Z}^d\}$, and $\{\lambda_s(\tau)\}$ be the eigenvectors and eigenvalues of $\mathcal{H}_\tau$, each $\lambda_s(\tau)$ continuous in τ. Let $u(t, x)$ be a solution of the Schrödinger equation (2), satisfying $u(0, x) = \varphi_{s_0}(0)$,

("a pure state initial data"), where s_0 is such that for each τ, $\lambda_{s_0}(\tau)$ is an isolated eigenvalue of $\mathcal{H}_\tau$ of a constant multiplicity. Decompose $u(t)$ in the basis $\{\varphi_s(\varepsilon t)\}$: $u(t, x) = \sum_s u_s(t)\varphi_s(\varepsilon t; x)$. The quantum adiabatic theorem says that $u(t, x)$ stays close to the eigenspace, corresponding to $\lambda_{s_0}(\varepsilon t)$:

Theorem 1 (M. Born - V. Fock (1928) and T. Kato (1950))

$$\sup_{0 \le t \le \varepsilon^{-1}} \sum_{s:\, \lambda_s(\varepsilon t) \neq \lambda_{s_0}(\varepsilon t)} |u_s(t)|^2 \to 0 \text{ as } \varepsilon \to 0.$$

The result remains true if $x \in \mathbb{R}^d$ and $\mathcal{H}_\tau$ has mixed spectrum, but $\lambda_{s_0}(\tau)$ always is an isolated eigenvalue of constant multiplicity.

Note that in difference with the classical adiabaticity, now we DO NOT assume that the Hamiltonians $|p|^2 + V(\tau, q)$ are integrable.

§3. Around Nekhoroshev's Theorem

Start with classical systems. Let $(p, q) \in \mathbb{R}^d \times \mathbb{T}^d$. Let $H^\varepsilon(p, q) = h_0(p) + \varepsilon h_1(p, q)$ and h_0 is steep (e.g., it is strictly convex). Let $(p(t), q(t))$ be a solution. Then there are $a, b > 0$ such that

(3) $$|p(t) - p(0)| \le \varepsilon^a \qquad \forall\, |t| \le e^{\varepsilon^{-b}}.$$

That is,

$(*)$ under perturbed hamiltonian dynamics integrals of unperturbed system change only a bit during exponentially long time.

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 $h_1(\xi; p, q), \xi \in \mathbb{T}^N$ $(N \ge 1)$ is analytic. Then for a typical ω estimate (3) is true. In particular, let us take

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

The corresponding quantised Hamiltonian is the operator $-\Delta + \varepsilon V(\omega t; x)$, and the corresponding evolutionary equation is $\dot{u} = -i(-\Delta u + \varepsilon V(\omega t; x)u)$.
Do we have any analogy of the Nekhoroshev estimate

under perturbed dynamics integrals of the unperturbed system

change only a bit during exponentially long time?

Yes, even with $\varepsilon = 1$! Consider $\dot{u} = -i(-\Delta u + V(t,x)u)$. Denote $\|u\|_r^2 = \sum |u_s|^2(1+|s|^2)^r,\ r \in \mathbb{R}$.

Theorem 2 (J. Bourgain, 90's). Let $V(t,x) = \tilde{V}(\omega t, x)$, $\omega \in \mathbb{R}^N$, where ω is a Diophantine vector and $\tilde{V}$ is a smooth function on $\mathbb{T}^N \times \mathbb{T}^d$. Then for each $r \geq 1$ there exists $c(r)$ such that

$$\|u(t)\|_r \leq (\ln t)^{c(r)} \|u_0\|_r, \qquad \forall\, t \geq 2.$$

So if u_0 is smooth, then the high states s stay almost non-excited for exponentially long time.

Is it important that $V(t,x)$ is time-quasiperiodic? Not really!

We discuss

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

Theorem $2'$ (J. B.) Let V be smooth and C^k-bounded uniformly in (t,x) for each k. Then for each $r \geq 1$ and $a > 0$ there exists C such that

$$\|u(t)\|_r \leq C\, t^a \|u_0\|_r, \qquad \forall\, t \geq 2.$$

Also see papers by J-M Delort and W-M Wang (and cf. Theorem 1).

Problem. Prove any long-time stability result for actions of an integrable classical system under nonautonomous perturbations which are smooth and bounded uniformly in t.

§3. Quantum KAM

Let $(p,q)\in\mathbb{R}^d\times\mathbb{T}^d$. Consider integrable hamiltonian $h_0(p)=|p|^2$. Consider its perturbation $H^\varepsilon(p,q)=h_0(p)+\varepsilon V(\omega t,q)$, $\omega\in\mathbb{R}^N$, V is analytic. For the corresponding Hamiltonian equation we have a KAM-like result:

for a typical $(p(0),q(0))$ and a typical ω the solution $(p(t),q(t)$ is time-quasiperiodic.

The quantised hamiltonian defines the dynamical equation:

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

We regard the vector ω as a parameter of the problem:

$$\omega\in U\Subset\mathbb{R}^n.$$

Denote $L^2=L^2(\mathbb{T}^d,\mathbb{C})$. Provide it with the exponential basis $\{e^{is\cdot x},s\in\mathbb{Z}^d\}$. 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 see in

$[EK1]$ H. Eliasson and S. Kuksin, CMP 286 (2009), 125-136.

The 1d case is due to Bambusi-Graffi (2001).

We talk about the equation $\dot{u} = -i\big(-\Delta u + \varepsilon V(t\omega, x)u\big).$

Theorem 3. If $\varepsilon \ll 1$, then for most ω we can find an φ-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 the perturbed equation if and only if $v(t) = \Psi(t\omega)u(t)$ satisfies

$$\dot{v} = -i\big(-\Delta v + \varepsilon Q v\big).$$

The matrix (Q_{ab}) is block-diagonal, i.e. $Q_{ab} = 0$ 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, for any $p \in \mathbb{N}$ we have $\|Q\|_{H^p,H^p} \leq C_1$ and $\|\Psi(\varphi) - \mathrm{id}\,\|_{H^p,H^p} \leq \varepsilon^{\gamma'} C_2,\ \gamma' > 0.$ “For most” means “for all $\omega \in U_\varepsilon \subset U$, where mes $(U \setminus U_\varepsilon) \leq \varepsilon^\kappa$ for some $\kappa > 0$”.

Corollary. For ω as in the theorem all solutions $u(t,x)$ are almost-periodic functions of time. For any p they satisfy

$$(1-C\varepsilon)\|u(0)\|_p \le \|u(t)\|_p \le (1+C\varepsilon)\|u(0)\|_p, \quad \forall\, t \ge 0$$

(this is the “dynamical localisation”).

Proof. Since Q is block-diagonal, then $\|v(t)\|_p =$ const. Since $v(t) = \Psi(t)u(t)$ and $\|\Psi - \mathrm{id}\,\|_{H^p,H^p} \le \varepsilon C_2$, then the estimate follows. $\square$

Remarks. 1) Let $n=0$. Then the perturbed equation is $\dot u = -i\big(-\Delta u + \varepsilon V(x)u\big).$ Theorem states that this equation may be reduced to a block-diagonal equation

$\dot u = -iAu$, where

$A_{ab} = 0$ if $|a| \ne |b|.$ This is a well known fact.

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

Proof. The perturbed equation is a non-autonomous linear Hamiltonian system in L^2:
$\dot{u} = -i\frac{\delta}{\delta \bar{u}} H^\varepsilon(u), \quad H^\varepsilon(u) = \frac{1}{2}\langle \nabla u, \nabla \bar{u}\rangle + \frac{1}{2}\varepsilon \langle V(\varphi_0 + t\omega, x)u, \bar{u}\rangle.$

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

$$\dot{u} = -i\frac{\delta}{\delta \bar{u}} H^\varepsilon(u, \varphi, r),$$
$$\dot{\varphi} = \nabla_r H^\varepsilon = \omega,$$
$$\dot{r} = -\nabla_\varphi H^\varepsilon,$$

where $H^\varepsilon(u, \varphi, r, \varepsilon) = \omega \cdot r + \frac{1}{2}\langle \nabla u, \nabla \bar{u}\rangle + \frac{1}{2}\varepsilon \langle V(\varphi, x)u, \bar{u}\rangle.$

H^ε is a small perturbation of the integrable quadratical hamiltonian
$h_0 = \omega \cdot r + \frac{1}{2}\langle \nabla u, \nabla \bar{u}\rangle$. To perturbations of h_0 applies the KAM-theorem from
$[EK2]$ Eliasson-Kuksin, “KAM for nonlinear Schrödinger equation”, Ann. Math. 2010.

How the theorem from [EK2] implies Theorem 3 ? 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 $f=\frac{1}{2}\langle V(\varphi,x)u,\bar u\rangle$.

KAM Theorem from [EK2]: There exists domain $\mathcal{O}=\{\|u\|<\delta\}\times\mathbb{T}^n\times\{|r|<\delta\}$ and symplectic transformation $\Phi:\mathcal{O}\to L^2\times\mathbb{T}^n\times\mathbb{R}^n$ which transforms 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 $f' = O(|u|^3)+O(|r|^2)$.

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. NOW it is trivial: it simply states that $u(t)\equiv 0$ is a solution on the original equation.

But KAM theorem above tells more! Simple analysis of the proof (see a Remark in [EK2]) shows that if the perturbation εf is quadratic in u and r-independent, then

the KAM-transformations are linear in u and do not change ω.

So the transformed hamiltonians stay quadratic in u. Hence, the transformed 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.

§4. Quantum diffusion.

Let $(p,q) \in \mathbb{R}^d \times \mathbb{T}^d$. Consider $H^\varepsilon(p,q) = |p|^2 + \varepsilon V(\omega t, q)$, $\omega \in \mathbb{R}^N$, V is analytic. Fix any initial data (p_0, q_0). Then

i) by KAM, for a typical ω a solution such that $(p(0), q(0)) = (p_0, q_0)$ is time-quasiperiodic;

ii) for exceptional ω we "should" have the Arnold diffusion: the action $p(t)$ of a corresponding solution "diffuses away" from p_0.

The quantised hamiltonian defines the dynamical equation:

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

Claim 4. Let $d = 1$, $N \geq 2$ and the potential V is nondegenerate in a suitable sense. Then there exist a smooth function $u(0,x)$ and $\omega \in \mathbb{R}^N$ such that

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

for some $s \geq 1$.

An *example* of a time-periodic potential V, satisfying the assertion, is given by Bourgain. It is conjectured by H. Eliasson that the validity of the Claim for a *typical* potential follows from the method of his paper

H. L. Eliasson, Ergod.Th. Dynam. Sys 22 (2002), 1429 - 449.

Proof of this assertion is a work under preparation.

§5. Perturbed harmonic and unharmonic oscillators.

※ Consider Schrödinger equation in $\mathbb{R}^1$:

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

where $\mu > 0,\ m \in \mathbb{N},\ m \geq 2$; $V(\varphi, x)$ is C^2-smooth in φ, x and analytic in φ, bounded uniformly in φ, x. An analogy of the KAM-Theorem 3 holds. See [SK1993] LNM 1556 (Section 2.5) for the needed KAM-theorem.

※ Due to Bambusi-Graffi (CMP **219** (2001), 465-480) the result holds for non-integer m. That is, for equations

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

where $Q(x) \sim |x|^\alpha, \alpha > 2$ as $|x| \to \infty$. Moreover, they allow $V \to \infty$ as $|x| \to \infty$.

※ Liu-Yuan (CPAM, 2010) allow faster growth of V in x. They proved an analogy of Theorem 3 for the *quantum Duffing oscillator*

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

※ Due to Grebert and Thomann (CMP 2011) the assertion holds for the perturbed harmonic oscillator

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

What happens in higher dimensions, $d \geq 2$? – Nobody knows.

§6. Quantum adiabatic theorem in semiclassical limit

Consider the classical system on $T^*\mathbb{R}^d = \mathbb{R}^d \times \mathbb{R}^d$ with a smooth Hamiltonian

$$H(p, q, \varepsilon t) = |p|^2 + V(\varepsilon t, q),$$

and the corresponding quantum system

$$i\hbar\, \dot{u} = -\hbar^2 \Delta u + V(\tau, x)u = \mathcal{H}_\tau u, \quad \tau = \varepsilon t.$$

We assume that for each τ the potential $V(\tau, x)$ grows to infinity with $|x|$, so the operator $\mathcal{H}_\tau = -\hbar^2\Delta + V(\tau, x)$ has a discrete spectrum.

We will fix ε so small that it allows to make some statements about the dynamics of the classical system, and then pass to the limit as $\hbar \to 0$. This limiting dynamics may be quite different from that in Section 2 on quantum adiabaticity when $\hbar$ is fixed and $\varepsilon \to 0$. This was first demonstrated by M. Berry.

Systems with one degree of freedom.

Let the classical Hamiltonian $H_\tau(p,q) = H(p,q,\tau) = -p^2 + V(\tau,q)$ has one degree of freedom. Assume that for each $\tau = \mathrm{const}$ in the phase plane of H_τ there is a domain filled by closed trajectories. In this domain we introduce action-angle variables $I = I(p,q,\tau)$, $\chi = \chi(p,q,\tau)$ ($\chi \in \mathbb{T}^1$), and express H_τ via the action variable and τ, $H_\tau(p,q) = E(I,\tau)$.

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

Theorem (classical averaging). There exist ε_0, c_1 such that for $0 < \varepsilon < \varepsilon_0$ we have

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

Bohr-Sommerfeld Quantisation Rule. Assume that for each $\tau = \mathrm{const} \in [0,1]$ and each $I_* \in [a,b]$ the classical Hamiltonian H_τ has a unique trajectory with the action $I = I_*$. Then the quantum operator $\mathcal{H}_\tau$ has a series of eigenfunctions $\varphi_s(\tau) = \varphi_s(\tau, x)$ such that the corresponding eigenvalues are $\lambda_s(\tau) = E(I_s, \tau) + O(\hbar^2)$, where $I_s = \hbar(s + 1/2) \in [a,b]$.

Let $u(t,x)$ be a solution of the Schrödinger equation with a pure state initial condition:

$$i\hbar\,\dot{u} = -\hbar^2 \Delta u + V(\varepsilon t, x)u, \qquad u(0,x) = \varphi_{s_0}(0;x).$$

Denote by $\mathbf{P}^\tau_{(\alpha,\beta)}$ the spectral projector in $L^2(\mathbb{R})$ onto the linear span of vectors $\varphi_s(\tau)$ with $I_s \in (\alpha, \beta)$.

Theorem 5. There exist ε_0, c_1 such that if $0 < \varepsilon < \varepsilon_0$ and $0 < \hbar \le \varepsilon$, then for any $m \ge 1$ and a suitable $c_2(m) > 0$ we have

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

Thus $u(t,\cdot)$ stays close to the eigenspace that corresponds to eigenvalues from the $O(\varepsilon)$-neighbourhood of $\lambda_{s_0}(\varepsilon t)$ (dimension of this space is $\sim \varepsilon/\hbar$). I recall that for $\hbar = 1$ it stays close to the eigenspace, corresponding to f $\lambda_{s_0}(\varepsilon t)$ (it has a finite dimension ~ 1).

Systems with many degrees of freedom. Now let $d \geq 2$. Assume that for any τ the Hamiltonian $H_\tau = |p|^2 + V(\tau, q)$ is integrable. Let $u(t,x)$ be a solution of the quantum system

$$i\hbar\,\dot{u} = -\hbar^2 \Delta u + V(\varepsilon t, x)u,$$

such that $u(0,x) = \varphi_{s_0}(0; x)$.

Conjecture. For $d \geq 2$ relation (4) is not in general true since the l.h.s. is $\sim C\varepsilon$, uniformly in $0 < \hbar < \varepsilon$, due to "the quantisation of the capture in resonance".

That is, with probability $\sim \varepsilon$ the quantum particle escapes the spectral vicinity of the original state s_0. There is a specific prediction what happens to this defect of probability.

Consider the Schrödinger equation

$$i\hbar\,\dot{u} = -\hbar^2\,\Delta u + \varepsilon V(t\omega, x)u, \quad x \in \mathbb{T}^d.$$

If $\hbar = 1$, it was treated in the KAM-Section 3. By analogy with the results above in this section:

Problem. Study solutions of this equation for typical ω with fixed $\varepsilon \leq \varepsilon_0$ (ε_0 sufficiently small), and $\varepsilon \geq \hbar \searrow 0$. Find their relations with KAM-properties of the classical hamiltonian system with the Hamiltonian $|p|^2 + \varepsilon V(\omega t, q)$.

(It may be that this is not just ”right scaling” of the question – e.g. it may be that $V(\omega t, q)$ has to be replaced by $V(\hbar^a \omega t, q)$ with a suitable exponent a.)

See

SK and A.Neishtadt, arXiv 2012