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VÝZKUMNÝ ÚKOL

EGOROV THEOREM FOR TIME DEPENDENT CASE

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1 Introduction

According to the Bohr's correspondance principle, the quantum evolution of an observable is close to its classical evolution as the Planck constant $\hbar$ is small. In the mathematical literature this result is known as Egorov Theorem [Ho], [Ro1]. There is a lot of semiclassical methods, which attack classical limit in quantum mechanics. Nice summary of these methods, with large overview of literature dealing with this topic is [Ro2]. There is also different point of view, WKB approximation in Feynman path integral [Sch].

The goal of this work is to prove that quantum evolution of an obbservable, in the system with time dependent Hamiltonian, may be computed (up to an error of order $\hbar^2$) with help of the classical flow, if the observable, Hamiltonian and the classical flow are bounded in suitable sense. Physical interpratention of this fact is clear. When the quantities of the dimension same as $\hbar$, like $E.t$, $p.q$ are much larger then numerical value of $\hbar$ (i.e. that is possible limit $\hbar \to 0$), then quantum evolution of an observable tends to the classical one. The theory of this type use so called Weyl-quantization, as powerfull tool to construct quantum observables (i.e. symmetric or even essentially self-adjoint operators) according to the principal of corespondance.

Starting point of this work is the preprint [BR]. This work deals only with C^∞ case, but the statement of the main theorem is improved. The assumptions on Hamiltonian are weaker (it is possible cubic increasment in infinity) and the error is estimated to order $\hbar^2$ instead of $\hbar$ in [BR].

The heart of this work is the time dependent case. It is schown (for Hamiltonian of the Schrödinger type) that even in this more general case the consequences of the semiclassical theorem are the same, if observable depends only on coordinate and momentum.

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2 Notation and conventions

Let us denote by $X = \mathbb{R}^n$ the configuration space of a classical mechanical system with n degrees of freedom. The corresponding phase space Z is identified with $\mathbb{R}^{2n}$ equipped with the symplectic form σ defined by

$$\sigma(z; z') = \langle Jz, z' \rangle. \tag{1}$$

where $\langle , \rangle$ is the Euclidean scalar product and J is the $2n \times 2n$ matrix

$$J = \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix}.$$

A generic point in Z is denoted z and its coordinates by (q, p) where $q, p \in \mathbb{R}^n$. We will also use notation $\langle x \rangle = (1 + |x|^2)^{1/2}$.
A classical Hamiltonian is a smooth real function $H : Z \to \mathbb{R}$. Our basic example will be $H(q,p) = \frac{\|p\|^2}{2m} + V(q)$ $(m > 0)$ where $\|p\|^2 =< p, p >$. In what follows we put emphasis on the case $X = \mathbb{R}^n$.
The motion of the classical system is determined by the system of Hamilton's equations

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}(q,p), \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q}(q,p). \tag{2}$$

The equations (2) generate a flow Φ^t on the phase space Z, defined by
$\Phi^t(q(0), p(0)) = (q(t), p(t))$; $\Phi^0 = \mathbb{1}$. Φ^t exists locally by the Cauchy-Lipchitz Theorem for O.D.E. But we need more assumptions on H to define Φ^t globally on Z.
Φ^t defines a symplectic diffeomorphism (canonical transformation) group of transformations on Z. Let us consider a classical observable A, i.e A a smooth real valued function defined on phase space Z. The time evolution of A can be easily computed

$$\frac{d}{dt} A(\Phi^t(z)) = \{H, A\}(\Phi^t(z)), \quad z = (q,p) \tag{3}$$

where $\{H, A\}$ is the Poisson bracket defined by

$$\{H, A\} = \partial_q H \cdot \partial_p A - \partial_p H \cdot \partial_q A.$$

Here we have used the notation $\partial_q = \frac{\partial}{\partial q}$. Now let us assume that H, A are quantizable. That means that we can associate to them the quantum observables $\hat{H}$ and $\hat{A}$
i.e self-adjoint operators in $L^2(X)$. By solving the Schrödinger equation :
$i\hbar\partial_t \psi_t = \hat{H}\psi_t$, we can define the one parameter group of unitary operators
$U(t) = \exp\left(-\frac{it}{\hbar}\hat{H}\right)$. The quantum time evolution of $\hat{A}$ is then given by

$$\hat{A}(t) = U(-t)\hat{A}\, U(t)$$

which satisfies the Heisenberg-von Neumann equation

$$\frac{d\hat{A}(t)}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{A}], \tag{4}$$

where $[A, B] = AB - BA$ is the commutator of A, B.

3 Weyl quantization

Definition 3.1 *$A \in \mathcal{O}(m)$, $m \in \mathbb{R}$, if and only if $Z \xrightarrow{A} \mathbb{C}$ is C^∞ in Z and for every multi-index $\gamma \in \mathbb{N}^{2n}$ there exists $C > 0$ such that*

$$|\partial_z^\gamma A(z)| \le C\langle z\rangle^m, \ \forall z \in Z.$$

Definition 3.2 *Let $A \in \mathcal{O}(m)$. We will define $\hat{A}$ as operator from $\mathcal{S}(X)$ to itself, called $\hbar$-Weyl quantization of A, by the following formula, with $\psi \in \mathcal{S}(X)$,*

$$\hat{A}\psi(x) = (2\pi\hbar)^{-n} \int_X \left(\int_X A\left(\frac{x+y}{2}, p\right) \mathrm{e}^{i\hbar^{-1}\langle x-y,p\rangle} \psi(y) dy \right) dp. \tag{5}$$

Example: Let us focus for example to observable $A := x.p$. To compute $\hat{A}$ we will use

$$p \exp(\frac{i}{\hbar}(x-y)p) = -\frac{\hbar}{i}\partial_y \exp(\frac{i}{\hbar}(x-y)p)$$

and after integration by parts we yeild

$$\hat{A} = \frac{1}{2}(\hat{p}\hat{q} + \hat{q}\hat{p}).$$

For $A \in \mathcal{S}(Z)$ we will compute, (with help of integral kernel) inverse prescription of Weyl symbol if operator is given as integral operator.

$$(\hat{A}\psi)(x) = (2\pi\hbar)^{-n} \iint_Z A\left(\frac{x+y}{2}, p\right) \mathrm{e}^{i\hbar^{-1}\langle x-y,p\rangle} \psi(y) dy dp = \int_{\mathbb{R}^n} \mathcal{K}_A(x,y)\psi(y) dy$$

$$\mathcal{K}_A(x,y) := (2\pi\hbar)^{-n} \int_{\mathbb{R}^n} A\left(\frac{x+y}{2}, p\right) \mathrm{e}^{i\hbar^{-1}\langle x-y,p\rangle} dp$$

After inverse Fourier transform.

$$A(x,\xi) = \int_{\mathbb{R}^n} \mathcal{K}_A\left(x + \frac{v}{2}, x - \frac{v}{2}\right) \mathrm{e}^{-\frac{i}{\hbar}\langle v,\xi\rangle} dv \tag{6}$$

The class $\mathcal{O}(m)$ has nice properties. For example, if $A \in \mathcal{O}(m)$ is real-valued function, then $\hat{A}$ is symmetric operator in $L^2(X)$, with domain $\mathcal{S}(X)$. Further there exists a product formula. For proof one can see [Ro1], [Fo] or [Ho].

Theorem 3.3 *Let $A \in \mathcal{O}(m)$, $B \in \mathcal{O}(p)$, then there exists $C \in \mathcal{O}(m+p)$, such that*

$$\hat{A} \cdot \hat{B} = \hat{C}$$

And there exists following asympotic expansion of Weyl symbol of this operator

$$C(q,p) = \exp\left(\frac{i\hbar}{2}\sigma(D_q, D_p; D_{q'}, D_{p'})\right) A(q,p)B(q',p')|_{(q,p)=(q',p')},$$

where σ is the symplectic bilinear form (1) and $D = i^{-1}\nabla$. By expanding the exponential term, we get

$$C(q,p) = \sum_{j\geq 0} \frac{\hbar^j}{j!}(\frac{i}{2}\sigma(D_q, D_p; D_{q'}, D_{p'}))^j A(q,p)B(q',p')|_{(q,p)=(q',p')}.$$

So that $C(q,p)$ is a formal power serie in $\hbar$ with coefficients given by

$$C_j(q,p) = \frac{1}{2^j}\sum_{|\alpha+\beta|=j} \frac{(-1)^{|\beta|}}{\alpha!\beta!}(D_q^\beta \partial_p^\alpha A).(D_q^\alpha \partial_p^\beta B)(q,p). \tag{7}$$

We will show this for $A, B \in \mathcal{S}(Z)$

$$\left(\hat{A}\cdot\hat{B}\psi\right)(x) = \int_{\mathbb{R}^n} \mathcal{K}_{A\cdot B}(x,y)\psi(y)dy$$

where

$$\mathcal{K}_{A\cdot B}(x,y) = \frac{1}{(2\pi\hbar)^{2n}}\int_{\mathbb{R}^{3n}} A\left(\frac{x+z}{2}, p\right) B\left(\frac{z+y}{2}, \eta\right) \mathrm{e}^{-\frac{i}{\hbar}\langle x-z,p\rangle + \langle z-y,\eta\rangle} dzdpd\eta$$

Let's define

$$\hat{C} := \hat{A}\cdot\hat{B}$$

then Weyl symbol of $\hat{C}$ can be computed with help of formula (6).

$$\begin{aligned} C(x,\xi) &= \int_{\mathbb{R}^n} \mathcal{K}_{A\cdot B}\left(x+\frac{v}{2}, x-\frac{v}{2}\right)\mathrm{e}^{-\frac{i}{\hbar}v\cdot\xi}dv \\ &= \frac{1}{(2\pi\hbar)^{2n}}\int_{\mathbb{R}^{4n}} A\left(\frac{x+z-\frac{v}{2}}{2}, p\right) B\left(\frac{z+y-\frac{v}{2}}{2}, \eta\right) \times \\ &\quad \times \mathrm{e}^{\frac{i}{\hbar}\left(\langle x+\frac{v}{2}-z,p\rangle + \langle z-x+\frac{v}{2},\eta\rangle - v\xi\right)} dzdpd\eta dv \end{aligned}$$

We apply the change of variables

$$s := \frac{1}{2}(x+z)+\frac{1}{4}v, \quad t := \frac{1}{2}(x+z)-\frac{1}{4}v \Rightarrow z = s+t-x, \quad v = 2(s-t), \quad dzdv = 4^n dsdt$$

to get

$$C(x,\xi) = \frac{1}{(\pi\hbar)^{2n}} \int_{\mathbb{R}^{4n}} A\,(s,p)\, B\,(t,\eta)\, \mathrm{e}^{\frac{2i}{\hbar}(\langle x-s,\xi-\eta\rangle - \langle x-t,\xi-p\rangle)} ds dp dt d\eta$$

Now using Taylor formula

$$A(s,p)B(t,\eta) = \sum_{|\alpha+\beta|<N} \partial_x^\alpha A(x,p)\ \partial_x^\beta B(x,\eta) \frac{(s-x)^\alpha}{\alpha!} \frac{(t-x)^\beta}{\beta!}$$
$$+ \sum_{|\alpha+\beta|=N} \int_0^1 (1-\sigma)^N \partial_x^\alpha A(x+\sigma(s-x),p)\ \partial_x^\beta B(x+\sigma(t-x),\eta) \frac{(s-x)^\alpha}{\alpha!} \frac{(t-x)^\beta}{\beta!} d\sigma$$

we obtain

$$\begin{aligned} C(x,\xi) \quad = \quad & \frac{1}{(\pi\hbar)^{2n}} \sum_{|\alpha+\beta|<N} \int_{\mathbb{R}^{4n}} \partial_x^\alpha A(x,p)\ \partial_x^\beta B(x,\eta) \frac{(s-x)^\alpha}{\alpha!} \frac{(t-x)^\beta}{\beta!} \times \\ & \times \mathrm{e}^{\frac{2i}{\hbar}(\langle x-s,\xi-\eta\rangle - \langle x-t,\xi-p\rangle)} ds dp dt d\eta + R_{N-1}(A,B;z;\hbar), \end{aligned}$$

where the remainder is defined by:

$$C(z) - \sum_{0\le j\le N} \hbar^j C_j(z) =: R_N(A,B;z;\hbar). \tag{8}$$

$$z = (x,\xi) \in Z$$

Using

$$(s-x)^\alpha (t-x)^\beta \mathrm{e}^{\frac{2i}{\hbar}(\langle x-s,\xi-\eta\rangle - \langle x-t,\xi-p\rangle)} = \left(\frac{\hbar}{2i}\right)^{|\alpha|+|\beta|} (-1)^{|\beta|}\ \partial_\eta^\alpha \partial_p^\beta\ \mathrm{e}^{\frac{2i}{\hbar}(\langle x-s,\xi-\eta\rangle - \langle x-t,\xi-p\rangle)}$$

and integrating by parts we get

$$\begin{aligned} & C(x,\xi) = \\ & \frac{1}{(\pi\hbar)^{2n}} \sum_{|\alpha+\beta|<N} \left(\frac{\hbar}{2i}\right)^{|\alpha|+|\beta|} (-1)^{|\alpha|} \int_{\mathbb{R}^{4n}} \frac{\partial_p^\beta \partial_x^\alpha A(x,p)}{\alpha!} \frac{\partial_\eta^\alpha \partial_x^\beta B(x,\eta)}{\beta!} \times \\ & \times\ \mathrm{e}^{\frac{2i}{\hbar}(\langle x-s,\xi-\eta\rangle - \langle x-t,\xi-p\rangle)} ds dp dt d\eta\ + R_{N-1}(A,B;z;\hbar). \end{aligned}$$

Finally

$$\begin{aligned} C(x,\xi) \quad = \quad & \sum_{|\alpha+\beta|<N} \left(\frac{\hbar}{2i}\right)^{|\alpha|+|\beta|} (-1)^{|\alpha|} \frac{\partial_\xi^\beta \partial_x^\alpha A(x,\xi)}{\alpha!} \frac{\partial_\xi^\alpha \partial_x^\beta B(x,\xi)}{\beta!} + \\ + \quad & R_{N-1}(A,B;z;\hbar). \end{aligned}$$

Remainder (8) can be also expressed as

$$R_{N-1}(A,B;z;\hbar) := \frac{1}{(\pi\hbar)^{2n}}\sum_{|\alpha+\beta|=N}\int_0^1 (1-\sigma)^N \partial_x^\alpha A(x+\sigma(s-x),p)\ \partial_x^\beta B(x+\sigma(t-x),\eta)\times$$
$$\times\frac{(s-x)^\alpha}{\alpha!}\frac{(t-x)^\beta}{\beta!}\mathrm{e}^{\frac{2i}{\hbar}(\langle x-s,\xi-\eta\rangle-\langle x-t,\xi-p\rangle)}d\sigma ds dp dt d\eta$$

After the change of variables

$$\sigma(s-x) =: s',\ \ \sigma(t-x) =: t',\ \ \eta-\xi =: \eta',\ \ p-\xi =: p'$$

and using the same trick with integrating by parts (and in what follows omitting primes) we finally get

$$R_{N-1}(A,B;z;\hbar) := \left(\frac{\hbar}{2i}\right)^N \int_0^1 \frac{(1-\sigma)^N}{(\pi\hbar\sigma)^{2n}}\sum_{|\alpha+\beta|=N}\frac{(-1)^\alpha}{\alpha!\beta!}\partial_p^\beta\partial_x^\alpha A(x+s,p+\xi)\ \partial_\eta^\alpha\partial_x^\beta B(x+t,\eta+\xi)\times$$
$$\times\exp\left(\frac{2i}{\hbar\sigma}\left(\langle s,\eta\rangle-\langle t,p\rangle\right)\right)d\sigma ds dp dt d\eta =$$
$$\left(\frac{\hbar}{2i}\right)^N\int_0^1\frac{(1-\tau)^N}{(\pi\hbar\tau)^{2n}}\int_{Z\times Z}\exp(-\frac{2i}{\tau\hbar}\sigma(u,v))\sigma^{N+1}(D_u,D_v)A(u+z)B(v+z)dudvd\tau.$$

Now we estimate this remainder and his derivatives.

Theorem 3.4 *There exists $K_n > 0$ and for every $m\in\mathbb{N}$, $m\geq 4n$, for every $s>4n$ there exists a constant $\rho_{n,m,s}$ such that for every $A,B\in\mathcal{S}(Z)$, for every $N\geq 1$, for every multi-index γ, the following estimate holds, for every $z\in Z$,*

$$|\partial_z^\gamma\left(C(z)-\sum_{0\leq j\leq N}\hbar^j C_j(z)\right)|\leq \hbar^{N+1}\rho_{n,m,s}K_{n,N,|\gamma|}\times$$
$$\times\sup_{(*)}\left[(1+u^2+v^2)^{(s-m)/2}|\partial_u^{(\alpha,\beta)+\mu}A(u+z)||\partial_v^{(\beta,\alpha)+\nu}B(v+z)|\right]\qquad(9)$$

where $\sup\limits_{(*)}$ means that the supremum holds under the conditions $u,v\in Z$, $|\mu|+|\nu|\leq m+|\gamma|$, $|\alpha|+|\beta|=N+1$ ($\mu,\nu\in\mathbb{N}^{2n}$, $\alpha,\beta\in\mathbb{N}^n$).

Proof :

We shall use the following lemma to estimate $R_N(A,B;z,\hbar)$.

Lemma 3.5 *Let us consider $F\in\mathcal{S}(Z\times Z)$ and the integral*

$$I(\lambda)=\lambda^{2n}\int_{Z\times Z}\exp[-i\lambda\sigma(u,v)]F(u,v)dudv.$$

Then for every real number $s > 4n$ and every integer $m \geq 4n$ there exists $\kappa(n,s,m) > 0$ depending only on n, s, m (but independent of F) such that the following estimate holds

$$|I(\lambda)| \leq \kappa(n,s,m) \sup_{\substack{u,v \in Z, \\ |\mu|+|\nu|\leq m}} (1+u^2+v^2)^{(s-m)/2} |\partial_u^\mu \partial_v^\nu F(u,v)|.$$

Proof : Let us introduce a cut-off χ_0, C^∞ on $\mathbb{R}$, $\chi_0(x) = 1$ for $|x| \leq 1/2$ and $\chi_0(x) = 0$ for $|x| \geq 1$. We split $I(\lambda)$ into three pieces

$$I_0(\lambda) = \lambda^{2n} \int_{Z\times Z} \exp[-i\lambda\sigma(u,v)]\chi_0(u^2+v^2)\chi_0(\lambda(u^2+v^2))F(u,v)dudv,$$

$$I_1(\lambda) = \lambda^{2n} \int_{Z\times Z} \exp[-i\lambda\sigma(u,v)] \left(1-\chi_0(\lambda(u^2+v^2))\right)\chi_0(u^2+v^2)F(u,v)dudv,$$

$$I_2(\lambda) = \lambda^{2n} \int_{Z\times Z} \exp[-i\lambda\sigma(u,v)](1-\chi_0(u^2+v^2))F(u,v)dudv.$$

For $I_0(\lambda)$, we easily have

$$|I_0(\lambda)| \leq \omega_{4n} \sup_{u^2+v^2\leq 1} |F(u,v)|,$$

where ω_{4n} is the volume of the unit ball in Z^2. For $I_1(\lambda)$ and $I_2(\lambda)$, we integrate by parts with the differential operator

$$L = \frac{i}{u^2+v^2}\left(Ju\frac{\partial}{\partial v} - Jv\frac{\partial}{\partial u}\right),$$

where J is the matrix associated to the symplectic form ($\sigma(u,v) =< Ju, v >$). It holds true that

$$L\left(\exp[-i\lambda\sigma(u,v)]\right) = \lambda \exp[-i\lambda\sigma(u,v)].$$

Performing $4n$ integrations by parts, we can see that it exists a constant c_n such that

$$|I_1(\lambda)| \leq c_n \sup_{\substack{u^2+v^2\leq 1 \\ |\mu|+|\nu|\leq 4n}} |\partial_u^\mu \partial_v^\nu F(u,v)|.$$

Similarly, performing m integrations by parts,

$$\begin{aligned} |I_2(\lambda)| &\leq \left| \int_{Z\times Z} \exp[-i\sigma(u,v)] \left(1-\chi_0(\frac{1}{\lambda}(u^2+v^2)\right) F(\frac{u}{\sqrt{\lambda}}, \frac{v}{\sqrt{\lambda}})\ dudv\right| \\ &\leq c_m \int_{Z\times Z} (\frac{|u|+|v|}{u^2+v^2})^m \sup_{|\mu|+|\nu|\leq m} |\partial_u^\mu \partial_v^\nu \left((1-\chi_0(\frac{1}{\lambda}(u^2+v^2))F(\frac{u}{\sqrt{\lambda}}, \frac{v}{\sqrt{\lambda}})\right)|dudv. \end{aligned}$$

Using the existence of integral

$$\int_{Z\times Z} (\frac{|u|+|v|}{u^2+v^2})^m (1+u^2+v^2)^{\frac{m-s}{2}} dudv$$

we get for a constant $c(n, s, m)$,

$$|I_2(\lambda)| \leq c_n \sup_{\substack{u,v \in Z \\ |\mu|+|\nu| \leq m}} (1 + u^2 + v^2)^{(s-m)/2} |\partial_u^\mu \partial_v^\nu F(u, v)|.$$

∎

Now we can complete the proof of the theorem by using Lemma 3.5, the Leibniz formula and the following elementary estimate, using in Z the coordinates $u = (x, \xi)$, $v = (y, \eta)$,

$$|\sigma^N(\partial_x, \partial_\xi; \partial_y, \partial_\eta))A(x,\xi)B(y,\eta)| \leq$$
$$(2n)^N \sup_{|\alpha|+|\beta|=N} |\partial_x^\alpha \partial_\xi^\beta A(x,\xi) \partial_y^\beta \partial_\eta^\alpha B(y,\eta)|.$$

∎

Remark 3.6 *We can easily extend the estimate (9) for observables A, B with polynomial growth at infinity, by choosing m large enough to get a finite r.h.s. Let us assume that $A \in \mathcal{O}(\mu_A)$, $B \in \mathcal{O}(\mu_B)$, where $\mu_A, \mu_B \in \mathbb{R}$. Then we can apply (9) to $A_\varepsilon(u) = \mathrm{e}^{-\varepsilon u^2} A(u)$ and $B_\varepsilon(v) = \mathrm{e}^{-\varepsilon v^2} B(v)$ for $\varepsilon > 0$ and pass to the limit $\varepsilon \to 0$ with $m - s \geq \mu_A + \mu_B$.*

4 Main theorem

Theorem 4.1 *Let us consider a Hamiltonian H and an observable A satisfying*

$$\begin{aligned} |\partial_z^\gamma H(z)| &\leq C_\gamma, \quad \text{for} \quad |\gamma| \geq 3 \\ |\partial_z^\gamma A(z)| &\leq C_\gamma, \quad \text{for} \quad |\gamma| \geq 1 \\ |\partial_z^\gamma \Phi^\tau(z)| &\leq K_\gamma(t), \quad \text{for} \quad |\gamma| \geq 1,\ \tau \in [0,t] \end{aligned} \tag{10}$$

We know that $\hat{H}, \hat{A}$ are symmetric operators on the Schwartz space. If they are moreover essentially self-adjoint operators in $L^2(X)$, with core $\mathcal{S}(X)$, then the quantum evolution

$$U(t) = \exp(-\frac{it}{\hbar}\bar{\hat{H}})$$

is well defined for all $t \in \mathbb{R}$. And the quantum evolution of observable $\hat{A}$ can be approximated by the operator with the Weyl symbol

$$A_0(t,z) = A(\Phi^t(z)) \tag{11}$$

in the following sense:

$$\|\hat{A}(t) - \widehat{A_0(t)}\|_{L^2} \leq t\hbar^2 K_{n,m,s}(t)$$

Proof: By Taylor formula

$$H \in \mathcal{O}(4)\ , \quad A \in \mathcal{O}(2)$$

For any $\psi \in \mathcal{S}(\mathcal{X})$ it holds true that

$$\frac{d}{dt}\widehat{A_0}\psi = (\widehat{\frac{d}{dt}A_0})\psi \tag{12}$$

Under assumptions propagator exists and conserves $\mathcal{S}(\mathcal{X})$, because Hamiltonian does. On Schwartz space holds equation

$$\begin{aligned} U(-t)\hat{A}U(t) - \widehat{A_0}(t) &= \int_0^t \frac{d}{ds}(U(-s)\widehat{A \circ \Phi^{t-s}}U(s))\ \mathrm{d}s \\ &= \int_0^t U(-s)\left(\frac{i}{\hbar}[\hat{H}, \widehat{A_0}(t-s)] - \widehat{\{H,A\} \circ \Phi^{t-s}}\right) U(s)\ \mathrm{d}s, \end{aligned} \tag{13}$$

where (3), (4), (12), conservation of Poisson bracket and Hamiltonian along the classical flow were used. With help of (7) we compute that the Weyl symbol of expression

$$\widehat{C} := \frac{i}{\hbar}[\hat{H}, \hat{A}]$$

is

$$C = 0 + \{H,A\} + 0 + 2\frac{i}{\hbar}R_2(H,A;z,\hbar)\ ,$$

where

$$R_2(H,A;z,\hbar) = \qquad (14)$$
$$\left(\frac{\hbar}{2i}\right)^3 \int_0^1 \frac{(1-\tau)^N}{(\pi\hbar\tau)^{2n}} \int_{Z\times Z} \exp(-\frac{2i}{\tau\hbar}\sigma(u,v))\sigma^3(D_u,D_v)A(u+z)B(v+z)dudvd\tau.$$

Aplying L^2 norm to (13) we obtain

$$\|\hat{A}(t) - \widehat{A_0(t)}\|_{L^2} \le 2\frac{t}{\hbar}\|\widehat{R_2}(H,A;z,\hbar)\|_{L^2}.$$

But there is a Calderon- Vaillancourt Theorem with improvement by A. Boulkhemair [Bo], which estimates the norm of Weyl-quantized operator

$$\|\hat{B}\|_{L^2} \le \gamma_n \sup_{\substack{|\alpha|,|\beta|\le[n/2]+1 \\ z\in Z}} |\partial_z^{\alpha,\beta} B(z)|. \qquad (15)$$

So we need to estimate

$$\sup_{\substack{|\alpha|,|\beta|\le[n/2]+1 \\ z\in Z}} |\partial_z^{\alpha,\beta} R_2(H,A;z,\hbar)|.$$

This is exactly what we have prepared in the **Theorem** 3.4. Using (10) we deduce that for each $s \le m$ there exist $K_{n,m,s}(t)$, such that:

$$K_{n,m,s}(t) :=$$
$$\sup_{(*)} \left[(1+u^2+v^2)^{(s-m)/2}|\partial_u^{(\alpha,\beta)+\mu}H(u+z)||\partial_v^{(\beta,\alpha)+\nu}A(\Phi^\tau(u+z)|\right] < \infty$$

where $\sup\limits_{(*)}$ means that the supremum holds under the conditions $u,v,z \in Z, \tau \in [0,t]$, $|\mu|+|\nu| \le m+[n/2]+4$, $|\alpha|+|\beta| = 3$ $(\mu,\nu \in \mathbb{N}^{2n},\ \alpha,\beta \in \mathbb{N}^n)$.
We have also used following estimate on derivatives of composition of functions

$$|\partial^\alpha(f\circ g)| \le K_{n,|\alpha|} \sup_{\substack{\beta,\gamma\ne 0 \\ |\beta|,|\gamma|\le|\alpha|}} |\partial^\beta f||\partial^\gamma g|$$

Combining all these facts we may finish the proof. ∎

5 Time dependent case

We will consider the time dependent Hamiltonian of special type

$$H = \frac{1}{2}p^2 + V(q,t)$$

on line. The trick is to extend the phase space about the time and energy (canonical momentum of time), to define new parameter σ which describes the trajectory and to take Floquet Hamiltonian instead of the original one.

$$K(q_1, q_2, p_1, p_2) := \frac{1}{2}p_1^2 + V(q_1, q_2) + p_2,$$

where

$$\begin{aligned} q_1 &= q \text{ is the original coordinate} \\ p_1 &= p \text{ is the original momentum} \\ q_2 &= t \text{ is time} \\ p_2 &= E \text{ is energy.} \end{aligned}$$

New Hamilton equations of motion will be

$$\begin{aligned} \frac{dq_1}{d\sigma} &= \frac{\partial K}{\partial p_1}, \quad \frac{dp_1}{d\sigma} = -\frac{\partial K}{\partial q_1} \\ \frac{dq_2}{d\sigma} &= \frac{\partial K}{\partial p_2}, \quad \frac{dp_2}{d\sigma} = -\frac{\partial K}{\partial q_2} \end{aligned}$$

Hence

$$\begin{aligned} \frac{dq}{d\sigma} &= p, \quad \frac{dp}{d\sigma} = -\frac{\partial V}{\partial q} \\ \frac{dt}{d\sigma} &= 1, \quad \frac{dE}{d\sigma} = -\frac{\partial V}{\partial t} \end{aligned} \tag{16}$$

We need initial conditions

$$q(\sigma = 0) = q_0,\ p(\sigma = 0) = p_0,\ t(\sigma = 0) = t_0,\ E(\sigma = 0) = E_0 \tag{17}$$

But because the right hand sides of Hamiltonian equations for q, p, t does not depend on energy E and so doesn't the initial conditions, we may conclude that the classical flow Φ^σ will be of this type

$$\Phi^\sigma \begin{pmatrix} q \\ p \\ t \\ E \end{pmatrix} = \begin{pmatrix} q(q_0, p_0, t_0, \sigma) \\ p(q_0, p_0, t_0, \sigma) \\ \sigma + t_0 \\ E(q_0, p_0, t_0, E_0, \sigma) \end{pmatrix}$$

So we see that the trajectories of q, p, t are independent on energy E. This cause that we can make weaker assumptions on potential V, then in case of $\mathbb{R}^4$.

Theorem 5.1 *Consider the time dependent Hamiltonian of type*

$$H = \frac{1}{2}p^2 + V(q,t)$$

on line. Denote the classical flow Φ, given by Hamilton equations in extended space (16). Suppose that

$$\begin{array}{rll} |\partial_x^{3+\alpha}\partial_t^{\beta}V(x,t)| \le C_{\alpha\beta}, & \text{for} & |\alpha|,\ |\beta| \ge 0 \\ |\partial_z^{\gamma}A(z)| \le C_{\gamma}, & \text{for} & |\gamma| \ge 1 \\ |\partial_z^{\gamma}\Phi^{\tau}(z)| \le K_{\gamma}(\sigma), & \text{for} & |\gamma| \ge 1,\ \tau \in [0,\sigma] \end{array}$$

If moreover $\hat{H}, \hat{A}$ are essentially self-adjoint operators in $L^2(X)$, with core $\mathcal{S}(X)$, then the quantum evolution

$$U(\sigma) = \exp(-\frac{i\sigma}{\hbar}\bar{\hat{H}})$$

is well defined for all $\sigma \in \mathbb{R}$. And the quantum evolution of observable $\hat{A}$ can be approximated by the operator with the Weyl symbol (11)

$$\|\hat{A}(\sigma) - \widehat{A_0(\sigma)}\|_{L^2} \le \sigma\hbar^2 K_{n,m,s}(\sigma)$$

Proof: The situation is almost the same as in the **Theorem** 4.1, except the expression (14), which may by substituted by the following better estimate

$$\begin{aligned} & R_2(K, A; z, \hbar) = \\ & \left(\frac{-\hbar}{3!2i}\right)^3 \int_0^1 \frac{(1-y)^N}{(\pi\hbar y)^{2n}} \int_{\mathbb{R}^8} \exp(-\frac{2i}{y\hbar}(ec + fd - ga - hb)) \times \\ & \times \partial_x^3 V(x+a, t+b)\partial_p^3 A \circ \Phi^{\tau}(x+e, t+f, p+g)\mathrm{d}a\mathrm{d}b\mathrm{d}c\mathrm{d}d\mathrm{d}e\mathrm{d}f\mathrm{d}g. \end{aligned}$$

End of the proof follows the proof of **Theorem** 4.1 . ∎

6 Examples

Example 1:
Firstly, we will deal with time independent harmonic oscilator. Hamiltonian is

$$H = \frac{1}{2}(p^2 + q^2)$$

Either by direct computations of the remainder (7), or by estimate (9), one can see that in this case semiclassical approximation of quantum evolution of an observable (11) is exact solution (even any observalbe $A \in \mathcal{O}(m)$ without restrictions (10)). If we observe expectation values $\langle \psi, \hat{A}\psi \rangle$ of such quantities as $\hat{q},\ \hat{p}$, which are linear, on wave packets

$$\Psi_{a,b,\ (\Delta a)^2}(x) := (2\pi(\Delta a)^2)^{-\frac{1}{4}} \exp(-\frac{(x-a)^2}{4(\Delta a)^2} + \frac{i}{\hbar} bx)$$

then thanks to relations

$$\langle \Psi_{a,b,\ (\Delta a)^2}, \hat{q}\ \Psi_{a,b,\ (\Delta a)^2} \rangle = a$$
$$\langle \Psi_{a,b,\ (\Delta a)^2}, \hat{p}\ \Psi_{a,b,\ (\Delta a)^2} \rangle = b$$

expactation values follow exactly the classical evolution of these quantities. On the other hand if we focus on hamiltonian, which is of course conserving, then because of dispersion of mimimalizing wave packets:

$$\begin{aligned} (\Delta_{\Psi_{a,b,\ (\Delta a)^2}}\ \hat{q})^2 &= (\Delta a)^2 \\ (\Delta_{\Psi_{a,b,\ (\Delta a)^2}}\ \hat{p})^2 &= \frac{\hbar^2}{4(\Delta a)^2} = (\Delta b)^2 \end{aligned}$$

we yield

$$\langle \Psi_{a,b,\ (\Delta a)^2}, \hat{H}\ \Psi_{a,b,\ (\Delta a)^2} \rangle = \frac{1}{2}(a^2+b^2) + (\Delta a)^2 + \frac{\hbar^2}{4(\Delta a)^2} = \frac{1}{2}(a^2+b^2) + (\Delta a)^2 + (\Delta b)^2$$

Additional terms are not quantum effects (although they contain terms propotional to $\hbar^2$), but they are the consequences of error during measuring.

Example 2:
Our next Hamiltonian will be

$$H := \frac{1}{2}p^2 - q\cos t$$

Hamilton equations in extended space (16) are

$$\frac{dq}{d\sigma} = p, \quad \frac{dp}{d\sigma} = \cos t$$
$$\frac{dt}{d\sigma} = 1, \quad \frac{dE}{d\sigma} = q \sin t$$

The solution with initial conditions (17) is desribed by relations:

$$\begin{aligned}
q(\sigma) &= q + (p - \sin t)\sigma - \cos(t+\sigma) + \cos t \\
p(\sigma) &= p + \sin(t+\sigma) - \sin t \\
t(\sigma) &= \sigma + t \\
E(\sigma) &= E + (\cos t + q)(\cos t - \cos(t+\sigma) + \frac{1}{4}(\cos 2(t+\sigma) - \cos 2t) + \\
&+ (p - \sin t)(\sin(t+\sigma) - \sigma\cos(t+\sigma) - \sin t)
\end{aligned}$$

We will not care about observables explicitly dependent on t, E. After Weyl quantization procedure (5) in extended space, we discover that the result would be the same (except the measuring of the time from point t, instead of 0), if we computeted it directly as time independent Hamiltonian.

Contents

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