Recent Results in Semiclassical Approximation with Rough Potentials

T. Paul

Quantum Mechanics was invented for stability reasons. In fact it is striking to notice the difference of regularity that needs the potential of a Schrödinger operator to insure unitary of the quantum flow (e.g. $V \in L^1_{\text{loc}}$, $\lim_{\epsilon\to 0} \sup_x \int_{|x-y|\leq\epsilon} |x-y|^{2-N}|V(y)|dy = 0$) compared to the classical Cauchy-Lipshitz condition for vector fields.

On the other side, tremendous progress have been done in the last 25 years concerning the theory of ODEs using PDE's methods: extension of the Cauchy-Lipshitz condition to Sobolev ones [5] and BV vector fields (Bouchut for the Hamiltonian case [4] and Ambrosio for the general case [1]) have been proved to provide well-posedness of the classical flow almost everywhere, through uniqness result for the corresponding Liouville equation in the space $L^\infty_+([0,T]; L^1(\mathbb{R}^{2n}) \cap L^\infty(\mathbb{R}^{2n}))$. Under these regularity conditions on the potential (in addition to some growing at infinity) the Schrödinger equation is well posed for all positive values of the Planck constant and it is therefore natural to ask what's happen at the classical limit. As we will see different answers will be given, according to the choice we make first on the topology of the convergence, and secondly on the asymptotic properties of the initial datum. The genral idea of the results we are going to present here can be summarized as follows:

For some $V \notin C^{1,1}$ both the quantum and the classical exist and

the diPerna-Lions-Ambrosio flow is the classical limit of the quantum flow

for non concentrating initial data.

For concentrating initial data

the multivalued bicharateristics are the classical limit of the quantum flow.

T. Paul (✉)
CNRS and CMLS, Ecole Polytechnique, Palaiseau cedex, France
e-mail: thierry.paul@math.polytechnique.fr

D. Grieser et al. (eds.), *Microlocal Methods in Mathematical Physics and Global Analysis*, Trends in Mathematics, DOI 10.1007/978-3-0348-0466-0_11,

All the results presented here will use a quantum formalsim on phase space, thanks to the notion of Wigner funtion. More precisely we will be concerned with the so-called Schrödinger and von Neumann equation

$$i\hbar\partial_t\psi = (-\hbar^2\Delta + V)\psi \text{ and } \partial_t D = \frac{1}{i\hbar}[-\hbar^2\Delta + V, D]$$

with $\psi^{t=0} \in L^2(\mathbb{R}^n)$ and $D^{t=0} \geq 0, TrD^{t=0} = 1$ (density matrix, e.g. $D^0 = |\psi^0\rangle\langle\psi^0|$). And we will consider the Wigner funtion associted to D^t (e.g. $= |\psi^t\rangle\langle\psi^t|$), defined by

$$W^\epsilon D(x,p) := \frac{1}{(2\pi)^n}\int_{\mathbb{R}^n} D^t(x + \frac{\epsilon}{2}y x - \frac{\epsilon}{2}y)e^{-ipy}dy$$

where $D^t(x,y)$ is the integral kernel of D^t (e.g. $= \overline{\psi^t(x)}\psi^t(y)$ in which case we write $W^\epsilon\psi^t_\epsilon$).

The well-known lack of positivity of W^ϵ suggests, in order to study evolution in spaces like L^∞_+, to use the so-called Husimi function of D^t, a molification of W^ϵ defined as $\widetilde{W^\epsilon D} := e^{\epsilon\Delta_{\mathbb{R}^{2n}}}W^\epsilon D$ which happens to be positive. But the only bound we have for $\widetilde{W^\epsilon D}$ is $\|\widetilde{W^\epsilon D}\|_{L^\infty} \leq \epsilon^{-n}\mathrm{Tr}D$, unuseful for the L^∞ condition needed for the existence of the classical solution. We formulate the

Conjecture. For an ϵ dependant family D_ϵ of density matrices we have

$$\mathrm{Tr}D_\epsilon = 1 \Longrightarrow \sup_{\epsilon>0}\|\widetilde{W^\epsilon D_\epsilon}\|_{L^\infty} = +\infty$$

In the general case of a potentials whose gradient is BV, the first idea will be to smeared out the initial conditions and consider a family of vectors $\psi^0_{\epsilon,w}$, w belonging to a probabilty space $(W, \mathcal{F}, \mathbb{P})$. Under the general assumptions

Assumptions on V	Assumptions on initial datum
globally bounded, locally Lipschitz	$\psi^\epsilon_{0,w} \in H^2(\mathbb{R}^n;\mathbb{C})$
$\nabla U_b \in BV_{loc}(\mathbb{R}^n;\mathbb{R}^n)$	$\sup_{\epsilon>0}\int_W\int_{\mathbb{R}^n}\lvert H_\epsilon\psi^0_{\epsilon,w}\rvert^2 dx\,d\mathbb{P}(w) < \infty$
$\mathrm{ess\,sup}_{x\in\mathbb{R}^n}\frac{\lvert\nabla U_b(x)\rvert}{1+\lvert x\rvert} < +\infty$	$\int_W \lvert\psi^0_{\epsilon,w} >< \psi^0_{\epsilon,w}\rvert\, d\mathbb{P}(w) \leq \epsilon^n\mathrm{Id}$
+ *finite repulsive Coulomb singularities*	$\lim_{\epsilon\downarrow 0}\widetilde{W^\epsilon\psi^0_{\epsilon,w}} = i(w) \in \mathcal{P}(\mathbb{R}^d)$ for $\mathbb{P} - a.e.\ w \in W$.

we have, any bounded distance $d_{\mathcal{P}}$ inducing the weak topology in $\mathcal{P}(\mathbb{R}^{2n})$, the

Theorem 1 ([2]).

$$\lim_{\epsilon\to 0}\int_W \sup_{t\in[-T,T]} d_{\mathcal{P}}\big(\widetilde{W^\epsilon\psi^t_{\epsilon,w}}), \boldsymbol{\mu}(t, i(w))\big)\, d\mathbb{P}(w) = 0,$$

where $\boldsymbol{\mu}(t,\nu)$ is a (regular Lagrangian) flow on $\mathcal{P}(\mathcal{P}(\mathbb{R}^{2n}))$ "solving" the Liouville equation.

In the case of the von Neumann equation, a more direct result can be obtained.

Assumptions on V	Assumptions on initial datum
globally bounded, locally Lipschitz	$sup_{\epsilon\in(0,1)}\mathrm{Tr}(H_\epsilon^2 D_\epsilon^o) < +\infty$
$\nabla U_b \in BV_{loc}(\mathbb{R}^n;\mathbb{R}^n)$	$D_\epsilon^o \leq \epsilon^n \mathrm{Id}$
$\text{ess sup}_{x\in\mathbb{R}^n} \frac{\vert\nabla U_b(x)\vert}{1+\vert x\vert} < +\infty$	$w-\lim_{\epsilon\to 0} W^\epsilon D_\epsilon^0 = W_0^0 \in \mathcal{P}\mathbb{R}^{2n}$

Theorem 2 ([6]). *Let $d_{\mathcal{P}}$ be any bounded distance inducing the weak topology in $\mathcal{P}(\mathbb{R}^{2n})$. Then*

$$\lim_{\epsilon\to 0}\sup_{[0,T]} d_{\mathcal{P}}(\widetilde{W^\epsilon D_\epsilon^t}, W_t^0) = 0,$$

W_t^0 is the unique solution in $L_+^\infty([0,T];L^1(\mathbb{R}^{2n})\cap L^\infty(\mathbb{R}^{2n}))$ of the Liouville equation.

The next result concern the semiclassical approximation in strong topology. Let us denote $\widetilde{V} := e^{\epsilon\Delta_{\mathbb{R}^n}}V$.

(new) Assumptions on V	(new) Assumptions on initial datum
$\int \vert\widehat{V}(S)\vert \frac{\vert S\vert^2}{1+\vert S\vert^2}\, dS < \infty$	$W_0^\epsilon \in H^2(\mathbb{R}^n)$
$\int_{\vert S\vert\in(a,b)} \vert\widehat{V}(S)\vert\,\vert S\vert^m dS \leq C\left(b^{m-1-\theta} - a^{m-1-\theta}\right)$	if $\partial_t\rho + k\partial_x\rho - \partial_x\widetilde{V}\cdot\partial_x\rho = 0,\ \rho_{t=0} := W_0^\epsilon$
$m = 0,1,2,\ 0<\theta<1$	$\exists T>0, \delta\in\left(0,\frac{\theta}{2+\theta}\right)$ such that $\vert\vert\rho(t)\vert\vert_{H^2} = O(\varepsilon^{-\delta}\vert\vert W_0^\varepsilon\vert\vert_{L^2})$ for $t\in[0,T]$

Theorem 3 ([3]). *Let ρ_1^ϵ be the solution of*

$$\partial_t\rho_1^\epsilon + k\partial_x\rho_1^\epsilon - \partial_x\widetilde{V}\cdot\partial_x\rho_1^\epsilon = 0.$$

$W_t^\epsilon := W^\epsilon D_\epsilon^t$ satisfies, uniformly on $[0,T]$,

$$||W_t^\epsilon - \rho_1^\varepsilon(t)||_{L^2} = O(\varepsilon^\kappa ||W_0^\varepsilon||_{L^2}),\ \kappa = min\{\ \frac{1+\theta}{2} - 1,\ \frac{\theta}{2+\theta} - \delta\ \}.$$

Let us now give a 1D example where the lack of unicity will be crucial.

Let V be a confining potentail such that $V = -|x|^{1+\theta}$ near 0. Near $(0,0)$ we obtain two solutions of the Hamiltonian flow:

$$(X^\pm(t), P^\pm(t)) = (\pm c_0 t^\nu, \pm c_0\nu t^{\nu-1}),$$

$\nu = \frac{2}{1-\theta}$ and $c_0 = \left(\frac{(1-\theta)^2}{2}\right)^{1-\theta}$, plus a continuum family of solutions by not moving up to any value of the time and then starting to move according to $(X^{\pm}(t), P^{\pm}(t))$.

The question now is to know which one is going to be selected the semiclassical limit. The answer is given by the following result.

Theorem 4 ([3]). *Let* $W^{\varepsilon} D_{\epsilon}^{0}(x,k) = \lambda^{\frac{7+3\theta}{30}} w(\lambda^{\frac{1+\theta}{6}} x, \lambda^{\frac{1-\theta}{15}} k)$, $\lambda = \log \frac{1}{\epsilon}$, *supp* $w \subseteq \{|x|^2 + |k|^2 < 1\}$.

Then $\exists T > 0 / t \in [0, T]$, $W^{\epsilon} D_{\epsilon}^{t}$ *converges in weak-$*$ sense to*

$$W_t^0 = c_+ \delta_{(X^+(t), P^+(t))} + c_- \delta_{(X^-(t), P^-(t))},$$

$$c_{\pm} = \int_{\pm x > 0} w(x,k) dx dk.$$

What these results show is the fact that, at the contrary of the case where the underlying classical dynamics is well-posed, the semiclassical limit of the qunatum evolution with non regular (i.e. not providing uniqness of the classical flow) potentials is not unique, and depends on the family itself of initial conditions, and not anymore only on their limit.

For non concentrating data the classical limit, in the general case of a potential whose gradient is BV, is driven (in the two senses expressed by Thoerems 1 and 2) by the DiPerna-Lions-Bouchut-Ambrosio flow.

Slowly concentrating data (Theorem 4) provide situations where the classical limit is ubiquous, and follows several of the non unique bi-charateritics, a typical quantum feature surviving in this situation the classical limit. It is important to remark that the speed of concentration governs the selections of the remaining trajectories. The case of fast concentration, in particular the pure states situations, is still open.

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