Singular classical transport and recent advances in semiclassical analysis

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December 13 2012

Classical particle in a potential force field:

$$\ddot{x}(t) = -\nabla V(x(t)),$$
$$x(0) = x_0, \dot{x}(0) = k_0$$

Statistical version
(non-interacting particles):

$$\partial_t \rho + k \cdot \partial_x \rho - \partial_x V \cdot \partial_k \rho = 0,$$
$$\rho(t = 0) = \rho_0$$

The two formulations are equivalent for $\rho(0) = \delta(x - x_0, k - k_0)$.

Basic framework:
$\rho_0 \in \mathcal{M}(\mathbb{R}^{2n}_{x,k})$, $V \in C^{1,1}$

Position/momentum distributions:
$\int \rho dk$, $\int \rho dk$
Observables are continuous functions,
$a(t) = \int A d\rho(t)$

Quantum particle in a potential force field

$$i\hbar \frac{\partial}{\partial t} u^\hbar(t) = \left(-\frac{\hbar^2}{2}\Delta + V(x)\right) u^\hbar(t),$$
$$u^\hbar(t = 0) = u_0^\hbar(x) \in L^2$$

(pure state), or more generally

$$i\hbar \frac{\partial}{\partial t} D^\hbar(t) = \left[-\frac{\hbar^2}{2}\Delta + V, D^\hbar(t)\right],$$
$$D^\hbar(t = 0) = D_0^\hbar \in \mathcal{S}_1$$

(mixed states). The two formulations are equivalent for $D = |u\rangle\langle u|$.

Basic framework: V in Kato's class

Position/momentum distributions:
$\sum |u_n^\hbar(x)|^2$, $\sum |\widehat{u}_n^\hbar(x)|^2$.
Observables are operators,
$a(t) = tr(A(D(t))$

Semiclassical analysis is the asymptotic study of $\hbar \to 0$.

$u^\hbar$ or $D^\hbar$ have no meaningful limit in $\hbar$; Building a formulation that presents one theory as a perturbation of the other is a way to do semiclassical analysis and also highlight the "correspondence".

To that end: if $K(x, y)$ is the integral kernel of the density matrix D, its Wigner transform is

$$W^\hbar(x,k) = \int e^{-2\pi iky} K(x + \frac{y\hbar}{2}, x - \frac{y\hbar}{2})dy = \hbar^{-n} \textit{Weyl symbol}(D).$$

For pure states this gives rise to the sesquilinear transform

$$W^\hbar[u](x,k) = \int e^{-2\pi iky} u(x + \frac{y\hbar}{2})\overline{u}(x - \frac{y\hbar}{2})dy$$

One constructs the equation for the WT

$$\frac{\partial}{\partial t} W^\hbar(x,k,t) + 2\pi k \frac{\partial}{\partial x} W^\hbar(x,k,t) + \underbrace{\frac{2}{\hbar} Re\left(i \int_S \hat{V}(S) e^{2\pi iSx} W^\hbar(x, k - \frac{\hbar S}{2}, t) dS \right)}_{T_V^\hbar W^\hbar} = 0.$$

The point is that the Wigner function converges (in an appropriate sense) to a classical state $W^\hbar \rightharpoonup \rho \in \mathcal{M}^+(\mathbb{R}^{2n})$, and moreover the formal $\hbar \to 0$ limit of the Wigner equation is the Liouville equation.

A fundamental result here is

Theorem 1, Lions & Paul, 1993

Let $V \in C^1$. Then (for "any meaningful" initial data) the solution of the problem

$$\partial_t W^\hbar + k \cdot \partial_x W^\hbar + T_V^\hbar W^\hbar = 0,$$
$$W^\hbar(0) = W_0^\hbar$$

converges (in weak-$*$ sense, and up to extraction of a subsequence) to $\rho^0(t) \in \mathcal{M}^+$,

$$\langle W^{\hbar_n}(t) - \rho^0(t), \phi \rangle \to 0 \quad \forall \phi \in \mathcal{A}, \ \ t \in \mathbb{R}$$

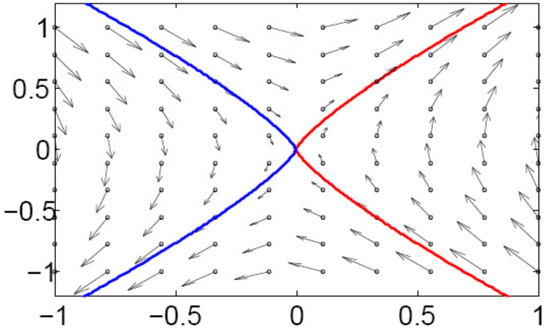
where

$$\partial_t \rho^0 + k \cdot \partial_x \rho^0 - \frac{1}{2\pi} \partial_x V(x) \cdot \partial_k \rho^0 = 0,$$
$$\rho^0(t=0) = w * -\lim_{\hbar \to 0} W_0^\hbar.$$

$$||f||_{\mathcal{A}} = \int_K \sup_x |\mathcal{F}_{k \to K} f(x,k)| dK$$

If $V \in C^{1,1}$, then Theorem 1 constitutes an explicit computation of the semiclassical limit. If $V \in C^1 \setminus C^{1,1}$, in general there is existence but not uniqueness for the Liouville equation with measure-valued initial data.
An example of what can go wrong: in this saddle point, the "stable" trajectories reach 0 in finite time, intersecting with the "unstable" ones.

$$n = 1, \qquad V(x) = -|x|^{1+\theta}, \ \ \theta \in (0,1)$$



More generally, the Schrödinger equation is well posed for very general potentials, while the respective/expected classical limit seems to require much more regularity.
Since the natural space for classical states is $\mathcal{M}^+(\mathbb{R}^{2n})$, anything below $V \in C^{1,1}$ will in general uniqueness issues, and below C^1 even existence in in question.

- What are some natural/physically relevant classes of potentials (in the context of semiclassical limits) not in $C^{1,1}$?
- Are there weak solutions for the respective classical equations? Is the semiclassical limit one of them?
- When they're not unique, can we construct selection principles?

Sufficient conditions for well-posedness of quantum dynamics:

Kato's conditions:
sufficient conditions for well-posedness of the quantum dynamics

Quantum dynamics are well posed for all meaningful initial data as soon as the potential satisfies

$$V(x) \in L^\infty + L^p, \quad \text{where} \;\; p > max\{\frac{n}{2}, 2\},$$

or

$$V(x) \in L^\infty + L^2_{loc}, \quad \exists A, B > 0 : |V(x)| \geqslant -A|x|^2 - B.$$

Physically relevant (in the semiclassical regime) potentials not in $C^{1,1}$:
Coulomb potentials, and
conical singularities, i.e. of the form $V(x) = a(x)|b(x)|$, a, b smooth.
They are contained in $\mathcal{B} = \{V|\partial_x^j V \in \mathcal{M} \text{ for } |j| = 2, \partial_x V \in L^1\}$.

Repulsive Coulomb potentials, $W^{1,\infty}$ effective potentials and eigenvalue crossings (see below) appear in the Born-Oppenheimer approximations for molecular dynamics.
The semiclassical parameter there is the ratio of electronic to nuclear mass, in the order of 10^{-2} to 10^{-4}, and therefore the question of the rate of convergence is relevant.
Vector-valued Schrödinger equations with real symmetric matrix valued potentials can in general be diagonalized

$$i\hbar u_t + \frac{\hbar^2}{2}\Delta u - Vu = 0, \;\; u \in L^2(\mathbb{R}^n, \mathbb{C}^d), \;\; V = \sum_{j=1}^{d} \lambda_j(x) J_j(x).$$

Even if all the functions involved are smooth, unless there is global separation of the eigenvalues, $\lambda_1(x) < \lambda_2(x) < \ldots < \lambda_d(x)\, \forall x$, conical-type singularities appear. E.g.

$$i\hbar u_t + \frac{\hbar^2}{2}\Delta u - \begin{bmatrix} x_1 & x_2 \\ x_2 & -x_1 \end{bmatrix} u = 0, \;\; u \in L^2(\mathbb{R}^2, \mathbb{C}^2),$$

decouples, *as long as the position density is essentially supported away from 0*, to

$$i\hbar u_t^{\pm} + \frac{\hbar^2}{2}\Delta u^{\pm} \mp |x| u^{\pm} = 0, \;\; u^{\pm} \in L^2(\mathbb{R}^2, \mathbb{C}).$$

So in particular conical singularities of the form $a(x)|b(x)|$ are **simplified** versions of eigenvalue crossings [Fermanian-Kammerer, Gérard & Lasser 2012]; they also appear when dealing with homogenization of lattices, e.g. [Mielke 2006].

Another reason that makes conical singularities (and more generally potentials of the class denoted earlier $\mathcal{B}$) natural comes from ODE theory. The problem of well-posedness for the Liouville equation is coupled with wellposedness for the respective ODE

$$\dot{x} = k, \ \ \dot{k} = -\nabla V(x(t)), \ \ x(0), k(0) \in \mathbb{R}^n.$$

Although $V \in C^{1,1}$ is in general needed for **all** trajectories to exist, there can be trade-offs when considering better initial data for the Liouville equation than $\mathcal{M}(\mathbb{R}^{2n})$; building on the Di Perna-Lions theory, more recently it was shown e.g. that

Well-posedness of the Liouville equation [Bouchut 2001; Ambrosio et al. 2010]

If $\nabla V(x) \in BV$,

$$\nabla V \in L^1, \quad \nabla^A V(x) \in \mathcal{M} \ \ \forall |A| = 2,$$

then the Liouville equation is well posed on $L^1 \cap L^\infty$.

In this context, one could say that the ODE for the trajectory of a single particle is well-posed for almost all initial states... It is natural to ask; in those cases, does this classical solution indeed capture the semiclassical limit?

A final motivation comes from a well-known nonlinear problem in semiclassical analysis: the Schrödinger-Poisson equation

$$i\hbar u_t + \frac{\hbar^2}{2}\Delta u - Vu = 0, \;\; \Delta V = b(x) - |u|^2, \;\; u \in L^2(\mathbb{R}^n)$$

gives rise to the so called Wigner-Poisson equation in phase-space, which is (formally) expected to converge to the Vlasov-Poisson equation

$$\rho_t + k \cdot \nabla_x \rho - \nabla V(x) \cdot \nabla_k \rho = 0, \Delta V = b - \int_k \rho(x,k,t)dk;$$

this is shown to be true for mixed state / small initial data, e.g. [Lions & Paul 1993]. However, in general, i.e. for $\rho(0) = w * -limW^{\hbar}(0) \in \mathcal{M}^+(\mathbb{R}^{2n})$ the Vlasov-Poisson equation isn't well posed.

The only result for pure states is the following is the following: for $n = 1$, the Vlasov-Poisson equation has (multiple) weak solutions [Majda, Majda & Zheng 1994], and the semiclassical limit for the Schrödinger-Poisson problem corresponds to one of them [Zhang, Zheng & Mauser 2002]

Observe that in $n = 1$ the Schrödinger-Poisson problem is

$$i\hbar u_t + \frac{\hbar^2}{2}\Delta u - (|x| * (b(x) - |u|^2))u = 0, \;\; u \in L^2(\mathbb{R}^n),$$

i.e. a conical singularity is a simplified version of this problem as well.

1st result: Ambrosio, Figalli, Friesecke, Giannoulis & Paul 2010

On a physical level, this work is mainly motivated from molecular dynamics and Born-Oppenheimer approximations. The effective electronic potential is, under certain assumptions, known to be in $W^{1,\infty}$, and there are the mutually repulsive Coulomb nucleus-nucleus interactions.

On a technical level, can one use the Bouchut-Ambrosio-Di Perna-Lions theory for the Liouville equation, and get (in some appropriate weak sense) a well-posed classical problem for those potentials?

As a first step, they show that the repulsive Coulomb singularities don't destroy the a.e. flow (which is plausible, and illustrates what the problem would be with an *attractive* strong singularity). However, as is well understood, it is impossible to speak about *each* trajectory in phase-space (equivalently, quantum states that tend to δ-functions in $\hbar$). Hence they consider a statistical population of pure states as initial data, and they construct semiclassical asymptotics for the population as a whole:

Corollary of [Ambrosio, Figalli, Friesecke, Giannoulis, Paul 2010]

Let $V(x)$ satisfy the Kato conditions, and

$$V(x) = \quad \text{repulsive Coulomb part} \quad + \quad \mathcal{B}$$

Assume the initial data is given by a coherent state $u^{\hbar}_{z,p}(x,k)$, centered on the point (z,p) in phase-space, which is distributed according to the probability density $f(x,k) \in L^1 \cap L^\infty$.

Denote $f(x,k,t)$ the propagation of $f(x,k)$ under the Liouville equation; then the probability distribution for $W^0(t)$ converges (as a measure on $\mathcal{M}^+(\mathbb{R}^{2n})$) to

$$\delta(x - z(t), k - p(t))$$

where $(z(t), k(t))$ are distributed according to $f(x,k,t)$.

Related, for appropriate *small* mixed states, $D^{\hbar} \leqslant C\hbar^n Id$: [Figalli, Ligabò & Paul 2011].

2nd result: Fermanian-Kammerer, Gérard & Lasser

The relevance of conical singularities in semiclassical limits is highlighted in this work, which treats the problem

$$i\hbar u_t + \frac{\hbar^2}{2}\Delta u - (a(x)|b(x)| + V_0(x))u = 0, \quad u \in L^2(\mathbb{R}^n), \quad a, b, V_0 \text{ smooth.} \quad (1)$$

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Obviously the bad set is where $\{g(x) = 0\}$.
However, the authors point out that for those points in phase-space that $\{g(x) = 0 \wedge \nabla g(x) \cdot k \neq 0\}$, there is a unique weak solution for a trajectory passing from / starting there (in general the trajectory may have a corner).
Therefore the "truly bad set" is $S = \{g(x) = 0 \wedge \nabla g(x) \cdot k = 0\}$.

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Therefore, for any point in phase-space $(x, k) \notin S$ there exists a time T so that the trajectory $\phi_t(x, k)$, $t \in [0, T]$ is well defined. Finally:

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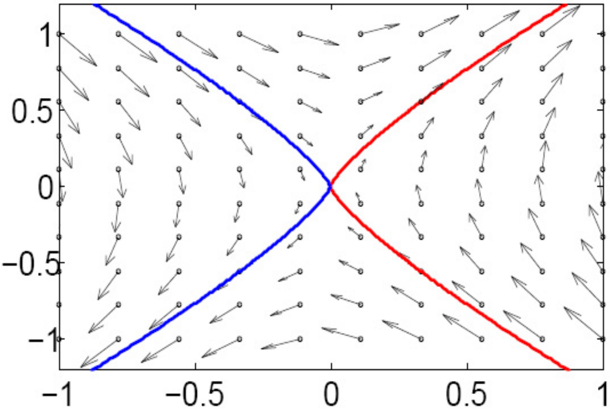
Theorem [Fermanian-Kammerer, Gérard & Lasser 2012]

If the initial data for eq. (1) has a unique Wigner measure W_0^0, and it is supported outside S, then there exists a time $T > 0$ so that all trajectories leaving $suppW_0^0$ do not enter S, and, for $t \in [0, T]$, $W^\hbar(u) \rightharpoonup W_0^0 \circ \phi_t$.

$$n = 1, \qquad V(x) = -|x|$$



The point here is that "generic" initial data do not reach S. In most cases that would be all initial data except a set of Lebesgue measure zero (always?). So the previous two results tell us that, loosely speaking, either with probability 1 or a.e., we can take semiclassical limits and compute trajectories in phase-space for $V \in \mathcal{B}$.

Still, those "atypical" cases, where e.g. trajectories intersect do exist, and they do present us with an ill-posed problem. In particular all the results mentioned so far cannot tell us anything about the semiclassical limit for a situation where the Wigner measure at $t = 0$ concentrates on the "stable branch" of the saddle point of $-|x|$ (previous slide). There is an essential loss of uniqueness there that needs to be better understood.

One should mention here that the Schrödinger-Poisson problem in $n = 1$ that was mentioned earlier corresponds exactly to this interaction, where you "carry" the bad region around with you, because of the convolution – and in particular it is not possible to avoid it "with probability 1" or anything like that.

Some case studies on problems where the Wigner measure concentrates on the "bad set"; following examples are from

- *"Strong and weak semiclassical limits for some rough Hamiltonians"*, with T. Paul, to appear in M^3AS, applies to $C^1 \setminus C^{1,1}$ potentials.
- *"On the selection of the classical limit for potentials with BV derivatives"*, with T. Paul, to appear in JDDE

An example [A. & Paul, 2011]

Let $n = 1$, $V(x) = -|x| \cdot \beta(x)$, where $C^\infty \ni \beta = 1$ on $[-1, +1]$, and $\beta(x) = 0$ for $|x| \geq 2$, and

$$W_0^\hbar(x,k) = \lambda^{\frac{5}{8}} w(\lambda^{\frac{1}{8}} x, \lambda^{\frac{1}{2}} k) * \left(\frac{2}{\hbar}\right)^n e^{-2\pi \frac{x^2+k^2}{\hbar}}$$

with $\lambda = log(\frac{1}{\hbar})$, $w \in H^2 \cap L^\infty \cap L^1$, $w(x,k) \geqslant 0$, $supp\, w \subseteq \{|x|^2 + |k|^2 < 1\}$, $\int w(x,k) dxdk = 1$.

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with $\lambda = log(\frac{1}{\hbar})$, $w \in H^2 \cap L^\infty \cap L^1$, $w(x,k) \geqslant 0$, $supp\, w \subseteq \{|x|^2 + |k|^2 < 1\}$, $\int w(x,k) dxdk = 1$.

Then $\exists T > 0$ such that for all $t \in [0, T]$, the Wigner function $W^\hbar(t)$ converges in weak-$*$ sense in $\mathcal{A}'$ to

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

with $(X^\pm(t), P^\pm(t)) = (\pm\frac{1}{2}t^2, \pm\frac{1}{2\pi}t)$, , and

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

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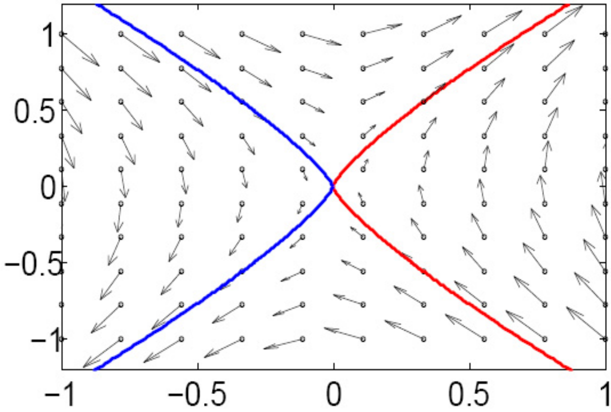

An example [A. & Paul, 2011]

Let $n = 2$, $V(x) = -|x_1| \cdot \beta(x_1)\beta(x_2)$, where $C^\infty \ni \beta = 1$ on $[-1, +1]$, and $\beta(x) = 0$ for $|x| \geq 2$, and

$$W_0^\hbar(x,k) = \lambda^3 w(\lambda^{\frac{1}{2}}(x + (0,1)), \lambda(k - (0, K_0)))$$

with $\lambda = log(\frac{1}{\hbar})^2$, $w \in H^2 \cap L^\infty \cap L^1$, $w(x,k) \geqslant 0$, $supp\, w \subseteq \{|x|^2 + |k|^2 < 1\}$, $\int w(x,k)dxdk = 1$.

Then for $t \in [0, T]$, the Wigner function $W^\hbar(t)$ converges in weak-$*$ sense to

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

with where $(X^\pm, K^\pm)$ is the limit as $\eta \to 0$ of

$$\begin{array}{ll} \dot{X}_\eta^\pm = 2\pi K_\eta^\pm, & \dot{K}_\eta^\pm = -\frac{1}{2\pi}\nabla V(X_\eta^\pm), \\ X_\eta^\pm(0) = (\pm\eta, -2), & K_\eta^\pm(0) = (0,1). \end{array}$$

and

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

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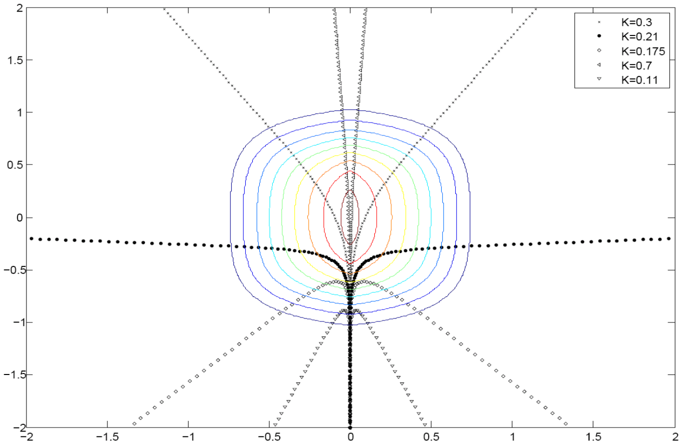

Ideas from the proof

Definition

$$||f||_{\mathcal{A}} = \int_K \sup_x |\mathcal{F}_{k\to K} f(x,k)| dK,$$

$$||f||_{\mathcal{A}'} = \sup_K \int_x |\mathcal{F}_{k\to K} f(x,k)| dx.$$

Lemma

$$||f||_{L^\infty} \leqslant ||f||_{\mathcal{A}}$$

$$||f||_{\mathcal{A}'} \leqslant ||f||_{\mathcal{M}} \leqslant ||f||_{L^1}$$

Lemma

For any trace class operator $D^\hbar$, with corresponding Wigner function $W^\hbar$,

$$||W^\hbar||_{\mathcal{A}'} \leqslant ||D^\hbar||_{tr} = tr(|D^\hbar|).$$

Moreover, if $D^\hbar \geqslant 0$, then

$$\int W^\hbar(x,k)dxdk = ||W^\hbar||_{\mathcal{A}'} = ||D^\hbar||_{tr} = tr(D^\hbar)$$

even if $W^\hbar \notin L^1$.

Therefore the conservation of trace for $W^\hbar(t)$ becomes a conservation of $\mathcal{A}'$ norm, *for density matrix initial data* only. There is no preservation of $\mathcal{A}'$ norm in general.

$$h(t) = U(t)(W_0^\hbar - \rho_2^\hbar(0)) + \int_{\tau=0}^{t} U(t-\tau)R^\hbar(\tau)d\tau$$

$$\mapsto \langle W_0^\hbar - \rho_2^\hbar(0), \phi\rangle + T\langle R^\hbar, \phi\rangle \leqslant ||W_0^\hbar - \rho_2^\hbar(0)||_{L^1}||\phi||_{\mathcal{A}} + o(1)$$

only if $W_0^\hbar - \rho_2^\hbar(0)$ is a density matrix.

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only if $W_0^\hbar - \rho_2^\hbar(0)$ is a density matrix.

Recall sufficient condition: $\exists \mu \in \mathcal{M}^+$ such that

$$W_0^\hbar - \rho_2^\hbar(0) = \left(\frac{2}{\hbar}\right)^n \int e^{-2\pi \frac{(x-x')^2+(k-k')^2}{\hbar}} d\mu(x', k').$$

For example if we had

$$W_0^\hbar - \rho_3^\hbar(0) = \Phi(W_0^\hbar \beta^\hbar(x)) \Leftrightarrow \rho_3^\hbar(0) = \Phi(W_0^\hbar(1-\beta^\hbar(x)))$$

things would work

$$h(t) = U(t)(W_0^\hbar - \rho_2^\hbar(0)) + \int_{\tau=0}^{t} U(t-\tau)R^\hbar(\tau)d\tau$$

$$\mapsto \langle W_0^\hbar - \rho_2^\hbar(0), \phi\rangle + T\langle R^\hbar, \phi\rangle \leqslant ||W_0^\hbar - \rho_2^\hbar(0)||_{L^1}||\phi||_{\mathcal{A}} + o(1)$$

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things would work; it suffices to observe

$$W_0^\hbar - \rho_2^\hbar(0) = \underbrace{W_0^\hbar - \rho_3^\hbar(0)}_{density\ \ matrix} + \underbrace{\rho_3^\hbar(0) - \rho_2^\hbar(0)}_{small\ \ in\ \ L^2}$$

Let $h(t) = W^\hbar(t) - \rho_2^\hbar(t)$,

$$\partial_t \rho_2^\hbar + 2\pi k \cdot \partial_x \rho_2^\hbar - \frac{1}{2\pi}\partial_x V(x) \cdot \partial_k \rho_2^\hbar = 0.$$

Then,

$$h(t) = U(t)(W_0^\hbar - \rho_2^\hbar(0)) +$$

$$+ \int_{\tau=0}^{t} U(t-\tau)\ \mathcal{F}^{-1}_{X,K}[\ \int \widehat{V}(S)(1 - \tfrac{sin(\hbar\pi S\cdot K)}{\hbar\pi S\cdot K})\pi S\cdot K\ \widehat{\rho}_2^\hbar(X-S,K,t)dS\ ]d\tau$$

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$$+ \int_{\tau=0}^{t} U(t-\tau)\ \mathcal{F}^{-1}_{X,K}[\ \int \widehat{V}(S)(1 - \tfrac{sin(\hbar\pi S\cdot K)}{\hbar\pi S\cdot K})\pi S\cdot K\ \widehat{\rho}_2^{\hbar}(X-S,K,t)dS\ ]d\tau$$

$$\mapsto ||\hbar R \int_{|S|<R} \widehat{V}(S)|S||K|^2|\widehat{\rho}_2^{\hbar}(X-S,K,t)|dS||_{L^2} +$$

$$+2||\ |K|\widehat{\rho}_2^{\hbar}(t)||_{L^2} \int_{|S|>R} |\widehat{V}(S)|\ |S|\ dS$$

$$h(t) = U(t)(W_0^{\hbar} - \rho_2^{\hbar}(0)) +$$

$$+ \int_{\tau=0}^{t} U(t-\tau)\ \mathcal{F}_K^{-1}[\ (\frac{V(x+\frac{\hbar K}{2})-V(x-\frac{\hbar K}{2})}{\hbar} - \partial_x V(x)\cdot K)\quad \mathcal{F}_k \rho_2^{\hbar}(x,K,t)\ ]d\tau$$

$$\mapsto \hbar || \sup_{\substack{|A|=2 \\ |K|<R}} |\partial_x^A V(x+\hbar K)|\ |K|^2 \mathcal{F}_k \rho_2^{\hbar}(t)||_{L^2} +$$

$$+ || \int_{s=-\frac{K}{2}}^{\frac{K}{2}} \int_{\tau=0}^{s} \sum_{i,j=1,\ldots,n} \partial_{x_i x_j} V(x+\tau) d\tau_i ds_j\ \chi_{[R,+\infty)}(|K|)\ \mathcal{F}_k \rho_2^{\hbar}(t)||_{L^2}$$

Conclusions - Open problems

- In a large class of problems (namely with potentials in $\mathcal{B}$ and "generic" initial data) where traditionally we said "we don't have semiclassical asymptotics", now the Wigner measure is known. Can we do more – coherent states; smooth observables, Ehrenfest times....?
- There seems to be no result for *pure states* concentrating on the "bad set"...
- Any result there could give insights to the 1-dimensional Schrödinger-Poisson semiclassical limit.