Mathematical Challenges in Quantum Mechanics

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On the optimal transport of semiclassical measures

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The main topics of this talk

- Schrödinger dynamics on the flat torus
- Wigner measures
- Optimal transport of measures

The Schrödinger dynamics

Let $\mathbb{T}^n := (\mathbb{R}/2\pi\mathbb{Z})^n$, $V \in C^\infty(\mathbb{T}^n)$ and

$$\widehat{H}_\hbar := -\frac{\hbar^2}{2}\Delta_x + V(x).$$

The dynamics is given by the one parameter group of unitary operators

$$U_\hbar(t) := e^{-i\widehat{H}_\hbar t/\hbar}$$

on $\varphi_\hbar \in L^2(\mathbb{T}^n)$. We look at

$$\psi_\hbar(t,x) = (U_\hbar(t)\varphi_\hbar)(x).$$

The object to study

Here we study the path of Borel probability measures

$$(\omega_t)_{0\leq t\leq 1} \in \mathcal{P}(\mathbb{T}^n \times \mathbb{R}^n)$$

given by semiclassical measures (Wigner measures) of $U_\hbar(t)\varphi_\hbar$, i.e.

$$\lim_{\hbar\to 0^+} \langle U_\hbar(t)\varphi_\hbar, \mathrm{Op}_\hbar^w(\phi) U_\hbar(t)\varphi_\hbar\rangle_{L^2} = \int_{\mathbb{T}^n\times\mathbb{R}^n} \phi(x,p)d\omega_t(x,p) \quad 0\leq t\leq 1,$$

for any test function $\phi(x,p)$ s.t. $\widehat{\phi} = F^{-1}(\phi)$ is compactly supported.
Remind The continuous path of semiclassical measures ω_t solves the Liouville equation in the measure sense,

$$\partial_t\,\omega_t + p\cdot\nabla_x\,\omega_t - \nabla_x V\cdot\nabla_p\,\omega_t = 0.$$

Equivalently, $\omega_t = (\phi_H^t)_\star\omega_0$ where ϕ_H^t is the Hamiltonian flow.

The class of symbols $b \in S^m_{\rho,\delta}(\mathbb{T}^n \times \mathbb{R}^n)$, $m \in \mathbb{R}$, $0 \leq \delta, \rho \leq 1$, consisting of those functions in $C^\infty(\mathbb{T}^n \times \mathbb{R}^n; \mathbb{R})$ which are 2π-periodic in x and for which for all $\alpha, \beta \in \mathbb{Z}^n_+$ there exists $C_{\alpha\beta} > 0$ such that $\forall (x, \eta) \in \mathbb{T}^n \times \mathbb{R}^n$

$$|\partial_x^\beta \partial_\eta^\alpha b(x,\eta)| \leq C_{\alpha\beta m} \langle \eta \rangle^{m-\rho|\alpha|+\delta|\beta|}$$

where $\langle \eta \rangle := (1 + |\eta|^2)^{1/2}$. In particular, the set $S^m_{1,0}(\mathbb{T}^n \times \mathbb{R}^n)$ is denoted by $S^m(\mathbb{T}^n \times \mathbb{R}^n)$. The toroidal Pseudodifferential Operator

$$b(X, D)\psi(x) := (2\pi)^{-n} \sum_{\kappa \in \mathbb{Z}^n} \int_{\mathbb{T}^n} e^{i\langle x-y,\kappa\rangle} b(x,\kappa)\psi(y)dy$$

(**M. Ruzhansky, V. Turunen, Quantization of pseudo-differential operators on the torus, J. Fourier Anal. Appl., 2010**).

The toroidal Weyl quantization

$$\mathrm{Op}^w_\hbar(b)\psi(x) := (2\pi)^{-n} \sum_{\kappa \in \mathbb{Z}^n} \int_{\mathbb{T}^n} e^{i\langle x-y,\kappa\rangle} b(y, \hbar\kappa/2)\psi(2y - x)dy$$

$$\mathrm{Op}^w_\hbar(b)\psi(x) = (\sigma(X, D) \circ T_x\, \psi)(x)$$

where $(T_x\psi)(y) := \psi(2y - x)$ and $\sigma \sim \sum_{\alpha \geq 0} \frac{1}{\alpha!} \triangle^\alpha_\eta D^{(\alpha)}_y b(y, \hbar\eta/2)\big|_{y=x}$.

The targets

• Select initial data $\varphi_\hbar \in L^2(\mathbb{T}^n)$ such that the projected measures on the torus by the canonical projection $\pi : \mathbb{T}^n \times \mathbb{R}^n \longrightarrow \mathbb{T}^n$

$$\sigma_t := \pi_\sharp(\omega_t), \qquad 0 \leq t \leq 1,$$

are optimal displacement interpolations of measures in the sense of the Optimal Transport theory.

• Conversely, for a given optimal displacement interpolation of measures σ_t look for $\varphi_\hbar \in L^2(\mathbb{T}^n)$ such that

$$\pi_\sharp(\omega_t) = \sigma_t, \qquad 0 \leq t \leq 1.$$

In other words, we study the link:

$$\text{Optimal path of measures} \Longleftrightarrow \text{path of semiclassical measures.}$$

A class of displacement interpolations of measures

Fix $\sigma_0, \sigma_1 \in \mathcal{P}(\mathbb{T}^n)$; we look at a continuous path $(\sigma_t)_{0\leq\tau\leq 1} \in \mathcal{P}(\mathbb{T}^n)$ which is a minimum curve for

$$\inf_{\gamma} \Big(\int_{\Omega} \int_0^1 \frac{m}{2} |\dot{\gamma}(\tau,\zeta)|^2 - V(\gamma(\tau,\zeta))\, d\tau \, \mathrm{d}\mathbb{P}(\zeta) \Big)$$

where the infimum is over all the random curves $\gamma : [0,1] \times \Omega \longrightarrow \mathbb{T}^n$ such that

$$\mathrm{Law}(\gamma(\tau,\cdot)) = \sigma_\tau.$$

More in general, here we fix $P \in \mathbb{R}^n$ and look at

$$\inf_{\gamma} \Big(\int_{\Omega} \int_0^1 \frac{m}{2} |\dot{\gamma}(\tau,\zeta)|^2 - V(\gamma(\tau,\zeta)) - P \cdot \dot{\gamma}(\tau,\zeta)\, d\tau \, \mathrm{d}\mathbb{P}(\zeta) \Big)$$

C. Villani: Optimal transport old and new, Springer (2008)

Transport maps

- Let $L(x,v) = \frac{1}{2}|v|^2 - V(x) - P \cdot v$ and

$$A^{0,t}(\gamma) := \int_0^t L(\gamma(\tau), \dot{\gamma}(\tau)) d\tau$$

the related Lagrangian Action. Define the cost function

$$c^{0,t}(x,y) := \inf_{\gamma} A^{0,t}(\gamma)$$

for cont. piecewise C^1 curves $\gamma : [0,t] \to \mathbb{T}^n$, $\gamma(0) = x$ and $\gamma(t) = y$.
- Fix $\sigma_0, \sigma_t \in \mathcal{P}_{ac}(\mathbb{T}^n)$ and look for the transport map T_t (Borel map) which is minimum for

$$\inf_{T_t} \int_{\mathbb{T}^n} c^{0,t}(x, T_t(x)) d\sigma_0(x)$$

when $\sigma_t = (T_t)_\star \sigma_0$.

P. Lee: Displacement Interpolation from a Hamiltonian point of view, J. Funct. Anal. (2013)

The initial data for the Schrödinger dynamics

For the phase of the wave functions, fix a Lipschitz continuous weak KAM solution of positive type for the stationary H-J equation (**A. Fathi: Weak KAM Theorem in Lagrangian Dynamics, Lecture Notes**) (**P. Bernard, B. Buffoni: Weak KAM Pairs and Monge-Kantorovich Duality, Adv. St. in Pure Math., 2007**)

$$\frac{1}{2}|P + \nabla_x S_+(x)|^2 + V(x) = \bar{H}(P), \quad P \in \mathbb{R}^n,$$

where

$$\bar{H}(P) = \sup_x \inf_{v \in C^1} \frac{1}{2}|P + \nabla_x v(x)|^2 + V(x)$$

is the so-called effective Hamiltonian (**L.C. Evans: some new PDE methods for weak KAM theory, Calc. Var. and PDE 2003**).
We assume that $\varphi_\hbar \in L^2(\mathbb{T}^n)$ is such that for some $\sigma_0 \in \mathcal{P}_{ac}(\mathbb{T}^n)$,

$$\lim_{\hbar \to 0^+} \langle \varphi_\hbar, \mathrm{Op}_\hbar^w(\phi)\varphi_\hbar \rangle_{L^2} = \int_{\mathbb{T}^n} \phi(x, P + \nabla_x S_+(x)) d\sigma_0(x).$$

In other words, we are assuming that there exists a semiclassical measure associated with $\varphi_\hbar$ taking the form

$$\omega_0(x,p) = \delta(p - P - \nabla_x S_+(x))\sigma_0(x), \quad \sigma_0 \in \mathcal{P}_{ac}(\mathbb{T}^n).$$

In the case $P \in \ell\mathbb{Z}^n$, $\ell > 0$, $\hbar^{-1} \in \ell^{-1}\mathbb{N}$ and a suitable subset of the above test functions, the typical example is given by WKB type wave functions

$$\varphi_\hbar(x) = a_\hbar(x)\, e^{i(P\cdot x + S_+(x))/\hbar}$$

where $a_\hbar \in H^1(\mathbb{T}^n;\mathbb{R})$ fulfills $\|a_\hbar\|_{L^2} = 1$, $\|\hbar\nabla a_\hbar\|_{L^2} \to 0$ as $\hbar \to 0$, $a^2(x)dx \rightharpoonup \sigma_0$ weakly as measures on $\mathbb{T}^n$ and $\mathrm{supp}(\sigma_0) \subseteq \mathrm{dom}(\nabla S_+)$.
In the case $P \notin \ell\mathbb{Z}^n$, another class of periodic wave function

$$\varphi_\hbar(x) = \int_{\mathbb{T}^n\times\mathbb{R}^n} \widetilde{\varphi}_{\hbar,y,\eta}(x)\, d\omega_0(y,\eta)$$

where $\widetilde{\varphi}_{\hbar,y,\eta}(x)$ are coherent states.

The reason of this choice

The nice property

$$\phi_H^t(\mathrm{Graph}(P + \nabla_x S_+)) \subseteq \mathrm{Graph}(P + \nabla_x S_+) \qquad \forall t \geq 0$$

has the following consequences

- $\omega_t := (\phi_H^t)_\star \omega_0(x,p) = \delta(p - \nabla_x S_+(x))\sigma_t(x)$.
- $\sigma \in C([0,1]; \mathcal{P}(\mathbb{T}^n))$ solves the continuity equation

$$\partial_t \sigma_t(x) + \mathrm{div}_x \Big(\frac{1}{m} (P + \nabla_x S_+(x)) \sigma_t(x) \Big) = 0$$

- For $\Psi^t(x) := \pi \circ \phi_H^t(x, P + \nabla_x S_+(x))$ the above path reads

$$\sigma_t = (\Psi^t)_\sharp(\sigma_0).$$

The first result

Theorem

Let $\varphi_\hbar \in L^2(\mathbb{T}^n)$ *as above,* $\omega_0 \in \mathcal{P}(\mathbb{T}^n \times \mathbb{R}^n)$ *be a linked semiclassical measure. Let* $\phi_H^t : \mathbb{T}^n \times \mathbb{R}^n \to \mathbb{T}^n \times \mathbb{R}^n$ *be the Hamiltonian flow of* $H = |p|^2/2m + V(x)$*. Then, the* $\omega_t := (\phi_H^t)_\sharp \omega_0$ *is a semiclassical measure associated to* $\psi_\hbar(t,\cdot)$ *and*

$$\omega_t(x,p) = \delta(p - P - \nabla_x S_+(x))\sigma_t(x)$$

and the path $(\sigma_t)_{0\le t\le 1} \in \mathcal{P}(\mathbb{T}^n)$ *equals for* $\mathcal{L}^1$ *- a.e.* $0 \le t \le 1$ *a continuous displacement interpolation between* σ_0 *and* σ_1*. By defining* $\Psi^t(x) := \pi \circ \phi_H^t(x, P + \nabla_x S_+(x))$*,*

$$\int_{\mathbb{T}^n} g(x)d\sigma_t(x) = \int_{\mathbb{T}^n} g(\Psi^t(x))d\sigma_0(x) \quad \forall g \in C^\infty(\mathbb{T}^n).$$

The complementary viewpoint

Theorem

Let $\sigma_0 \in \mathcal{P}_{ac}(\mathbb{T}^n)$ *and assume the uniqueness for solutions* $\sigma \in C([0,1]; \mathcal{P}(\mathbb{T}^n))$ *of*

$$\partial_t \sigma_t(x) + \operatorname{div}_x\Big(\frac{1}{m}(P + \nabla_x S_+(x))\sigma_t(x)\Big) = 0.$$

Define the lift $\omega_t := \delta(p - P - \nabla_x S_+)\sigma_t \in \mathcal{P}(\mathbb{T}^n \times \mathbb{R}^n)$. *Then, there exists* $\varphi_\hbar$ *such that* ω_0 *is the unique linked semiclassical measure. Any* ω_t *is a semiclassical measure linked to* $\psi_\hbar(t,x) := (U_\hbar(t)\varphi_\hbar)(x)$.

Remark 1: works for smooth S_+, for example in the one-dim case.
Remark 2: several open problems: can we recover all the optimal displacement interpolations? What are the related wave functions?

References

Download at my webpage http://www.math.unipd.it/∼lzanelli

L. Zanelli: Schrödinger dynamics and optimal transport of measures on the torus. Preprint.

L. Zanelli: On the optimal transport of semiclassical measures. Applied Mathematics and Optimization, online first october 2015.

Perspectives

Further studies of the link

$$\text{Optimal paths of measures} \iff \text{paths of semiclassical measures.}$$

This is part of a more general Project (2016-2018) involving

- Optimal transport theory
- Schrödinger operators
- Spectral theory
- Weak solutions of the H-J equation

Scientific collaborations:

- F. Cardin (Univ. Padova)
- A. Parmeggiani (Univ. Bologna)
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Thank you for the attention