Aspectos matemáticos del límite semiclásico de la mecánica cuántica en una variedad compacta

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Classical Mechanics

Let (M, g) be a complete Riemannian manifold.

The **position** $x(t)$ and **momentum** $\xi(t)$ of a **free Newtonian particle** in M, vary according to:

$$\begin{cases} \dot{x} = \partial_\xi H(x, \xi), \\ \dot{\xi} = -\partial_x H(x, \xi); \end{cases}$$

where H, defined on T^*M, is given in coordinates by:

$$H(x, \xi) := \frac{1}{2} \sum_{i,j=1}^{d} g^{ij}(x) \xi_i \xi_j + V(x);$$

with $\left(g^{ij}\right) := (g_{ij})^{-1}$.

When $V = 0$, this defines the **geodesic flow** ϕ_t of (M, g) on T^*M.

The Liouville formulation

The Hamiltonian system of O.D.E.'s may also be written as a P.D.E. for the density of particles $\mu_t(x, \xi)$ at time t:

$$\partial_t \mu_t + \frac{1}{2} \operatorname{div}(\mu_t X_H) = 0,$$

once an initial density $\mu_t|_{t=0} = \mu_0$ on T^*M is prescribed.

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The solution μ_t is then

$$\mu_t(x,\xi) = \delta_{x(t)}(x)\,\delta_{\xi(t)}(\xi),$$

where $(x(t), \xi(t))$ is the corresponding classical trajectory.

Classical Mechanics

A **quantum free particle** moves according to Schrödinger's equation:

$$i h \partial_t u(t,x) + \frac{h^2}{2} \Delta_x u(t,x) - V(x) u(t,x) = 0 \qquad \text{for } (t,x) \in \mathbb{R} \times M.$$

Now, Δ_x is the Laplace-Beltrami operator associated to g. In coordinates:

$$\Delta_x u(x) = \frac{1}{\rho(x)} \sum_{i,j=1}^{d} \partial_{x_i} \rho(x) g^{ij}(x) \partial_{x_j} u(x),$$

with $\rho(x) := (\det g(x))^{1/2}$.

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Interpretation

- $|u(t,x)|^2$ is the **position** probability density;
- "$|\widehat{u}(t,\xi)|^2$" is the **momentum** probability density.

Solutions to the Schrödinger equation

Suppose $\Delta - V$ has *discrete spectrum* (*e.g.*, if M is compact or $V(x) \underset{x\to\infty}{\longrightarrow} +\infty$).

Then there exists a sequence of eigenvalues $0 \leq \lambda_j \nearrow +\infty$ and an orthonormal basis in $L^2(M)$ consisting of eigenfunctions:

$$-\frac{h^2}{2}\Delta\psi_{\lambda_j}(x) + V(x)\psi_{\lambda_j} = \lambda_j\psi_{\lambda_j}, \qquad x \in M.$$

The solutions to the Schrödinger equation are of the form:

$$\boxed{u(t,x) = \sum_{\lambda_j} e^{-it\lambda_j}\widehat{u}(\lambda_j)\psi_{\lambda_j}(x).}$$

The Classical-Quantum correspondence I

Heuristically

As the characteristic oscillation frequencies $1/h^2$ of a solution $u(t,x)$ to the Schrödinger equation tend to infinity, the behavior of $|u(t,x)|^2$ is determined by classical mechanics.

The Classical-Quantum correspondence II

A little bit more precise

If (u_h) is an *h-oscillatory* sequence:

$$u_h(t,x) = \sum_{r/h^2 \le \lambda_j \le R/h^2} e^{-it\lambda_j} \widehat{u_h}(\lambda_j)\,\psi_{\lambda_j}(x),$$

for some $0 < r < R$ (this means that (u_h) oscillates at frequencies $\sim 1/h^2$) then the limit of

$$|u_h(t,x)|^2, \qquad \text{as } h \to 0^+,$$

propagates according to a law related to the classical dynamics (if $V = 0$, this is the geodesic flow of (M,g)).

Realizations of the C-Q

Times $t \sim 1$ - **The Semiclassical Limit**

$$|u_h(t,x)|^2 \text{ propagates following classical mechanics.}$$

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Uniform in time - Eigenfunction concentration

If $u_h(0,\cdot) = \psi_\lambda$ is an eigenfunction, then the solution of the evolution problem satisfies

$$|e^{it\lambda}\psi_\lambda|^2 = |\psi_\lambda|^2 .$$

The limit $\lambda = 1/h^2 \to \infty$ depends on fine dynamical properties of the geodesic flow.

Realizations of the C-Q

Times $t \sim 1/h$ - *Long-time* semiclassical limit

This is the intermediate regime we shall be interested in.
It requires an analysis of the full propagator for long times:

$$|u_h(t/h, x)|^2.$$

One expects that the dispersive effects associated to the Schrödinger equation become effective.

Classical approach

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The W.K.B. method constructs an **approximate solution** with this initial data.

The Ansatz

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then

$$ih\partial_t v_h + \frac{h^2}{2} \Delta v_h = \frac{h^2}{2} \Delta \rho e^{iS(t,x)/h}.$$

Therefore, the difference between the exact and approximate solutions satisfies:

$$\lim_{h \to 0^+} \sup_{t \in [-T,T]} \| u_h(t, \cdot) - v_h(t, \cdot) \|_{L^2(M)} = 0.$$

Times of order one?

As a conclusion

$$\lim_{h\to 0^+} \left| e^{iht\Delta/2} u_h^0 \right|^2 dm = \lim_{h\to 0^+} \left| v_h(t,\cdot) \right|^2 dm = \left| \rho(t,x) \right|^2 dm.$$

By solving the transport equation, one sees that $\rho(t,x)$ is transported along classical trajectories corresponding to $(x, dS_0(x))$.

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Times of order one?

This leads formally to considering $v_h(t/h, x)$. And therefore:

$$S(t/h, x), \qquad \text{for } h \text{ small.}$$

Or, in other words, long time behavior for solutions to the Hamilton-Jacobi equation.

Wigner measures: motivation

We want to compare

$$|u_h|^2 \ \text{(a density in } M\text{)}$$

with

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via the Liouville equation, for densities in T^*M.

Therefore, we shall replace $|u_h(x)|^2$ by a phase-space density $W_{u_h}^h(x,\xi)$ called the **Wigner measure** of u_h.

Wigner measures: motivation (techincal)

It is not convenient to analyze directly $|u_h(t,x)|^2$.

Main reason

Even for times of order one, the limits of $|u_h(t,\cdot)|^2$ are not determined by those of $|u_h(0,\cdot)|^2$.

An example in $\mathbb{R}^d$ with $V=0$:

$$u_h(0,\cdot)=\rho(x)\,e^{i\xi_0/h\cdot x}\Rightarrow |u_h(t,x)|^2=\left|e^{it\Delta_x/2}\rho(x-t\xi_0/h)\right|^2.$$

Therefore $|u_h(t,\cdot)|^2$ does not only depend on $|u_h(0,\cdot)|^2=|\rho(x)|^2$ **but also on ξ_0.**

This is because $|u_h(t,x)|^2$ does not detect the directions of oscillations of the sequence (u_h).

Wigner measures: general definition

We replace the measure $|u_h|^2$ on M:

$$\int_M \varphi(x) |u_h(t,x)|^2 \, dx = (\varphi u_h(t,\cdot) | u_h(t,\cdot))_{L^2(M)},$$

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by the measure $W^h_{u_h}$ on T^*M:

$$\int_{T^*M} a(x,\xi) W^h_{u_h}(t, dx, d\xi) := (\mathrm{op}_h(a) u_h(t,\cdot) | u_h(t,\cdot))_{L^2(M)}.$$

Where, for a continuous $a(x,\xi)$ defined on T^*M,

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This is called the **Wigner measure** of u_h.

Properties

1. It contains more information than $|u_h|^2$:

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3. Fundamental example, **coherent states**. If $u_h(0, x) = h^{-d/4} \rho\left(\frac{x - x_0}{\sqrt{h}}\right) e^{i\xi^0/h \cdot x}$ then

$$W_{u_h}^h(0, \cdot) \rightharpoonup \delta_{x_0}(x) \, \delta_{\xi^0}(\xi),$$

is concentrated on a point (x_0, ξ_0) in phase-space $T^* M$.

Egorov's theorem

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The Wigner measure $W_{u_h}^h$ solves:

$$\partial_t W_{u_h}^h + \frac{1}{2}\operatorname{div}\left(W_{u_h}^h X_H\right) = h\mathcal{L}_h W_{u_h}^h \qquad \text{on } \mathbb{R}_t \times T^*M,$$

where $\mathcal{L}_h W_{u_h}^h$ is locally uniformly bounded in t.

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The limiting Wigner measure solves the **Liouville equation**:

$$\partial_t \mu_t + \frac{1}{2}\operatorname{div}(\mu_t X_H) = 0.$$

Eigenfunction limits

Let (ψ_{λ_k}) be a sequence of normalized eigenfunctions of $-\Delta$ corresponding to eigenvalues $\lambda_k \to \infty$.

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Their limits μ are:

1. probability measures,
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3. supported on $S^*M := \{(x,\xi) \in T^*M : \|\xi\|_x = 1\}$.

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Some examples

- On the torus $\mathbb{T}^d$: the projection of $\mu(x, \xi)$ is absolutely continuous wrt Lebesgue measure (Bourgain). Complete characterization for $d = 2$ (Jakobson). Open for $d \geq 3$.

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- If (M, g) has negative curvature then the geodesic flow is Anosov. Most eigenfunctions tend to $dxd\xi$ (Schnirelman, Zelditch, Colin de Verdière, Rudnick-Sarnak...). Exceptional sequences may concentrate on sets of positive entropy (Anantharaman, Nonnenmacher).

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Theorem (D. Azagra and F.M., 2008)

The same holds if (M, g) is homogeneous and of constant sectional curvature $K > 0$.

Times of order $t \sim 1/h$

Theorem (F.M. 2006)

The following holds:

1. *The rescaled Wigner measures* $W_{u_h}^h(t/h,\cdot)$ *converge in average to a measure* $\mu \in L^\infty(\mathbb{R}_t; \mathcal{M}_+(T^*M))$*:*

$$\int_{\mathbb{R}} \varphi(t)\, W_{u_h}^h(t/h,\cdot)\, dt \rightharpoonup \int_{\mathbb{R}} \varphi(t)\, \mu(t,\cdot)\, dt, \qquad \forall \varphi \in L^1(\mathbb{R}).$$

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2. *Every* $\mu(t, \cdot)$ *is invariant by the classical flow.*
3. *A weak form of Egorov's theorem holds. If* $a \in C^\infty_c(T^*M)$ *is invariant, then:*

$$\lim_{h\to 0^+} \int_{T^*M} a W^h_{u_h}(t/h, \cdot) = \lim_{h\to 0^+} \int_{T^*M} a W^h_{u_h}(0, \cdot)$$
$$= \int_{T^*M} a(x,\xi)\, d\mu_0(x,\xi).$$

Manifolds with periodic geodesic flow

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The following holds:

$$\int_{T^*M} a(x,\xi)\, \mu(t, dx, d\xi) = \int_{T^*M} \langle a \rangle (x,\xi)\, \mu_0(dx, d\xi)\,.$$

Here

$$\langle a \rangle (x,\xi) := \lim_{T\to\infty} \frac{1}{T} \int_0^T a(\phi_s(x,\xi))\, ds,$$

ϕ_s *being the geodesic flow in* T^*M.

As a consequence:

Corollary

If $W^h_{u_h}(0,\cdot) \rightharpoonup \delta_{x_0}\delta_{\xi_0}$ *then*

$$\mu(t,x,\xi) = \delta_\gamma(x,\xi)$$

where γ *is the geodesic issued from* (x_0,ξ_0).

Corollary

The set of Wigner measures associated to solutions to Schrödinger's equation in a Zoll manifold coincides with the set of invariant measures in T^*M.

Analysis in $\mathbb{T}^d$

Consider the set of **resonant** frequencies:

$$\Omega := \left\{ \xi \in \mathbb{R}^d \ : \ \xi \cdot k = 0 \text{ for some } k \in \mathbb{Z}^d \setminus \{0\} \right\}.$$

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We have,

Theorem (F.M. 2007. Non-resonant case)

If $\mu^0 \left(\mathbb{T}^d \times \Omega \right) = 0$ *then,*

$$\int_{T^*\mathbb{T}^d} a(x,\xi)\, \mu(t, dx, d\xi) = \int_{T^*\mathbb{T}^d} \langle a \rangle (x,\xi)\, \mu_0(dx, d\xi)$$

$$= \int_{T^*\mathbb{T}^d} \left(\frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} a(y,\xi)\, dy \right) \mu_0(dx, d\xi)$$

Resonant case

If $\mu_0\left(\mathbb{T}^d \times \Omega\right) > 0$ then $\mu\left(t, x, \xi\right)$ may be non-constant in time.

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Example

Let $\xi^0 \in \Omega$. Take $\rho \in C_c^\infty\left(\mathbb{R}^d\right)$ and let $u_h\left(x\right)$ be the periodization of

$$\rho\left(x\right) e^{i\xi^0/h\cdot x}.$$

Then

$$\mu_0\left(x, \xi\right) = \left|\rho\left(x\right)\right|^2 dx \delta_{\xi^0}\left(\xi\right)$$

but

$$\mu\left(t, x, \xi\right) = \left\langle \left| e^{it\Delta_x/2}\rho\left(x\right)\right|^2 \right\rangle_{\xi^0} dx \delta_{\xi^0}\left(\xi\right).$$

Above,

$$\langle a \rangle_{\xi^0}\left(x\right) := \lim_{T\to\infty} \frac{1}{T}\int_0^T a\left(x + t\xi^0\right) dt$$

Resonant case

If $\mu_0\left(\mathbb{T}^d \times \Omega\right) > 0$ then $\mu\left(t, x, \xi\right)$ does not depend solely on μ_0.

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Example

Let $\xi^0 \in \Omega$ and $\eta^0 \in \mathbb{R}^d \setminus \Omega$. Suppose now that $u_h\left(x\right)$ is the periodization of

$$\rho\left(x\right) e^{i\left(\xi^0+\varepsilon\eta^0\right)/h\cdot x}$$

where $h \ll \varepsilon$. Then

$$\mu\left(t, x, \xi\right) = \left(\frac{1}{(2\pi)^d}\int_{\mathbb{T}^d}\left|\rho\left(y\right)\right|^2 dy\right) dx\delta_{\xi^0}\left(\xi\right).$$

Therefore, *two* **distinct** *sequences with the same* μ_0 *can give rise to* **different** *measures* μ.

General result

Let $\mathcal{P}$ be the set of periodic geodesics of $\mathbb{T}^d$ that pass through the origin.

Theorem (F.M. 2008)

The following formula holds:

$$\mu(t,x,\xi) = \sum_{\gamma\in\mathcal{P}} \mu_\gamma(t,x,\xi) + \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d} \mu_0(dx,\xi),$$

where

$$\mu_\gamma(t,x,\xi) = \left[e^{it\Delta_x/2} m_\gamma(x,y,\xi)\, e^{-it\Delta_y/2}\right]|_{x=y},$$

and m_γ are measures on $\mathbb{R}^d_\xi$ taking values in the space of symmetric, trace-class operators on $L^2(\gamma)$ that only depend on the initial data $(u_h(0,\cdot))$.

Structure

- Since m_γ is trace-class, the projection of $\mu_\gamma(t,x,\xi)$ on x is in $L^1(\mathbb{T}^d)$.

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Structure

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- The term
$$\sum_{\gamma \in \mathcal{P}} \mu_\gamma(t, x, \xi)$$
is concentrated on the set Ω of resonant frequencies.
- The measures $\mu_\gamma(0, x, \xi)$ are two-micolocal objects that characterize the concentration of energy of the initial data on the hyperplane orthogonal to γ.