Some mathematical manifestations of the quantum-classical relationship

Alejandro Uribe
University of Michigan

22 October 2005

Plan of this talk:
1. Physical origins and “early” results.
2. What is the big picture?
3. Ex. involving large matrices:
   (a) The pseudospectrum.
   (b) Asymptotics of orthogonal polynomials.
4. Ex. related to symplectic geometry.
1.- Physical Origins:
Classical Mechanics

The motion of a particle of mass $m$ under the influence of the force $F$ is:

$$\vec{F}(\vec{q}(t)) = m \frac{d^2 \vec{q}}{dt^2}$$

As a first-order system, with $\vec{F} = -\nabla V$:

$$\frac{d\vec{q}}{dt} = \frac{1}{m}\vec{p}, \quad \frac{d\vec{p}}{dt} = -\nabla V(\vec{q}(t)).$$

---

Hamiltonian formulation:

Phase space: $X = \{ (\vec{q}, \vec{p}) \}$. The total energy function, or Hamiltonian:

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

the equations of motion are:

$$\dot{\vec{q}} = \frac{\partial H}{\partial \vec{p}}, \quad \dot{\vec{p}} = -\frac{\partial H}{\partial \vec{q}},$$

Key object:

$$\omega = \sum_{j=1}^{n} dp_j \wedge dq_j$$
**Symplectic manifolds:** $(X, \omega)$

$\omega$ a non-degenerate two form, $d\omega = 0$.

Given $H : X \to \mathbb{R}$, get vector field $\xi_H$ on $X$ by:

$$\omega(\xi, \cdot) = dH(\cdot).$$

$\phi_t : X \to X, \quad \phi_t^* \omega = \omega, \quad H(\phi_t)$ constant in $t$.

Classical mechanics: differential geometry.

---

**Quantum mechanics:**

- States: Parametrized by wave functions:
  $$\psi \in \mathcal{H}, \quad \mathcal{H} \text{ a Hilbert space.}$$

- Observables: (energy, coordinates of position or momentum) are self-adjoint operators,
  $$F : \mathcal{H} \to \mathcal{H}.$$

- On average, the result of observing $F$ on $\psi$ is:
  $$\langle F\psi, \psi \rangle \quad \text{over} \quad \langle \psi, \psi \rangle.$$
Basic example:

\[ X = \mathbb{R}^{2n} \ni (q, p), \quad \mathcal{H} = L^2(\mathbb{R}^n), \]

Basic observables:
- \( q_j \mapsto Q_j = \) multiplication by \( q_j \)
- \( p_j \mapsto P_j = \frac{\hbar}{i} \frac{\partial}{\partial q_j} \)
- \( F(q, p) \): H. Weyl's quantization

Note: CCR:

\[ [P_j, Q_k] = \frac{\hbar}{i} \delta_{jk}. \]

Schrödinger’s equation

Quantum hamiltonian is an operator, \( \mathbf{H} \). Evolution:

\[ i\hbar \frac{d\psi}{dt} = \mathbf{H}(\psi). \]

Basic example:

\[ X = \mathbb{R}^{2n}, \quad H = \frac{1}{2m} ||p||^2 + V(q), \]

\[ \mathbf{H} = \frac{\hbar^2}{2m} \Delta + V \]

Fundamental solution (quantum propagator):

\( U_t : \mathcal{H} \to \mathcal{H}, \) unitary one-parameter group.
The semiclassical limit:

- Quantum mechanics is a “finer” theory than classical mechanics.
- Both are fantastically successful theories.
- If $\hbar = 0$ we would not have quantum effects.
- So, if we let $\hbar \to 0$, quantum $\to$ classical...

An old result (1980's):

The semi-classical trace formula

Let $(X, \omega)$ a symplectic manifold, quantized by $\mathcal{H}$.
Examples:

- $X = \mathbb{R}^{2n}$, $\mathcal{H}$ as above.
- $X = T^* M$, $M$ any configuration space,
  \[ \mathcal{H} = L^2(M). \]

Let $H : X \to \mathbb{R}$ a Hamiltonian, quantized by

\[ H : \mathcal{H} \to \mathcal{H}. \]
Theorem:
Suppose $H$ has discrete spectrum:
\[ E_1^{(h)} \leq E_2^{(h)} \leq \ldots \]
If $\phi$ is a band-limited test function then the asymptotics of
\[ \sum_j \phi[h^{-1}(E_j^{(h)} - E)] \]
is governed by the periodic trajectories of the Hamilton flow of $f$ on the energy surface
\[ X_E := f^{-1}(E). \]

Some details:
- Leading term:
  \[ h^{n-1} \hat{\phi}(0) \text{Vol}(X_E) = h^{n-1} \hat{\phi}(0) \int_{X_E} \nu, \]
  where $\nu \wedge df = \frac{\omega_n}{m!}$ (Liouville measure).
- A closed trajectory $\gamma$ contributes:
  \[ \hat{\phi}(T_\gamma) e^{h^{-1} i \int_{\gamma} p dq} \frac{T^\dagger}{2\pi} \frac{1}{\sqrt{I - P_\gamma}} \]
A few references:

1. M. Gutzwiller.
2. Chazarin, Colin de Verdière, Duistermaat-Guillemin.
4. Guillemin-U.
5. Brummelhuis, Paul, U.
7. Camus.

A recent result:

Joint work with V. Guillemin

- Consider a Schrödinger operator with discrete spectrum.
- Assume the potential has a unique minimum, highly non-degenerate and “symmetric”.
- Then the bottom of the spectrum (for $\hbar \in (0, \epsilon]$) determines the Taylor expansion of $V$ at the minimum.

We use a result of Iantchenko-Sjöstrand-Zwoński.
2.- Towards a "Theory" (b. late 70’s):

<table>
<thead>
<tr>
<th>Classical</th>
<th>Quantum</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X, \omega$</td>
<td>$\mathcal{H}, \langle, \rangle$</td>
</tr>
<tr>
<td>$F : X \to \mathbb{R}$</td>
<td>$F : \mathcal{H} \to \mathcal{H}$</td>
</tr>
<tr>
<td>Hamilton’s eqn.</td>
<td>Schrödinger’s eqn.</td>
</tr>
<tr>
<td>$\phi_t : X \to X$</td>
<td>$U(t) : \mathcal{H} \to \mathcal{H}$</td>
</tr>
<tr>
<td>${,}$</td>
<td>$\frac{i}{\hbar}[\cdot,\cdot]$</td>
</tr>
</tbody>
</table>

Quantization $\implies$ Semiclassical limit

-the table continues-

<table>
<thead>
<tr>
<th>Classical</th>
<th>Quantum</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Lambda \subset X$ B.S.Lagrangians</td>
<td>States $</td>
</tr>
<tr>
<td>Hamiltonian $G$ actions</td>
<td>Rep. $\rho_\hbar : G \to U(\mathcal{H}_\hbar)$</td>
</tr>
<tr>
<td>Symp$(\mathfrak{X})$</td>
<td>“$U$”$(\mathcal{H}_\hbar)$</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>Periodic orbits ?</td>
<td>Eigenfunctions ?</td>
</tr>
<tr>
<td>Chaos ??</td>
<td>?? (long story)</td>
</tr>
<tr>
<td>... ??</td>
<td>... ??</td>
</tr>
</tbody>
</table>
Some references:

- B. Kostant, A. Kirillov.
- J.M. Souriau.
- V.I. Maslov.
- A. Weinstein
- Guillemin and Sternberg.

Today's point:

- Quantization and its inverse appear in many branches of mathematics, in ways that are surprising (at first anyway).
- I want to discuss some new(er) examples/theorems of this phenomenon.
3.- Large matrices

- The first results have to do with certain (highly structured) sequences of large matrices.
- These sequences correspond to quantum observables on Hilbert spaces quantizing compact symplectic manifolds.
- The size of the matrices is correlated with $\frac{1}{\hbar}$.

(a) The Pseudospectrum:

**Definition 1:** Let $A$ be a matrix, $\lambda \in \mathbb{C}$ and $\epsilon > 0$. Then

$$\lambda \in \Sigma_\epsilon(A) \iff \| (A - \lambda I)^{-1} \| > \frac{1}{\epsilon}. $$

$$\iff \exists v \neq 0, \frac{\|(A - \lambda I)v\|}{\|v\|} < \epsilon. $$

**Definition 2:** Let $A = \{A_N\}$ be a sequence of matrices of growing dimension and let $\lambda \in \mathbb{C}$. Then

$$\lambda \in \Sigma(A) \iff \forall p > 1 \quad \| (A_N - \lambda I)^{-1} \| > C_p N^p. $$
A surprising phenomenon:

If $A$ is Hermitian, then $\Sigma(A)$ is the limit the spectrum of $A_N$. NOT SO if $A$ is not Hermitian!

Example: Let: $\sigma_j \in \text{su}(2), j = 1, 2, 3$ the Pauli matrices, and

$$A_N = -i\sigma_3 + i\epsilon(\sigma_1\sigma_3 + \sigma_3\sigma_1)$$

in the $N$-dimensional unirrep of SU(2)...
What is the Theorem?

- Let $(X, \omega)$ a Kähler manifold.
- Assume there exists $L \to X$ a Hermitian holomorphic line bundle with curvature $i\omega$.
- Let $\mathcal{H}_N := H^0(X, L^N)$ with its natural inner product, $\Pi_N : L^2(X, L^N) \to \mathcal{H}_N$ the projector.
- Given $f : X \to \mathbb{C}$, let $A^f_N : \mathcal{H}_N \to \mathcal{H}_N$,
  \[ A^f_N = \Pi_N(-i\nabla_\xi f + f)\Pi_N. \]

Theorem:

Assume $X$ compact, and $f$ is smooth. Then the pseudospectrum of the sequence $A^f = \{A^f_N\}$ contains the image under $f$ of the set

\[ X_0 = \{ x \in X : df(x) \neq 0 \text{ and } \{\Re f, \Im f\}(x) < 0 \}. \]

In the movie example, $X = \mathbb{C}\mathbb{P}^1$ and $f(X_0)$ is the interior of a lemniscate.
Why?

- Rough model for $A_N - \lambda I$ near a point $x$, $f(x) = \lambda$ and $df_x \neq 0$, is either $\frac{d}{dz}$ or $z$.
- $X_0$ corresponds to the model: $\frac{d}{dz}$, which has a kernel.
- $\lambda$ is in the pseudospectrum iff
  $$\text{Inf Spec}(A_N^* - \overline{\lambda}I) (A_N - \lambda I) = O(N^{-\infty}).$$
- Can construct approximate kernel of $(A_N^* - \overline{\lambda}I) (A_N - \lambda I)$ (which is s. a.) to all orders.

References

- Trefethen and Chapman.
- Sjostrand-Zworski, pseudodifferential case.
- Borthwick-U.
(b) Asymptotics of discrete orthogonal polynomials:

Given: A Jacobi matrix,

\[
A_N = \begin{pmatrix}
  a_1 & b_1 & 0 & \cdots & 0 \\
  b_1 & a_2 & b_2 & \cdots & 0 \\
  0 & b_2 & a_3 & b_3 & \cdots & 0 \\
  \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
  0 & \cdots & b_{N-1} & a_N \\
\end{pmatrix},
\]

\[b_j > 0.\]

Lemma:

For every \(z \in \mathbb{C}\) there exists a unique vector \(\psi(z) \in \mathbb{C}^N\) such that:

\[S_+ (A - zI) \psi = 0.\]

and of the form

\[\psi(z) = (1, p_1(z), \ldots, p_{N-1}(z))^T.\]

\(\forall j = 0, \ldots, N - 1, \ p_j(z)\) is a polynomial in \(z\) of degree \(j\):

\[p_j(z) = \frac{1}{\prod_{k=1}^{j} b_{k-1}} z^j + \cdots\]
Orthogonality:

Let \( \lambda_1, \ldots, \lambda_N, \psi_1, \ldots, \psi_N \) the eigenvalues/vectors of \( A \) (normalized), and

\[ w_j = |\langle e_1, \psi_j \rangle|^2 \]

Define

\[ d\mu(z) = \sum_{j=1}^{N} w_j \delta(z - \lambda_j). \]

Then the polynomials \( p_j \) are orthogonal with respect to \( d\mu \).

---

A semi-classical picture:

Think \( N = 1/\hbar \). Is there a semi-classical setting associated with this structure?

\( S_+ \) suggests: \( X = \mathbb{C}P^1 \). Action-angle coordinates \((I, \theta)\) on \( X \),

\[ 0 \leq I \leq 1, \quad 0 \leq \theta < 2\pi, \quad \omega = d\theta \wedge dI \]:

---
Assumptions:

Assume that, in $A_N$, 

$$a_j = a(j/N), \quad b_j = b(j/N), \quad a, b \in C^\infty(0,1)$$

and such that:

$$f(I, \theta) = a(I) + \cos(\theta) b(I) \in C^\infty(\mathbb{CP}^1).$$

Then we have a conclusion...
Asymptotics of the zeroes:

Theorem: Fix $\ell \in (0, 1)$, and let

$$X_\ell = \{ I \leq \ell \}.$$ 

Then the weak$^*$ limit of the zeroes of the polynomials $p_j(z)$, as

$$N \to \infty, \quad j \to \infty \quad \text{with} \quad \frac{j}{N} \approx \ell$$

is the push-forward

$$f_\ast\left(\omega|_{X_\ell}\right).$$

Why?

- The quantization of $\mathbb{CP}^1$ with $\hbar = 1/N$ is the space of homogeneous polynomials of degree $N$ in two variables. $SU(2)$ representation space.

- The quantization of $I$ is $J_z + \frac{1}{2}$ its eigenvectors:

$$e_j = C_{j,N} z_1^j z_2^{N-j}.$$ 

- In this basis, $A_N^f \cong A_N$. 

- $p_j(z)$ is the characteristic polynomial of the j-th principal minor, $M_N^j$, of $A_N$; therefore the zeroes of $p_j$ are the eigenvalues of $M_N^j$.
- So if $P_N^j$ is the projector onto the span of the first $j$ eigenvectors, we are asking about the spectral measure of $P_N^j A_N P_N^j$.
- Semiclassically, the range of $P_N^j$ corresponds to: $X_\ell = \{ I \leq \ell \}$.

**References:**
- Kuijlaars- Van Assche.
- Koornwinder (connection with Lie groups)
- Bloch-Golse-Paul-U (Toda lattice)
3.- Ex. from Symplectic Geometry:
- D. Auroux
- ...

**Almost-Kähler Quantization**
- $X, \omega$ an integral symplectic manifold.
- $L \to X$ a Hermitian line bundle with connection $\nabla$, such that $\text{curv}(\nabla) = i\omega$

Choose $J$ a compatible almost complex structure on $X$:
\[ \omega(J(u), J(v)) = \omega(u, v) \quad \text{and} \]
\[ g(Ju, v) := \omega(u, v) \]

is a Riemannian metric on $X$:
\[ (X, \omega, J) \text{ is an almost Kähler manifold.} \]
The Main Operator:

$$\Box = \nabla^{(N)} \nabla^{(N)} - nN$$

the shifted Laplace-Beltrami operator on $C^\infty(L^N)$.

If $J$ is integrable then

$$\Box = \bar{\partial}^* \partial,$$  

$$\partial : C^\infty(X, L^N) \rightarrow \Omega^{0,1}(X, L^N).$$

**Theorem** There exist $C > 0$, $C_1 > 0$ such that $\forall N > 1$ the spectrum of $\Box$ is contained in

$$(-C, C) \cup [NC_1, \infty).$$

---

The bounded eigenvalues

The eigenvalues of $\Box$ in $(-C, C)$:

$$\lambda_j^{(N)}, \ j = 1, \ldots, d_N$$  

(with multiplicities)

satisfy:

1. $d_N = \int_X e^{N\omega} \tau$, the Riemann-Roch polynomial of $X$.

2. **The Hilbert spaces**: $\mathcal{H}_N :=$ the span of the eigenfunctions of $\Box$ with eigenvalues in $(-C, C)$.

3. In the Kähler case $\mathcal{H}_N = H^0(X, L^N)$. 
Main structural result


The sequence of projectors \( \{ \Pi_N \} \) has the structure of a semi-classical Hermite FIO, with the same symbolic properties as in the integrable case:

$$
\Pi_N(x, y) = e^{-Nd(x, y)^2/2} \left( e^{iN\theta(x, y)} \left( \frac{N}{2\pi} \right)^n + O(N^{n-1}) \right).
$$

Further results:

**Theorem**: The assignment

$$
f \mapsto A_N^f := \Pi_N(-i\nabla^{(N)}_{\xi_f} + f) : \mathcal{H}_N \to \mathcal{H}_N
$$

has good properties:

- \( A_N^f \circ A_N^g = A_N^{fg} + O(1/N) \)
- \([A_N^f, A_N^g] = \frac{i}{N} A_N^{[f, g]} + O(1/N^2)\).
Remarks:
The $\mathcal{H}_N$ are naturally associated with $J$. So if we let
$$J = \{ \text{all compatible a.c. structures on } (X, \omega) \}$$
we get bundles $E_N \to J$ whose fibers are the $\mathcal{H}_N$.
$J$ is a Kähler manifold, and
$$\wedge^{\text{top}} E_N \to J$$
"pre-quantizes" $J$.

Applications?
Complexify $\text{Ham}(X)$?
Idea: Take $f : X \to \mathbb{C}$, quantize it to $A_N^f$ and solve the Schrödinger equation:
$$V_N(t) = \exp \left( -itNA_N^f \right).$$
Then, let $N \to \infty$ and recover from $V_N(t)$ a dynamical system on $X$...
If $f$ is real-valued this can be done: Recover the Hamilton flow of $f$. 
At the infinitesimal level:

Define the (coherent state) maps:

\[ \Psi_N : X \rightarrow \mathbb{P}(\mathcal{H}_N) \quad \text{by:} \]

\[ \Psi_N(x) = \{ \psi \in \mathcal{H}_N : \psi(x) = 0 \}^\perp. \]

**Theorem:** \( \Psi_N \) are asymptotically symplectic and isometric.

Note that \( V(t) \) induces a flow on \( \mathbb{P}(\mathcal{H}_N) \).

**Theorem:** Let \( \Xi \) be the component of the infinitesimal generator of \( V(t) \) that is tangential to the image of \( \Psi_N \). Then

\[ d\psi_N(\xi_R f + \nabla \Im f) = \Xi + O(1/\sqrt{n}). \]

and of \( V \).

**However:** \( f \mapsto \xi_R f + \nabla \Im f \) is *not* a Lie algebra morphism.
There is nonetheless a way of tracking the “classical path” of $V(t)$.

But the complexification of $\text{Ham}(\mathcal{X})$ does not exist as a Lie group (Donaldson).

Still, Q.M. provides insights and an “exponential map”.