Quantum dynamics of a particle constrained to lie on a surface

Gustavo de Oliveira[1]

SISSA – Trieste

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In this talk we will

- Recall the Schrödinger equation on $\mathbb{R}^3$.
- Present a Schrödinger-type equation on a surface of $\mathbb{R}^3$.
- Relate the solution to the latter to the solution to the former.

Outline

1. Introduction
2. Main result
3. Sketch of proof

Quantum mechanics for a particle in $\mathbb{R}^3$

Wave function

$$\psi(x,t) \in \mathbb{C}, \qquad x \in \mathbb{R}^3, \qquad t \in \mathbb{R}.$$

- Square-integrable:

$$\psi(\cdot\,,t) \in L^2(\mathbb{R}^3, dx).$$

- Normalized:

$$\int_{\mathbb{R}^3} |\psi(x,t)|^2 \, dx = 1.$$

Quantum dynamics of a particle in $\mathbb{R}^3$

Schrödinger equation

$$\begin{cases} i\partial_t \psi = H\psi \\ \psi|_{t=0} = \psi_0 \end{cases} \iff \psi(\cdot\,, t) = e^{-itH}\psi_0.$$

- Hamiltonian with $A(x) \in \mathbb{R}^3$ and $V(x) \in \mathbb{R}$:

$$\begin{aligned} H\psi &= \left[(i\nabla + A)^2 + V\right]\psi \\ &= i\,\mathrm{div}(i\,\mathrm{grad}(\psi) + A\psi) + \langle A, i\,\mathrm{grad}(\psi) + A\psi\rangle + V\psi. \end{aligned}$$

Calculus in a manifold S^k

- Coordinates:

$$x_1(p), \ldots, x_k(p) \quad \text{for} \quad p \in S^k.$$

- Metric:

$$[g_{ij}], \qquad [g^{ij}] = [g_{ij}]^{-1}, \qquad g = \det[g_{ij}].$$

- Gradient:

$$(\text{grad}\, f)^i = g^{ij} \frac{\partial}{\partial x_j} f.$$

- Divergent:

$$\text{div}\, Y = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x_j} (\sqrt{g}\, Y^j).$$

What if the particle is constrained to lie on Σ?

- Suppose
$$x \in \Sigma, \qquad \text{surface } \Sigma \subset \mathbb{R}^3.$$
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- Natural candidate:

$$\text{Replace} \qquad \mathbb{R}^3 \text{ and } \langle \cdot\,, \cdot \rangle \qquad \text{by} \qquad \Sigma \text{ and } \langle \cdot\,, \cdot \rangle|_\Sigma.$$

On Σ we have:

$$L^2(\Sigma, \mathrm{dvol}), \quad \mathrm{div}, \quad \mathrm{grad}, \quad A, \quad V, \quad H.$$

Equation:

$$\begin{cases} i\partial_t \psi = H\psi \\ \psi|_{t=0} = \psi_{0,\Sigma} \end{cases} \qquad \Longleftrightarrow \qquad \psi(\cdot\,, t) = e^{-itH}\psi_{0,\Sigma}.$$

Is this the right equation on Σ?

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- The solution of this equation on Σ must agree with Schrödinger on $\mathbb{R}^3$.
- How do we check?
- In $\mathbb{R}^3$, consider

$$H_\lambda = H + \lambda^4 W \quad \text{on} \quad L^2(\mathbb{R}^3)$$

with

$$\text{large } \lambda \in \mathbb{R}, \qquad W|_\Sigma = 0, \qquad W|_{\mathbb{R}^3 \setminus \Sigma} > 0.$$

The potential $\lambda^4 W$ traps the particle near Σ.

We want to compare solutions

- Is it true that

$$\underbrace{e^{-itH}\psi_{0,\Sigma}}_{\text{candidate}} \quad \simeq \quad \underbrace{e^{-itH_\lambda}\psi_{0,\lambda}}_{\text{Schrödinger}} \quad \text{as} \quad \lambda \to \infty,$$

where $\psi_{0,\lambda}$ is supported near Σ?

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$$H_\Sigma = H + K \quad \text{on } L^2(\Sigma),$$

  then yes.

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  then yes.

$$\begin{aligned} K = s - h^2 &\equiv \text{geometric potential}, \\ s &\equiv \text{Gaussian curvature}, \\ h &\equiv \text{mean curvature (not intrinsic)}. \end{aligned}$$

  s, h, K are functions of $\sigma \in \Sigma$.

Examples

- Sphere of radius r:

$$s = \frac{1}{r^2}, \qquad h = \frac{1}{r}, \qquad K = 0.$$

- Torus:

$$K \neq 0.$$

Motivation

- Effective evolution equations:

  One-particle system embedded in a larger system.
- Lab applications (physics literature).
- Comparison to classical dynamics.

Previous work (among others)

Physics

- da Costa, Phys. Rev. A, (1981). Others...
- Ferrari and Cuoghi, Phys. Rev. Lett. (2009).

Math-phys

- Froese and Herbst, Comm. Math. Phys. (2001).
- Dell'Antonio and Tenuta (2004) (semiclassics).
- Wachsmuth and Teufel (2009) (adiabatic).

Our contribution

- More general W.
- Magnetic potential A.
- H_Σ doesn't depend on $A_{\perp\Sigma}$.

Continuing... We will use

Normal bundle

$$N\Sigma = \{(\sigma, n) \mid \sigma \in \Sigma,\ n \in N_\sigma\Sigma\},$$
$$N\Sigma_\delta = \{(\sigma, n) \mid |n| < \delta\}.$$

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Change of variables

$$E : N\Sigma \to \mathbb{R}^3,$$
$$E(\sigma, n) = \sigma + n.$$

$$U_\delta \equiv \text{tubular neighborhood of } \Sigma \text{ in } \mathbb{R}^3,$$
$$E : N\Sigma_\delta \to U_\delta \quad \text{is a diffeomorphism.}$$

Rewriting the problem

We want to study

$$e^{-itH_\lambda}\psi_{0,\lambda} \quad \text{on} \quad L^2(\mathbb{R}^3) \quad \text{near } \Sigma \qquad \text{(Euclidean metric).}$$

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We do

Restrict to $L^2_0(U_\delta)$	Error $O(\lambda^{-1})$
Change variables to $L^2(N\Sigma_\delta)$	No error
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We end up with

$$e^{-itH_\lambda}\psi_{0,\lambda} \quad \text{on} \quad L^2(N\Sigma) \qquad \text{(metric } g_{N\Sigma}\text{).}$$

Decomposition of velocities

Tangent space of $N\Sigma$ at (σ, n)

$$T_{\sigma,n}N\Sigma.$$

Horizontal and vertical components of $T_{\sigma,n}N\Sigma$

$$T_{\sigma,n}N\Sigma \simeq (T_{\sigma,n}N\Sigma)_H \oplus (T_{\sigma,n}N\Sigma)_V,$$
$$(X, Y) = P_H(X, Y) + P_V(X, Y).$$

$$\langle (X_1, Y_1), (X_2, Y_2) \rangle_{N\Sigma_\delta} = \langle X_1 + Y_1, X_2 + Y_2 \rangle_{\mathbb{R}^3}.$$

Gauge transformation

Function γ on $N\Sigma$. Unitary transformation:

$$S_\gamma = e^{i\gamma} \quad \text{on} \quad L^2(N\Sigma),$$
$$S_\gamma^* H_\lambda S_\gamma,$$
$$A \rightsquigarrow A - \text{grad}(\gamma).$$

Proposition

$$P_H(A - \text{grad}(\gamma))|_\Sigma = P_H A,$$
$$P_V(A - \text{grad}(\gamma)) = 0.$$

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Proof:

$$\gamma(x,y) = \int_0^y A_3(x,s)\, ds$$

does the job in each chart. Check that works globally. □

Dilation in the normal directions

Unitary transformation:

$$U_\lambda : L^2(N\Sigma, \mathrm{dvol}_{N\Sigma}) \to L^2(N\Sigma, \mathrm{dvol})$$
$$(U_\lambda \psi)(\sigma, n) = \sqrt{\lambda}\, m(\sigma, n)\psi(\sigma, \lambda n)$$

Ignore $\mathrm{dvol}_{N\Sigma}$ and $m(\sigma, n) > 0$ for the moment.

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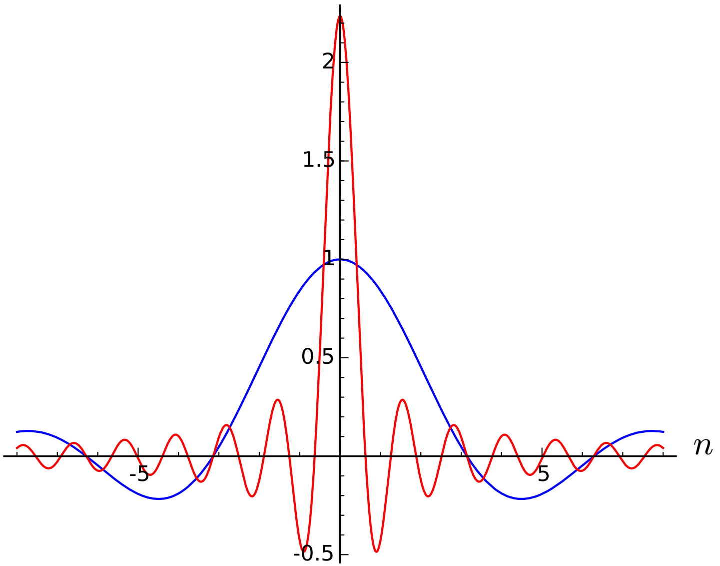
Initial data

$$e^{-itH_\lambda}\psi_{0,\lambda} \quad \text{on} \quad L^2(N\Sigma, \mathrm{dvol}), \qquad \psi_{0,\lambda} = S_\gamma U_\lambda \psi_0.$$

$\psi_{0,\lambda}$ is squeezed towards Σ.

Plot of $\psi(\sigma, \cdot\,)$ (blue) and $(U_\lambda \psi)(\sigma, \cdot\,)$ (red)



Putting all together

We arrive at

$$e^{-itL_\lambda}\psi_0 \quad \text{on} \quad L^2(N\Sigma, \mathrm{dvol}_{N\Sigma})$$

with

$$L_\lambda = U_\lambda^* S_\gamma^* H_\lambda S_\gamma U_\lambda.$$

Large λ expansion

Local coordinates

$$
\begin{aligned}
\Sigma : &\qquad x(\sigma) \\
N\Sigma : &\qquad \begin{cases} x(\sigma, n) = x(\sigma) \\ y(\sigma, n) = \langle \nu(\sigma), n \rangle \end{cases} \\
TN\Sigma : &\qquad \partial/\partial x,\ \partial/\partial y
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Expand the metric in $y\lambda^{-1}$

$$g_{N\Sigma_\delta}(x, y\lambda^{-1}) = \begin{pmatrix} G_\Sigma(x)(I - y\lambda^{-1}M(x))_{2\times 2} & 0 \\ 0 & 1 \end{pmatrix}_{3\times 3}$$

Hamiltonians

Hypothesis and notation

- A, V, W smooth functions of (σ, n).
- Set $\mathbb{A}(\sigma) = P_H A(\sigma, 0)$ and $\mathbb{V}(\sigma) = V(\sigma, 0)$.

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Expansion for L_λ

$$L_\lambda = H_\Sigma + \lambda^2 H_{O,\lambda} + O(\lambda^{-1}).$$

Hamiltonian on Σ:

$$H_\Sigma \psi = i\,\mathrm{div}_\Sigma(i\,\mathrm{grad}_\Sigma(\psi) + \mathbb{A}\psi) + \langle \mathbb{A}, i\,\mathrm{grad}_\Sigma(\psi) + \mathbb{A}\psi\rangle_\Sigma + (\mathbb{V} + K)\psi.$$

Oscillator in the normal directions:

$$H_{O,\lambda}\psi = -\Delta_n \psi + (\langle n, Bn\rangle_{\mathbb{R}^3} + \underbrace{O(\lambda^{-1})}_{\text{will not depend on } \sigma})\psi.$$

Main result

Theorem (J. Math. Phys. (2014))

- W has local minimum at Σ.
- $\partial_\sigma W(\sigma, n) = O(|n|^5)$ as $|n| \to 0$.
- $W(\sigma, n) \geq c|n|^2$.
- $g_{N\Sigma}$ complete metric.

Then for any ψ_0, $T > 0$, and large λ:

$$\sup_{t\in[0,T]} \left\| e^{-itL_\lambda}\psi_0 - e^{-it(H_\Sigma+\lambda^2 H_{O,\lambda})}\psi_0 \right\| \leq \frac{C}{\sqrt{\lambda}}.$$

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Remarks

- Neither orbits converge. Only their difference.
- Implies a statement on $\mathbb{R}^3$.

Interpretation

Since

$$L^2(N\Sigma, \mathrm{dvol}_{N\Sigma}) = L^2(\Sigma, \mathrm{dvol}) \otimes L^2(\mathbb{R}, dy),$$
$$[H_\Sigma, H_{O,\lambda}] = 0,$$

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we have

$$H_\Sigma = h_\Sigma \otimes I,$$
$$H_{O,\lambda} = I \otimes h_{O,\lambda},$$

and

$$\begin{aligned}\exp(-it(H_\Sigma + \lambda^2 H_{O,\lambda})) &= \exp(-itH_\Sigma)\exp(-it\lambda^2 H_{O,\lambda}) \\ &= \exp(-ith_\Sigma) \otimes \exp(-it\lambda^2 h_{O,\lambda}).\end{aligned}$$

Motion on Σ superposed by normal oscillations.

Sketch of proof

- Energy cutoff:

$$E_< \text{ equals 1 if } \langle \psi, L_\lambda \psi \rangle < \mu\lambda^2 \text{ and 0 otherwise.}$$

- $|n|$ cutoff:

$$N_< \text{ equals 1 if } |n| < \delta\lambda \text{ and 0 otherwise.}$$

- Partition of unity for Σ:

$$\{\chi_j\}.$$

- Resolution of identity:

$$\begin{aligned} 1 &= 1 \cdot 1 \cdot 1 \\ &= \Big[\sum_{j=1}^{m} \chi_j(\sigma)^2 \Big] \cdot [N_< + N_\geq] \cdot [E_< + E_\geq] \\ &= \chi_1 \cdot N_< \cdot E_< \; + \; \text{Reminder.} \end{aligned}$$

We want to estimate

Notation: $L_{0,\lambda} = H_\Sigma + \lambda^2 H_{O,\lambda}$.

$$\left\| e^{-itL_\lambda}\psi_0 - e^{-itL_{0,\lambda}}\psi_0 \right\|^2$$

$$\leq \Big| \int_0^t ds \frac{d}{ds} \langle e^{-isL_\lambda}\psi_0, 1 \cdot e^{-isL_{0,\lambda}}\psi_0 \rangle \Big|$$

$$\leq Ct \sup_s \left\langle \chi_1 E_< e^{-isL_\lambda}\psi_0, \underbrace{[L_{0,\lambda}, N_<]}_{\sim\{\partial_y N_<\}D_y} + N_< \big(\underbrace{L_\lambda - L_{0,\lambda}}_{\sim D_x^* D_x}\big) e^{-isL_{0,\lambda}}\psi_0 \right\rangle$$

$$+ O(\lambda^{-1})$$

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\begin{aligned}
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&\leq Ct \sup_s \langle \chi_1 E_< e^{-isL_\lambda}\psi_0, \underbrace{[L_{0,\lambda}, N_<]}_{\sim\{\partial_y N_<\} D_y} + N_< (\underbrace{L_\lambda - L_{0,\lambda}}_{\sim D_x^* D_x}) e^{-isL_{0,\lambda}}\psi_0 \rangle \\
&\quad + O(\lambda^{-1})
\end{aligned}
$$

Using Cauchy-Schwarz, we reduce the problem to

$$\lambda^2 \|(\chi_1 N_< E_<)\{\partial_y N_<\} D_y e^{-isL_{0,\lambda}}\psi_0\| \leq C\lambda^{-1} \quad \text{(Energy bounds).}$$

$$\|(\chi_1 N_< E_<)\underbrace{D_x e^{-isL_{0,\lambda}}}_{[D_x, W]}\psi_0\| \leq C\lambda^{-1/2} \qquad \text{(Propagation bounds).}$$

Appendix

Energy bounds

Schematically

We have

$$D_x^* D_x + V(x,y) + K(x,y) + \lambda^2 (D_y^* D_y + \lambda^2 W(x, y\lambda^{-1})) = L_\lambda \leq \lambda^2 \mu.$$

Use conservation of expected value of energy and positivity.
We obtain

$$(\lambda^{-1} D_x^*)^\alpha (\lambda^{-1} D_x)^\alpha + (D_y^*)^p D_y^p + (\lambda^2 W(x, y\lambda^{-1}))^l \leq C(\lambda^{-2} L_\lambda)^{l+1},$$

where $|\alpha| + p \leq 2$ and $l \geq 1$.

Propagation bounds

Let

$$f(t) \equiv \text{expected value of } D_x^* D_x \text{ on } e^{-itL_\lambda}\psi_0.$$

Use:

- Gronwall's inequality:

$$\frac{d}{dt} f(t) \leq Cf(t), \qquad f(0) \leq C \quad \Longrightarrow \quad \sup_t f(t) \leq C.$$

- Energy bounds.

Thank you for your attention.