An inverse problem for data-driven prediction in quantum mechanics

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Mathematical Challenges in Quantum Mechanics
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Outline

Forgetting the physics and predicting only with data

Data determine the evolution

The initial-to-final-state inverse problem

A scheme to solve this inverse problem

Restriction-extension of the Fourier transform and Strichartz inequalities

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- Wave functions describe the dynamics of quantum particles:

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- Such type of solutions are called **physical solutions**.

The playground for suitable $V(\mathrm{t}, \mathrm{x})$

- In the free-space $V = 0$ and with initial state f, the solution u

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\begin{aligned}
u(t,x) &= \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{ix\cdot\xi} e^{-it|\xi|^2} \widehat{f}(\xi)\,\mathrm{d}\xi \\
&= \frac{1}{(4\pi i t)^{n/2}} \int_{\mathbb{R}^n} e^{i\frac{|x-y|^2}{4t}} f(y)\,\mathrm{d}y
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- Strichartz estimates are derived from

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- Restriction-extension to the paraboloid $\tau = -|\xi|^2$

$$\phi(t,x) = \frac{1}{(2\pi)^{\frac{n+1}{2}}} \int_{\mathbb{R}\times\mathbb{R}^n} e^{i(t\tau + x\cdot\xi)} \widehat{\phi}(\tau,\xi)\,\mathrm{d}(\tau,\xi)$$

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- General phenomena: $e^{i(k\cdot\mathrm{x}-\omega\mathrm{t})}$ angular frequency $\omega = \omega(k)$ depends on the wave vector k.

The data-driven approximate prediction problem

- For $N \in \mathbb{N}$, we define the **initial-to-final-state set with N elements**

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so that

$$u_N(t, \cdot) \approx u(t, \cdot) \text{ as } N \to \infty?$$

with u solution with initial state f.

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- $\mathcal{D}_N$ consists of N points in the graph of $\mathcal{U}_T$.

Outline

Data determine the evolution map when

Theorem (C & Ruiz)

Assume $V_1(\mathrm{t},\mathrm{x})$ and $V_2(\mathrm{t},\mathrm{x})$ to have local critical singularities and super-exponential decay with $n \geq 2$. Then,

$$\mathcal{U}_T^1 = \mathcal{U}_T^2 \Rightarrow \mathcal{U}^1 = \mathcal{U}^2.$$

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Consider $V = V(\mathrm{t},\mathrm{x})$ so that for some compact $K \subset \mathbb{R}^n$:

- it has **local critical singularities**:

$$\mathbf{1}_K(\mathrm{x})V \in \begin{cases} L^a((0,T);L^b(\mathbb{R}^n)) & 2 - \dfrac{2}{a} = \dfrac{n}{b} \quad (a,b) \neq (\infty, n/2) \\ C([0,T];L^{n/2}(\mathbb{R}^n)) & n \geq 3 \end{cases}$$

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- it has **super-exponential decay**

$$\mathbf{1}_{\mathbb{R}^n \setminus K}(\mathrm{x}) e^{\rho|\mathrm{x}|} V \in L^\infty((0,T) \times \mathbb{R}^n) \quad \forall \rho > 0.$$

Some comments

- The need of $C([0,T];L^{n/2}(\mathbb{R}^n))$ for $n \geq 3$ instead of $L^\infty((0,T);L^{n/2}(\mathbb{R}^n))$ appears in the phenomenological resolution of the IVP.

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- The need of $C([0,T];L^{n/2}(\mathbb{R}^n))$ for $n \geq 3$ instead of $L^\infty((0,T);L^{n/2}(\mathbb{R}^n))$ appears in the phenomenological resolution of the IVP.
- What does it mean that $\mathcal{U}_T$ determines $\mathcal{U}$ with $H = -\Delta + V$?

$$\left.\begin{array}{l} i\dfrac{d}{d\mathrm{t}}\mathcal{U}^j_\mathrm{t} = H_j\mathcal{U}^j_\mathrm{t} \quad \text{in } \ (0,T), j \in \{1,2\} \\ \mathcal{U}^1_T = \mathcal{U}^2_T. \end{array}\right\} \ \Rightarrow \ \mathcal{U}^1_t = \mathcal{U}^2_t \ \ \forall t(0,T).$$

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The initial-to-final-state inverse problem

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- The resolution of inverse problem solves the data-driven prediction problem.

Uniqueness: unbounded potentials

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Uniqueness: stationary potentials

Theorem (Cañizares, C, Parissis & Zacharopoulos)

Assume $V_1(\mathrm{x})$ and $V_2(\mathrm{x})$ to be bounded and have super-linear decay with $n \geq 2$. Then,

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- Assume $V \in L^1(\mathbb{R}^n) \cap L^\infty(\mathbb{R}^n)$ to have a **super-linear decay**

$$\sum_{j \in \mathbb{N}_0} 2^j \|V\|_{L^\infty(D_j)} < \infty,$$

where

$$D_0 = \{x \in \mathbb{R}^n : |x| \leq 1\}, \;\; D_j = \{x \in \mathbb{R}^n : 2^{j-1} < |x| \leq 2^j\}, \forall j \in \mathbb{N}.$$

Related results

- In a joint collaboration with Cañizares, Parissis and Zacharopoulos we have improved this result showing that, for uniqueness, it is enough to have
$$V_1, V_2 \in L^1(\mathbb{R}^n) \cap L^p(\mathbb{R}^n)$$
with $p \geq n/2$ for $n \geq 3$ and $p > 1$ for $n = 2$.
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- Time-dependent Hamiltonian by Aïcha, Choulli, Eskin, Kian, Soccorsi, Tetlow...

Outline

The orthogonality relation

Proposition

We have

$$\mathcal{U}_T^1 = \mathcal{U}_T^2 \quad \Longrightarrow \quad \int_\Sigma (V_1 - V_2) u_1 \overline{v_2} = 0,$$

for all u_1 *and* v_2 *physical solutions of*

$$(i\partial_{\mathrm{t}} + \Delta - V_1)u_1 = (i\partial_{\mathrm{t}} + \Delta - \overline{V_2})v_2 = 0 \ \text{ in } \ \Sigma = (0, T) \times \mathbb{R}^n.$$

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- Density of the product $u_1\overline{v_2}$ would allow to conclude

$$V_1 = V_2.$$

Simplification of the problem

Assume to $F \in L^1(\mathbb{R}; L^1(\mathbb{R}^n)) \cap L^1(\mathbb{R}; L^\infty(\mathbb{R}^n))$ satisfy that

$$\int_{\mathbb{R}\times\mathbb{R}^n} Fu\overline{v} \; = 0$$

for all physical solutions $(i\partial_{\mathrm{t}} + \Delta)u = 0$ and $(i\partial_{\mathrm{t}} + \Delta)v = 0$.

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- The problem becomes

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- Hence $\widehat{F}(|\kappa|^2 - |\eta|^2, \eta - \kappa) = 0$ for all $\kappa, \eta \in \mathbb{R}^n$.

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  - Given $(\tau, \xi) \in \mathbb{R} \times \mathbb{R}^n$ so that $\xi \neq 0$, we choose

$$\kappa = -\frac{1}{2}\Big(1 + \frac{\tau}{|\xi|^2}\Big)\xi, \qquad \eta = \frac{1}{2}\Big(1 - \frac{\tau}{|\xi|^2}\Big)\xi;$$

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Simplification of the problem

- If $\widehat{F}(|\kappa|^2 - |\eta|^2, \eta - \kappa) = 0$ for all $\kappa, \eta \in \mathbb{R}^n$,
  - Given $(\tau, \xi) \in \mathbb{R} \times \mathbb{R}^n$ so that $\xi \neq 0$, we choose

$$\kappa = -\frac{1}{2}\Big(1 + \frac{\tau}{|\xi|^2}\Big)\xi, \qquad \eta = \frac{1}{2}\Big(1 - \frac{\tau}{|\xi|^2}\Big)\xi;$$

  - since $\eta - \kappa = \xi$ and $|\kappa|^2 - |\eta|^2 = \tau$, we obtain $\widehat{F}(\tau, \xi) = 0$.
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- Since the $\widehat{F}$ is continuous in $\mathbb{R} \times \mathbb{R}^n$ we can conclude that $\widehat{F}(\tau, \xi) = 0$ for all $(\tau, \xi) \in \mathbb{R} \times \mathbb{R}^n$.
- By the injectivity of the Fourier transform, we have that $F(t, x) = 0$ for a.e. $(t, x) \in \mathbb{R} \times \mathbb{R}^n$.

Back to the full problem

- Recall that
$$\int_\Sigma (V_1 - V_2) u_1 \overline{v_2} = 0,$$
for all u_1 and v_2 physical solutions of $(i\partial_t + \Delta - V_1)u_1 = 0$ and $(i\partial_t + \Delta - \overline{V_2})v_2 = 0$.

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- How can we do that?

Complex geometrical optics

- Solutions with exponential growth

$$(t, x) \in \mathbb{R} \times \mathbb{R}^n \mapsto e^{i|\nu|^2 t + \nu \cdot x}$$

with $\nu \in \mathbb{R}^n \setminus \{0\}$.

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$$u_1(t, x) = e^{i|\nu|^2 t + \nu \cdot x}\big(e^{-i(|\kappa|^2 t - \kappa \cdot x)} + u_1^\flat(t, x)\big),$$
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  These solutions are called **complex geometrical optics** (CGO).

The stationary vs dynamical potentials

- Complex geometrical optics

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- Stationary states at fix energy

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with

$$\kappa = -\frac{\xi}{2} + \Big(\lambda^2 - \frac{|\xi|^2}{4}\Big)^{1/2}\nu, \qquad \eta = \frac{\xi}{2} + \Big(\lambda^2 - \frac{|\xi|^2}{4}\Big)^{1/2}\nu,$$

where $\xi \in \mathbb{R}^n$ is arbitrary, $\nu\cdot\xi = 0$, $|\nu| = 1$ and $\lambda > |\xi|/2$.

Challenges of the proof

- Construction of the correction terms $u_1^\flat$ and $v_2^\flat$ of

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- For the construction, we use a trick[1] inspired in the Birman–Schwinger principle.
- CGO solutions are not physical. Hence, the orthogonality relation has to be extended. This is why we need the potentials to decay super-exponentially.
- This has been previously addressed in the literature Novikov, Khenkin, Uhlmann, Vasy... However, some difficulties have arisen in our situation because of the lack of ellipticity.

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Outline

Correction term of the CGO solution

Recall that CGO is a solution of

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in the form

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Since $(i\partial_t + \Delta)(e^{i|\nu|^2 t + \nu \cdot x} u^\sharp) = 0$ in $\mathbb{R} \times \mathbb{R}^n$ we have that

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- Is the operator $S_\nu \circ V$ quantitatively or qualitatively smaller than Id?

$$(\mathrm{Id} - S_\nu \circ V)u^\flat = S_\nu(Vu^\sharp).$$

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The operator S_ν is the Fourier multiplier

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which solves $(i\partial_{\mathrm{t}}+\Delta+2\nu\cdot\nabla)u=f$ in $\mathbb{R}\times\mathbb{R}^n$.

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which solves $(i\partial_\mathrm{t}+\Delta+2\nu\cdot\nabla)u=f$ in $\mathbb{R}\times\mathbb{R}^n$. The set

$$\Gamma_\nu=\{(\tau,\xi)\in\mathbb{R}\times\mathbb{R}^n : -\tau-|\xi|^2+i2\nu\cdot\xi=0\}$$

is a paraboloid of codimension 2.

How to bound S_ν

There are two types of situations: near and far from Γ_ν.

- Far from Γ_ν the symbol

$$\frac{\mathbf{1}_{\mathrm{far}(\Gamma_\nu)}}{-\tau - |\xi|^2 + i2\nu \cdot \xi}$$

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- When the symbol is supported near Γ_ν, the multiplier can be understood as a restriction-and-then-extension set-up in two different sense:

$$\frac{1}{(2\pi)^{\frac{n+1}{2}}} \int_{\mathbb{R}\times\mathbb{R}^n} e^{i(t\tau + x\cdot\xi)} \frac{\mathbf{1}_{\mathrm{near}(\Gamma_\nu)}}{-\tau - |\xi|^2 + i2\nu \cdot \xi} \widehat{f}(\tau,\xi)\, \mathrm{d}(\tau,\xi)$$

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- Restriction-and-then-extension either in the paraboloid

$$\{(\tau,\xi)\in\mathbb{R}\times\mathbb{R}^n : \tau = -|\xi|^2\},$$

  or the hyperplane

$$\{(\tau,\xi)\in\mathbb{R}\times\mathbb{R}^n : \nu\cdot\xi = 0\}.$$

Estimates with gain in $|\nu|$

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Theorem

Consider $n \in \mathbb{N}$. There exists an absolute constant $C > 0$ such that

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- This inequality can be understood as a local smoothing if $|\nu|$ is interpreted as a derivative.

Estimates with no gain in $|\nu|$: Strichartz inequalities

Theorem

Consider $n \in \mathbb{N}$ and $(q, r) \in [1, 2] \times [1, 2]$ such that

$$2 - \frac{2}{q} = \frac{n}{r} - \frac{n}{2} \iff \frac{2}{q'} = \frac{n}{2} - \frac{n}{r'},$$

with

$$(q, r, n) \neq (2, 1, 2) \iff (q', r', n) \neq (2, \infty, 2).$$

There exists a constant $C > 0$ that only depends on n, q and r such that

$$\|S_\nu f\|_{L^{q'}(\mathbb{R}; L^{r'}(\mathbb{R}^n))} \leq C \|f\|_{L^q(\mathbb{R}; L^r(\mathbb{R}^n))}$$

for all $f \in \mathcal{S}(\mathbb{R} \times \mathbb{R}^n)$.

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- To ensure that the correction terms become negligible we exploit the trace properties of the Fourier transform on hyperplanes.
- In order for the potentials to present local critical singularities, we need to prove suitable Strichartz inequalities.