Mathematical Aspects of Quantum Mechanics

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The Schrödinger equation

$$i\frac{\partial}{\partial t}\psi(x,t) = H\psi(x,t), \quad \psi(x,0) = \psi(x).$$

In $\mathbb{R}^3$, usually $\mathrm{L}^2(\mathbb{R}^3)$ (or a in separable Hilbert space $\mathcal{H}$).

Symbols explanations and Born interpretation.

H=energy and must be self-adjoint (s-a), i.e., $H = H^*$.

Time evolution $\psi(x,t) = e^{-itH}\psi$, and must be unitary, i.e.,

$$\int_{\mathbb{R}^3} |e^{-itH}\psi(x)|^2 \mathrm{d}x = \|e^{-itH}\psi\|^2 = \|\psi\|^2 = \int_{\mathbb{R}^3} |\psi(x)|^2 \mathrm{d}x,$$

so that total probability is preserved.

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Self-adjointness

Usually one starts with a symmetric operator (always densely defined) $T : \operatorname{dom} T \subset \mathcal{H} \to \mathcal{H}$, i.e.,

$$\langle \psi, T\phi \rangle = \langle T\psi, \phi \rangle, \quad \forall \psi, \phi \in \operatorname{dom} T.$$

This guarantees that eigenvalues are real, but not other kinds of spectra.

Definition

The $\operatorname{dom} T^*$ is the set of elements $\eta \in \mathcal{H}$ so that there is $\zeta \in \mathcal{H}$ with

$$\langle \eta, T\xi \rangle = \langle \zeta, \xi \rangle, \quad \forall \xi \in \operatorname{dom} T,$$

and action $T^*\eta = \zeta$ (maximality). Again, T is self-adjoint if $T = T^*$.

Theorem (Hellinger-Toeplitz, 1910)

If $T : \mathcal{H} \to \mathcal{H}$ satisfies $\langle \eta, T\xi \rangle = \langle T\eta, \xi \rangle$, for all $\xi, \eta \in \mathcal{H}$, then T is self-adjoint and bounded.

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Self-adjointness

How to check if a symmetric operator is s-a, or if it has self-adjoint extensions?

- T is symmetic iff $T \subset T^*$.
- If $S \subset T$, then $T^* \subset S^*$.
- If A is a s-a extension of T, then $T \subset A \Rightarrow A = A^* \subset T^*$.
- If T^* is s-a and A as above, then $T^{**} = T^* \subset A$ and $T^* = A$ is the unique s-a extension of T (essentially s-a).

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Self-adjointness

Observe that if T is symmetric, then for all $\xi \in \operatorname{dom} T$,

$$\|(T \pm i)\xi\|^2 = \|T\xi\|^2 + \|\xi\|^2 = \|\xi\|_T^2 \text{ (graph norm)},$$

and its *Cayley transform*

$$U(T) : (T - i)(T + i)^{-1} : \operatorname{img}(T + i) \to \operatorname{img}(T - i)$$

is an isometry.

Consider the *deficiency subspaces*

$$K_\pm(T) = \mathrm{N}(T^* \pm i) = \operatorname{img}(T \mp i)^\perp$$

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Key result for a symmetric T:

Proposition

T is self-adjoint iff $\mathrm{img}\,(T \pm i) = \mathcal{H}$ *iff* $U(T)$ *is a unitary operator.*

Proof.

(a) If $T = T^*$ (so T is closed), pick $\xi \in \mathrm{img}\,(T \pm i)^\perp = \mathrm{N}(T \mp i)$ and so $T\xi = \pm i\xi \Rightarrow \xi = 0$.

(b) If $\mathrm{img}\,(T \pm i) = \mathcal{H}$, pick $\eta \in \mathrm{dom}\,T^*$, so, for all $\phi \in \mathrm{dom}\,T$,

$$\langle \eta, (T+i)\phi \rangle = \langle (T^* - i)\eta, \phi \rangle.$$

There is $\xi \in \mathrm{dom}\,T$ with $(T^* - i)\eta = (T - i)\xi$ so that

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Theorem

A symmetric T *has self-adjoint extensions iff* $n_-(T) = n_+(T)$, *and is essentially self-adjoint iff* $n_-(T) = n_+(T)$=*0.*

Moment

Example

The linear momentum operator in one dimension has the action $\dot{P} = -i\mathrm{d}/\mathrm{d}x$. Is it self-adjoint?

(a) $\mathrm{L}^2(\mathbb{R})$. dom $\dot{P} = \mathrm{C}_0^\infty(\mathbb{R})$, which is symmetric. One checks that $\dot{P}^* = -i\mathrm{d}/\mathrm{d}x$ but dom $\dot{P}^* = \mathcal{H}^1(\mathbb{R})$.

(a1) $u \in K_+(T) \Rightarrow -i\mathrm{d}u/\mathrm{d}x = -iu$ and so $u(x) = Ce^x \notin \mathrm{L}^2(\mathbb{R})$, hence $n_+(\dot{P}) = 0$.

(a2) $v \in K_-(T) \Rightarrow -i\mathrm{d}v/\mathrm{d}x = iv$ and so $v(x) = Ce^{-x} \notin \mathrm{L}^2(\mathbb{R})$, hence $n_+(\dot{P}) = 0$.

Conclusion: $\dot{P}$ has exactly one self-adjoint extension, with domain $\mathcal{H}^1(\mathbb{R})$.

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(b) $L^2(0,1)$. dom $\dot{P} = C_0^\infty(0,1)$. Now both $u(x)$ and $v(x)$ are in the space, so $n_\pm(\dot{P}) = 1$ and this operator has infinitely many self-adjoint extensions.

(c) $L^2(0,\infty)$. dom $\dot{P} = C_0^\infty(0,\infty)$. Now whereas $v(x)$ is in the space, $u(x)$ is not, so $n_-(\dot{P}) = 1$, $n_+(\dot{P}) = 0$ and this operator has no self-adjoint extension.

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Examples

Let's mention important examples, whose proofs use different techniques.

Example

The free Schrödinger operator $H_0 = -\Delta$, with $\operatorname{dom} H_0 = \mathcal{H}^2(\mathbb{R}^d)$ is self-adjoint (and e-s-a).

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The typical Schrödinger operator $H = -\Delta + V$, with $V \in \mathrm{L}^2(\mathbb{R}^d)$ or $V \in \mathrm{L}^\infty(\mathbb{R}^d)$, $d \leq 3$, $\operatorname{dom} H = \mathcal{H}^2(\mathbb{R}^d)$, is self-adjoint (and e-s-a).

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The free Schrödinger operator $H_0 = -\Delta$, with $\operatorname{dom} H_0 = \mathcal{H}^2(\mathbb{R}^d)$ is self-adjoint (and e-s-a).

Example

The typical Schrödinger operator $H = -\Delta + V$, with $V \in \mathrm{L}^2(\mathbb{R}^d)$ or $V \in \mathrm{L}^\infty(\mathbb{R}^d)$, $d \leq 3$, $\operatorname{dom} H = \mathcal{H}^2(\mathbb{R}^d)$, is self-adjoint (and e-s-a).

Example

The typical Schrödinger operator $\dot{H} = -\Delta + V$, with $V \in \mathrm{L}^2_{\mathrm{loc}}(\mathbb{R}^d)$, has self-adjoint extensions.

H-atom

The H-atom initial operator in $\mathrm{L}^2(\mathbb{R}^3)$,

$$\dot{H} = -\Delta + \frac{\kappa}{|x|}, \quad \mathrm{dom}\, \dot{H} = \mathrm{C}_0^\infty(\mathbb{R}^3),$$

is essentially s-a, and its unique s-a extension has domain $\mathcal{H}^2(\mathbb{R}^3)$. An important result of Kato in the 1950's.

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Spectrum

The spectrum of the s-a operator are the possible experimental values that are measured in experiments.

Given a s-a T, its resolvent set is

$$\rho(T) = \{z \in \mathbb{C} \mid (T - z)^{-1} \text{ exists and is bounded}\},$$

and its spectrum is $\sigma(T) = \mathbb{C} \setminus \rho(T)$.

Roughly:

- *point:* closure of eigenvalues.
- *absolutely continuous:* intervals.
- *singular continuous:* fractal.

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More precisely: For each $\xi \in \operatorname{dom} T$, there exists a unique (finite) Borel measure $\mu_\xi^T = \mu_\xi$ on $\mathbb{R}$, the so-called spectral measure, so that

$$\langle \xi, T\xi \rangle = \int_{\sigma(T)} \lambda \, \mathrm{d}\mu_\xi^T(\lambda).$$

And for the time evolution

$$\langle \xi, e^{-itT}\xi \rangle = \int_{\sigma(T)} e^{-it\lambda} \, \mathrm{d}\mu_\xi^T(\lambda) = \text{Fourier transform of } \mu_\xi^T.$$

Hence, the above classification is precisely obtained from the Lebesgue decomposition of

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Suppose $T\xi_1 = \lambda_1\xi_1$ and $T\xi_2 = \lambda_2\xi_2$, with orthonormalized $\{\xi_1, \xi_2\}$ and $\lambda_1 \neq \lambda_2$.

Consider $\xi = a_1\xi_1 + a_2\xi_2$, with $|a_1|^2 + |a_2|^2 = 1$. Then

$$\langle \xi, T\xi \rangle = \lambda_1 |a_1|^2 + \lambda_2 |a_2|^2 = \int_{\sigma(T)} \lambda \, \mathrm{d}\mu_\xi^T(\lambda),$$

and one sees that $\mu_\xi^T(\lambda) = \delta_{\lambda_1}|a_1|^2 + \delta_{\lambda_2}|a_2|^2$.

This gives us an interpretation of the spectral measures!

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Return probability

H-atom: No $\sigma_{\rm sc}$. Bound states ($\sigma_{\rm p}$) and ionized atom ($\sigma_{\rm ac}$).

To be more precise, consider the return probability

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$$W_\xi^T(t) = \frac{1}{t}\int_0^t P_\xi^T(s)\,\mathrm{d}s.$$

Mentioning H-atom.

Next we mention the general behavior of these dynamical quantities for large t and different spectral types.

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Dynamical behavior

- If μ_ξ is a point measure, the function $t \mapsto P_\xi(t)$ is almost periodic. E.g., for ξ_1, ξ_2 as before,

$$e^{-itT}\xi = a_1 e^{-it\lambda_1}\xi_1 + a_2 e^{-it\lambda_2}\xi_2.$$

- If $\mu_\xi \ll \ell$, say, $\mathrm{d}\mu_\xi(\lambda) = f(\lambda)\mathrm{d}\lambda$,

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Two topics

Let's consider two rather recent topics (UFSCar):

- Aharonov-Bohm effect.
- correlation dimension.

We will describe each of them and just present some results, to illustrate those research areas.

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AB effect

Consider a unit charge in a magnetic field $\mathbf{B}$ in the plane or space.

Since $\operatorname{div} \mathbf{B} = \mathbf{0}$, one has $\mathbf{B} = \operatorname{rot} \mathbf{A}$, and $\mathbf{A}$ is the *magnetic potential*, an auxiliary quantity.

The classical dynamics is ruled by Lorenz force

$$\mathbf{F} = \mathbf{v} \times \mathbf{B}.$$

So, if $\mathbf{B}$ vanishes (e.g., $\mathbf{A} = \nabla\varphi$), there is no influence on dynamics.

Remark: There is a freedom $\mathbf{A} \mapsto \mathbf{A} + \nabla\varphi$, the so called "gauge choice."

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However, in QM it is the potential that appears in the Shcrödinger operator action

$$H = -(\nabla + i\mathbf{A})^{\mathbf{2}},$$

and if $\mathbf{A} = \nabla\varphi$, it may be removed by a unitary operator (gauge transform).

Aharonov and Bohm presented a situation in which $\mathbf{B} = \mathbf{0}$ but $\mathbf{A}$ is not a gradient and $\mathbf{A}$ influences the system physics!! Scattering and energy values.

For this, the space may not be simply connected. They have taken an *infinitely long* and *completely shielded* solenoid (two idealizations).

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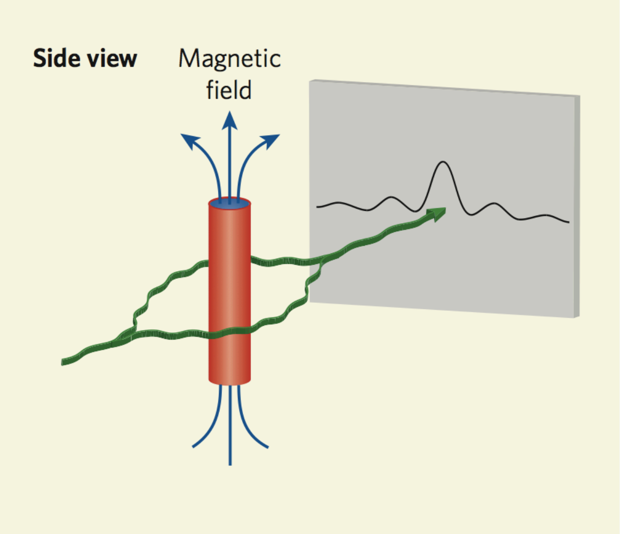

Figure: AB interference (figure borrowed from Tonomura & Nori).

AB effect 1

Notation:

1. The solenoid $\mathcal{S}$: the surface.
2. Its interior $\mathcal{S}^\circ$ (with $\mathbf{B} \neq \mathbf{0}$).
3. Its exterior $\mathcal{S}'$ (with $\mathbf{B} = \mathbf{0}$ but $\mathbf{A} \neq \mathbf{0}$).

How to justify the action $H = -(\nabla + i\mathbf{A})^2$, even in such situation, including the application of Stokes Theorem?

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we have proposed to consider a permeable and finite (size $2L$) solenoid, and to include a diverging sequence of potentials ("traditional") in the solenoid interior, e.g., $V_n(x) = n\chi_{S^\circ}(x)$.

Let $H_{L,n}$ denote the corresponding operator.

So, no problem with this model

$$H_{L,n} \text{ is s-a with } \operatorname{dom} H_{L,n} = \mathcal{H}^2(\mathbb{R}^2).$$

The limits $L \to \infty$ and $n \to \infty$ approach the idealizations.

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The limits $L \to \infty$ and $n \to \infty$ approach the idealizations.

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we have proposed to consider a permeable and finite (size $2L$) solenoid, and to include a diverging sequence of potentials ("traditional") in the solenoid interior, e.g., $V_n(x) = n\chi_{\mathcal{S}^\circ}(x)$.

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Theorem

Let $H_{\mathrm{AB}} = -(\nabla + i\mathbf{A})^{\mathbf{2}}$ *in the plane,* $\operatorname{dom} H_{\mathrm{AB}} = \mathcal{H}^2(\mathcal{S}') \cap \mathcal{H}^1_0(\mathcal{S}')$.
Then, in the sense of strong resolvent convergence

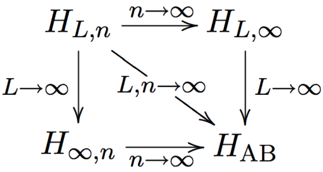

Figure: Commutative diagram for the the limits $L, n \to \infty$ in the plane.

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$$\begin{array}{ccc} H_{L,n} & \xrightarrow{n\to\infty} & H_{L,\infty} \\ {\scriptstyle L\to\infty}\downarrow & \searrow^{L,n\to\infty} & \downarrow{\scriptstyle L\to\infty} \\ H_{\infty,n} & \xrightarrow[n\to\infty]{} & H_{\mathrm{AB}} \end{array}$$

Figure: Commutative diagram for the the limits $L, n \to \infty$ in the plane.

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With R. Romano,

we have considered a zero radius solenoid and an additional potential $V_\alpha(x) = \alpha/|x|^2$, resulting in

$$H_{\alpha,\kappa} = -(\nabla + i\mathbf{A}_\kappa)^2 + V_\alpha, \quad \mathrm{dom}\, H_{\alpha,\kappa} = \mathrm{C}_0^\infty(\mathbb{R}^2 \setminus \{0\}).$$

$\kappa = \int_{C(0;r)} \mathbf{A}_\kappa \cdot \mathrm{d}\mathbf{r} = \Phi/(2\pi)$, with Φ the magnetic flux.

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Theorem (A new version of the AB effect)

$H_{\alpha,\kappa}$ always has self-adjoint extensions, but the values of its deficieny indices $n_\pm$ depend on the circulation κ (so on the magnetic potential).

For example: if $\alpha = -p^2/4 + 1$ ($p \in \mathbb{N}$), then $n_\pm = p - 1$ for $\kappa \in \mathbb{Z}$.

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Correlation dimension

The second topic is related to the **correlation dimension** of spectral measures and **dynamics**.

Given a finite Borel measure μ on $\mathbb{R}$, consider

$$I_\mu(\epsilon) = \int_{\mathbb{R}} \mu(x-\epsilon, x+\epsilon)\,\mathrm{d}\mu(x) \sim \epsilon^D$$

and its correlation dimension is given by

$$D_\mu = \lim_{\epsilon\to 0} \frac{\ln I(\epsilon)}{\ln \epsilon}.$$

It should be lim sup (D_μ^+) and lim inf (D_μ^-).

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- If the support(μ) is bounded, then $0 \leq D_\mu \leq 1$.

A little bit of intuition.

- If μ is a pure point measure, then $D_\mu^\pm = 0$.
- If μ Lipschitz (i.e., $\mu(a,b) \leq L|b-a|$), then $D_\mu^\pm = 1$.
- Hence, $0 < D_\mu^\pm < 1$ is an indication of a singular continuous measure.

Usually, it is hard to compute $D_\mu^\pm$!!

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For T s-a, recall the time average of the return probability

$$W_\xi^T(t) = \frac{1}{t}\int_0^t P_\xi^T(s)\,\mathrm{d}s \sim \left(\frac{1}{t}\right)^\gamma$$

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Let's study this dimension of spectral measures in a space of discrete Schrödinger operators on $l^2(\mathbb{Z})$,

$$(h_v u)(n) = u(n+1) + u(n-1) + v(n)u(n), \quad \|v\|_\infty \leq r.$$

If $v = 0$, the spectrum of the free (Laplacian) operator is $\sigma(h_0) = [-2, 2]$ and purely abs continuous. Let $I = (-2, 2)$.

Notation.

1. Let X_r be the metric space of such operators with the metric of pointwise convergence.
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In this complete metric space of operators X_r, what would be the typical value of the correlation dimension $D_{\mu_j^v}$?

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Theorem (S. Carvalho, CRdO)

For each $r > 0$, the set

$$\{h_v \in X_r \mid \sigma(h_v) = [2-r, 2+r] \text{ is sc},\ D^-_{\mu^v_j} = 0 \text{ and } D^+_{\mu^v_j} = 1,\ \forall k\}$$

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Another application

Let $Y_{a,b} = \{T \in B(\mathcal{H}) \text{ s-a } \mid \sigma(T) = [a,b]\}$ with the metric

$$d(T,T') = \|T - T'\|.$$

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Let h_v as before, but restricted to $\{0, 1, 2, 3, \cdots\}$ with $u(0) = 0$ (Dirichlet).

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If h_v is purely absolutely continuous with Lipschitz spectral measures (so $D_\mu^\pm = 1$), then such properties are preserved, up to the spectrum boundary, under suitable exponentially decaying perturbations $b(n)$.

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