An Invitation to Mathematical Quantum Physics

Lancaster University Postgraduate Forum

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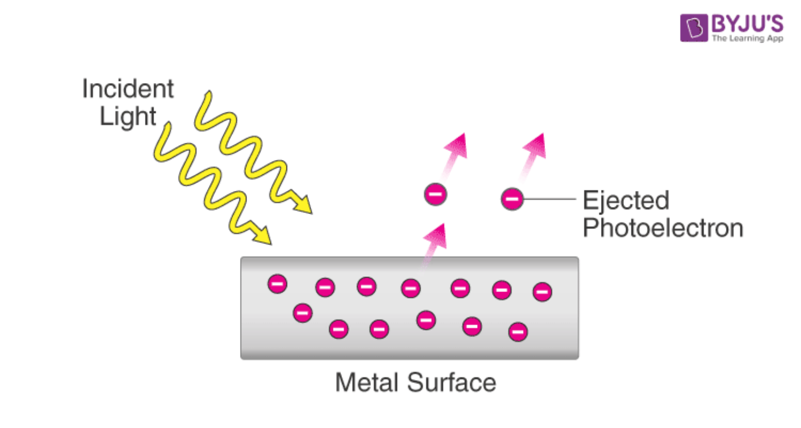
A quantum particle living in $\mathbb{R}$

Suppose that we have a quantum particle contained inside of $\mathbb{R}$.

This particle has things we can observe: e.g. *position*, *momentum*, and *energy*. Such things are called *observables*.

Wave-particle duality

Quantum objects can be observed to have both wave-like and particle-like properties. This is known as *wave-particle duality*.



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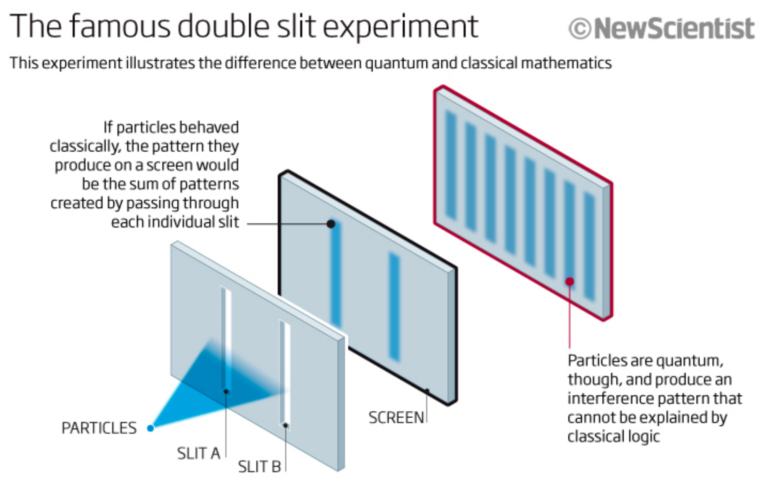

Probabilistic behaviour of quantum objects

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This suggests that we *cannot predict the outcome* of a quantum experiment; we can only predict *the probabilities of an outcome* of a quantum experiment.

The wavefunction

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- $\mathbb{P}\big(\text{The position of the particle is in } E \subset \mathbb{R}\big) = \int_E |\psi(x)|^2 \, \mathrm{d}x$.
- The *time-evolution* of the particle is *wave-like*:

$$\frac{\partial \psi}{\partial t} = \frac{1}{i\hbar} H\psi.$$

  This is the famous *Schrödinger equation*.

An underlying space for wavefunctions

As $\mathbb{P}\big(\text{The position of the particle is in } E \subset \mathbb{R}\big) = \int_E |\psi(x)|^2 \,\mathrm{d}x$, clearly

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$$\mathbb{P}\big(\text{The position of the particle is in } \mathbb{R}\big) = 1 = \int_{\mathbb{R}} |\psi(x)|^2 \,\mathrm{d}x.$$

Therefore, it makes sense to associate the wavefunctions with the space $\mathrm{L}^2(\mathbb{R})$, where

$$f \in \mathrm{L}^2(\mathbb{R}) \longleftrightarrow \int_{\mathbb{R}} |f(x)|^2 \,\mathrm{d}x < \infty.$$

This is not technically the definition of $\mathrm{L}^2(\mathbb{R})$, but it is good enough as a working definiton. To make this more precise, we need measure theory.

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- $\langle \phi, \psi \rangle := \int_{\mathbb{R}} \overline{\phi(x)} \psi(x) \, \mathrm{d}x$ is an inner product on $\mathrm{L}^2(\mathbb{R})$, and

$$\|\psi\| := \left(\int_{\mathbb{R}} |\psi(x)|^2 \, \mathrm{d}x \right)^{\frac{1}{2}} = \sqrt{\langle \psi, \psi \rangle}$$

  defines a norm on $\mathrm{L}^2(\mathbb{R})$ where *every Cauchy sequence converges*.

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  defines a norm on $\mathrm{L}^2(\mathbb{R})$ where *every Cauchy sequence converges*.
- $\mathrm{L}^2(\mathbb{R})$ has a non-trivial *dense subset*.

The position operator

As $\langle \phi, \psi \rangle = \int_{\mathbb{R}} \overline{\phi(x)} \psi(x) \, \mathrm{d}x$, we can express the expectation of the position as

$$\mathbb{E}(x) := \int_{\mathbb{R}} x |\psi(x)|^2 \, \mathrm{d}x = \langle \psi(x), x\psi(x) \rangle .$$

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We therefore have a natural operator describing the position of our particle:

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An issue: $\mathrm{Dom}(X) \neq \mathrm{L}^2(\mathbb{R})$, as

$$\frac{1}{x} \chi_{[1,\infty)}(x) \in \mathrm{L}^2(\mathbb{R}) \quad \text{but} \quad \chi_{[1,\infty)}(x) \notin \mathrm{L}^2(\mathbb{R})$$

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- Quantum particles behave both as *waves* and *particles*, and have a *probabilistic nature*. We describe this through *wavefunctions, which encode everything we know about the particle*.

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- A natural space for wavefunctions is $\mathrm{L}^2(\mathbb{R})$.
- For a wavefunction ψ, $|\psi|^2$ can be interpreted as a *probability density function*.
- Through the inner product of $\mathrm{L}^2(\mathbb{R})$, we can get an operator describing the position of a particle. This operator *cannot be defined on the whole space*.

Hilbert spaces

A (complex, infinite-dimensional) *Hilbert space* $\mathcal{H}$ is a (complex, infinite-dimensional) vector space such that:

- For a given inner product $\langle \cdot, \cdot \rangle$, $\|\cdot\| := \sqrt{\langle \cdot, \cdot \rangle}$ is a norm.
- Every Cauchy sequence converges with respect to this norm ($\mathcal{H}$ is *complete*).
- If $\mathcal{H}$ has a dense countable subset, then it is *separable*.

A linear map $T\colon \mathcal{H} \to \mathcal{H}$ is a *bounded operator* if there exists some $M > 0$ such that for all $x \in \mathcal{H}$,

$$\|Tx\| \leq M\|x\|.$$

Operators on Hilbert Spaces

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For a subspace $\mathrm{Dom}\,(T) \subset \mathcal{H}$, an *(unbounded) operator* is any linear map $T \colon \mathrm{Dom}\,(T) \to \mathcal{H}$.

An (unbounded) operator is *densely-defined* if $\mathrm{Dom}\,(T)$ is dense in $\mathcal{H}$.

Adjoints of bounded operators

For a bounded operator $T \colon \mathcal{H} \to \mathcal{H}$, there exists an *adjoint* operator $T^* \colon \mathcal{H} \to \mathcal{H}$ defined by

$$\langle x, Ty \rangle = \langle T^* x, y \rangle$$

for any $x, y \in \mathcal{H}$. Furthermore, *the adjoint operator is unique*.

Existence of adjoints of bounded operators

Theorem (Riesz-Fréchet theorem)

For a Hilbert space $\mathcal{H}$ and a continuous linear map $\psi : \mathcal{H} \to \mathbb{C}$, there is a unique $z \in \mathcal{H}$ such that for all $y \in \mathcal{H}$,

$$\psi(y) = \langle z, y \rangle .$$

Fix $x \in \mathcal{H}$. Then, $\psi \colon \mathcal{H} \to \mathbb{C}$, $\psi(y) = \langle x, Ty \rangle$ is a continuous linear map.

By the Riesz-Fréchet theorem, there exists a unique $z \in \mathcal{H}$ such that

$$\langle z, y \rangle = \langle x, Ty \rangle .$$

Define T^* by $T^* x = z$ to get a linear bounded operator.

What about adjoints of unbounded operators?

Let $T\colon \mathrm{Dom}(T) \to \mathcal{H}$ be a *densely-defined* operator. Define

$\mathrm{Dom}(T^*) := \{x \in \mathcal{H} \colon y \mapsto \langle x, Ty\rangle$ where $y \in \mathrm{Dom}(T)$ is a continuous map$\}$.

- $\mathrm{Dom}(T^*)$ is a subspace.
- As $\mathrm{Dom}(T)$ is dense, there exists a unique extension of $x \mapsto \langle x, Ty\rangle$

  to the entirety of $\mathcal{H}$ for every $y \in \mathcal{H}$.

  By the Riesz-Fréchet theorem, there then exists a unique vector

  $z \in \mathcal{H}$ such that

$$\langle z, y\rangle = \langle x, Ty\rangle$$

  for all $y \in \mathrm{Dom}(T)$ and $x \in \mathrm{Dom}(T^*)$. Define T^* by $T^*x = z$.

Consequences of this construction

- We need the denseness of $\mathrm{Dom}\,(T)$ or else the uniqueness of the adjoint fails. Therefore, *only densely-defined operators have adjoints*.

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    1. $\mathrm{Dom}\,(T^*)$ may not be dense, so $(T^*)^*$ *may not exist*.
    2. There exist operators such that $\mathrm{Dom}\,(T) \cap \mathrm{Dom}\,(T^*) = \{0\}$.
    3. For two densely-defined operators T and S on $\mathcal{H}$, as

    $$\mathrm{Dom}\,(T+S) = \mathrm{Dom}\,(T) \cap \mathrm{Dom}\,(S)\,,$$

    $T+S$ may have no adjoint.

Symmetric and self-adjoint operators

An operator $T\colon \mathrm{Dom}\,(T) \to \mathcal{H}$ is *symmetric* if for all $x, y \in \mathrm{Dom}\,(T)$,

$$\langle x, Ty \rangle = \langle Tx, y \rangle \,.$$

If T is densely-defined, symmetric, and if $\mathrm{Dom}\,(T) = \mathrm{Dom}\,(T^*)$, then T is *self-adjoint*.

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Theorem

A densely-defined operator $T \colon \operatorname{Dom}(T) \to \mathcal{H}$ is symmetric if and only if T^* is an extension of T.

Essentially self-adjoint operators

An operator $T\colon \mathrm{Dom}\,(T) \to \mathcal{H}$ is *essentially self-adjoint* if:

- T is symmetric: $\langle x, Ty\rangle = \langle Tx, y\rangle$ for all $x, y \in \mathrm{Dom}\,(T)$.
- The operator $\overline{T}$ whose *graph* is given by the *closure of the graph of T*,

$$\mathrm{G}(\overline{T}) = \overline{\mathrm{G}(T)} = \overline{\{(x, Tx) \in \mathcal{H} \oplus \mathcal{H} \colon x \in \mathrm{Dom}\,(T)\}},$$

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If T is essentially self-adjoint, then $\overline{T}$ is *the unique self-adjoint extension of T*.

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- X is not self-adjoint but is essentially self-adjoint on

$$\mathcal{S}(\mathbb{R}) \coloneqq \left\{\psi \in \mathrm{C}^\infty(\mathbb{R})\colon \forall \alpha, \beta \in \mathbb{N}, \sup_{x\in\mathbb{R}}\left| x^\alpha \frac{\mathrm{d}^\beta \psi(x)}{\mathrm{d}x^\beta}\right| < \infty\right\}.$$

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- *Bounded operators always have an adjoint* and are always either *self-adjoint or not self-adjoint*.
- For unbounded operators, *only densely-defined operators have adjoints*. There are *different families of unbounded operators between self-adjoint and not self-adjoint*.
- *Changing the domain* of an unbounded operator *can change key properties* of the operator.

The axioms of quantum mechanics

To formalise what we originally saw in quantum physics, we introduce the following 'axioms':

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1. The *possibile states* of a quantum system are *associated with vectors* in a complex and separable Hilbert space that have *norm 1*.
2. *Observables* in our quantum system are associated with *self-adjoint linear operators*.
3. If an observation a has the corresponding operator A and if our quantum system is in the state $\psi \in \mathrm{Dom}\,(A)$, then the *expected value for the measurement of a* is

$$\mathbb{E}_{\psi}(A) = \langle \psi, A\psi \rangle \,.$$

The 1D quantum harmonic oscillator

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For the quantum harmonic oscillator, it is the operator

$H\colon \mathrm{Dom}\,(H) \to \mathrm{L}^2(\mathbb{R})$ given by

$$H = \frac{1}{2m}\big(P^2 + (m\omega X^2)\big),$$

where:

- $P\psi = -i\hbar \frac{\mathrm{d}\psi}{\mathrm{d}x}$ is the *momentum operator*
- $X\psi = x\psi(x)$ is the *position operator*

The mathematical problem

A natural domain for our Hamiltonian is the *Schwartz space*,

$$\mathrm{Dom}\,(H) = \mathcal{S}(\mathbb{R}) = \left\{\psi \in \mathrm{C}^\infty(\mathbb{R}) \colon \forall \alpha, \beta \in \mathbb{N},\ \sup_{x\in\mathbb{R}} \left| x^\alpha \frac{\mathrm{d}^\beta \psi(x)}{\mathrm{d}x^\beta} \right| < \infty \right\}.$$

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Our goals:

- Find the *eigenvalues* (if they exist) of our Hamiltonian on $\mathcal{S}(\mathbb{R})$: these are *the energy levels of the quantum harmonic oscillator*.

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Our goals:

- Find the *eigenvalues* (if they exist) of our Hamiltonian on $\mathcal{S}(\mathbb{R})$: these are *the energy levels of the quantum harmonic oscillator*.
- Confirm that the Hamiltonian is either *essentially self-adjoint* or *self-adjoint* on $\mathcal{S}(\mathbb{R})$ so that we *satisfy our axioms*.

Simplifying our problem

We introduce the following two operators:

$$\text{Lowering Operator:} \quad a\colon \mathcal{S}(\mathbb{R}) \to \mathrm{L}^2(\mathbb{R}), \quad a = \frac{1}{\sqrt{2\hbar m\omega}}\Big(m\omega X + iP\Big)$$

$$\text{Raising Operator:} \quad a^*\colon \mathcal{S}(\mathbb{R}) \to \mathrm{L}^2(\mathbb{R}), \quad a^* = \frac{1}{\sqrt{2\hbar m\omega}}\Big(m\omega X - iP\Big)$$

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- a^*a is symmetric on $\mathcal{S}(\mathbb{R})$.
- $H = \hbar\omega\left(a^*a + \frac{1}{2}I\right)$ on $\mathcal{S}(\mathbb{R})$.
- $\lambda \mapsto \hbar\omega\left(\lambda + \frac{1}{2}\right)$ takes us from the eigenvalues of a^*a to all of the eigenvalues of H on $\mathcal{S}(\mathbb{R})$.

Eigenvalue results

Suppose (λ, ψ) is an eigenvalue-eigenvector pair for a^*a when defined on $\mathcal{S}(\mathbb{R})$. Then,

- $a^*a(a\psi) = (\lambda - 1)a\psi$.
- $a^*a(a^*\psi) = (\lambda + 1)a^*\psi$.

Therefore,

- $a\psi = 0$ or $(\lambda - 1, a\psi)$ is an eigenvalue-eigenvector pair for a^*a.
- $a^*\psi = 0$ or $(\lambda + 1, a^*\psi)$ is an eigenvalue-eigenvector pair for a^*a.

Important consequence: *if we have an eigenvalue-eigenvector pair for a^*a, we can repeatedly apply a to the eigenvector to get an eigenvalue of 0*.

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Furthermore, for $n \geq 0$ define the *excited states* by $\psi_n := (a^*)^n\psi_0$.

1. Any distinct pair (ψ_n, ψ_m) are orthogonal.
2. $a^*\psi_n = \psi_{n+1}$ and $a\psi_n = n\psi_{n-1}$, so $a^*a\psi_n = n\psi_n$.

The eigenvalues

The ground state of $a^* a$ when defined on $\mathcal{S}(\mathbb{R})$ is

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega}{2\hbar}x^2\right).$$

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The excited states are given by

$$\psi_n(x) = H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right)\psi_0(x),$$

where H_n is the physicist's Hermite polynomial

$$H_n(y) = \begin{cases} 1 & \text{if } n = 1. \\ \frac{1}{\sqrt{2}}\left(2xH_{n-1}(y) - \frac{\mathrm{d}}{\mathrm{d}x}H_{n-1}(y)\right) & \text{if } n \geq 2. \end{cases}$$

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The energy levels of the Hamiltonian on $\mathcal{S}(\mathbb{R})$ are given by

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \qquad \text{for } n \in \mathbb{N}.$$

Thanks for listening!

References i