Mathematical Foundations of Quantum Mechanics

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Remarks about the exercises

- The excercises are written on the transparencies.
- Try to solve as many exercises as you can.

Some History

The Old Quantum Mechanics

- N. Bohr (1913)

The Q.M.

- W. Heisenberg, M. Born and P. Jordan: Matrix Mechanics
- E. Schrödinger: Wave Mechanics
- P.A.M. Dirac: Relativistic Equation for the Electron
- J. Von Neumann and M.H. Stone: Rigorous mathematical formulation of Q.M.

Outline

Part I

Preliminaries

- Hilbert Space
- Total Orthonormal Sets
- Unbounded Linear Hilbert Adjoint, Symmetric and Self-Adjoint Operators
- Spectral Proprerties of Self-Adjoint Operators

Outline

Part II

- Basic Ideas of Quantum Mechanics
- The Spectral Theorem for Unbounded Self-Adjoint Operators
- J. Von Neumann's Postulates for Quantum Mechanics
- Heisenberg's Uncertainty Principle
- The Virial Theorem for Quantum Mechanics

Part III

Application

- The Quantum Harmonic Oscillator in One Spatial Dimension

PART I

Hilbert Space

Definition

Let $(\mathcal{H}(K), \langle\cdot,\cdot\rangle)$ be an *inner product space* where

$$\langle\cdot,\cdot\rangle : \mathcal{H} \times \mathcal{H} \to K.$$

If $\mathcal{H}$ is *complete* w.r.t. $\|\cdot\| = \sqrt{\langle\cdot,\cdot\rangle}$ it is called a **Hilbert space**.

Examples:

(1) $l^2 = \{(a_j)_{j=1}^{\infty},\ a_j \in \mathbb{C} : \sum_{j=1}^{\infty} |a_j|^2 < \infty\}$ with inner product $\langle a, b\rangle = \sum_{j=1}^{\infty} a_j \bar{b}_j < \infty$.

(2) $L^2(\mathbb{R}, d\mu) = \{f \text{ compex-valued measurable functions on } \mathbb{R} : \int_{\mathbb{R}} |f(x)|^2 d\mu < \infty\}$ with inner product $\langle f, g\rangle = \int_{\mathbb{R}} f(x)\bar{g}(x) d\mu$.

Remark: Additionally we will assume that $\mathcal{H}$ is *separable*.

Total orthonormal sets and sequences

Definition

A total orthonormal set in a an inner product space $(\mathcal{H}, \langle \cdot, \cdot \rangle)$ is a subset $M \subset \mathcal{H}$ for which:

(1) its span is dense in $\mathcal{H}$

(2) it is orthonormal

Proposition

Let $\mathcal{H}$ be a Hilbert space then:

(α) *If $\mathcal{H}$ is separable, every orthonormal set in $\mathcal{H}$ is countable.*

(β) *If $\mathcal{H}$ contains a countable orthonormal set which is total in $\mathcal{H}$ then $\mathcal{H}$ is separable.*
Exc.: Prove this

Continued

Example: Hermite polynomials of order n. Consider $L^2(\mathbb{R}, dx)$ with inner product $\langle f, g\rangle = \int_{\mathbb{R}} f(x)g(x)dx$ and the sequence of functions

$$\{x^n e^{-\frac{x^2}{2}}\},\ n \in \mathbb{N}_0.$$

Applying Gram-Schmidt

$$\begin{aligned} e_n(x) &= \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} e^{-\frac{x^2}{2}} H_n(x), \\ H_0(t) &= 1, \quad H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}, \quad n = 1, 2, \cdots . \end{aligned}$$

Eigenstates of the Schrödinger operator $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}k\hat{X}^2$.

Unbounded Linear Operators

Definition (Bounded Linear Operators)

Let X, Y be two normed spaces and $T : \mathcal{D}(T) \subset X \to Y$ a linear operator. The operator T is called bounded is there exists real number $c > 0$ such that

$$\|Tx\|_Y \leq c \|x\|_X , \forall x \in \mathcal{D}(T).$$

Definition (Hilbert-Adjoint)

Let $T : \mathcal{D}(T) \to \mathcal{H}$ be an unbounded, densely defined linear operator on a complex Hilbert space. Then the Hilbert-adjoint $T^* : \mathcal{D}(T^*) \to \mathcal{H}$ is defined as follows:

$$\begin{aligned} \mathcal{D}(T^*) &= \{y \in \mathcal{H} : \exists y^* \in \mathcal{H} \text{ satisfying} \\ &\quad \langle Tx, y\rangle = \langle x, y^*\rangle, \forall x \in \mathcal{D}(T), y^* = T^* y, \text{un. det.}\} \end{aligned}$$

Proposition

Let $S : \mathcal{D}(S) \to \mathcal{H}$ and $T : \mathcal{D}(T) \to \mathcal{H}$ be linear operators densely defined in a complex Hilbert space $\mathcal{H}$, then:

$$\textit{if } S \subset T \Rightarrow T^* \subset S^*$$

Definition (Symmetric linear operator)

Let $T : \mathcal{D}(T) \to \mathcal{H}$ be a linear operator densely defined in a complex Hilbert space $\mathcal{H}$. T is called a symmetric linear operator if

$$\langle Tx, y\rangle = \langle x, Ty\rangle, \forall x, y \in \mathcal{D}(T)$$

Lemma

A densely defined linear operator T in a complex Hilbert space $\mathcal{H}$ is symmetric iff $T \subset T^*$.

Exc.: Prove this

Definition (Self-adjoint linear operator)

A densely defined linear operator T in a complex Hilbert space $\mathcal{H}$ is called self-adjoint if $T = T^*$.

Remark: Every self-adjoint operator is symmetric.

Examples:

(α) The multiplication operator (or position operator). The operator $X : \mathcal{D}(X) \to L^2(\mathbb{R}, dx)$ with $(Xf)(x) = xf(x)$ and domain

$$\mathcal{D}(X) = \{\psi \in L^2(\mathbb{R}, dx) : \; X\psi \in L^2(\mathbb{R}, dx)\}$$

is unbounded and self-adjoint

Exc.: Prove this

Continued

(β) The differentiation operator (or momentum operator). The operator $P:\ \mathcal{D}(P) \subset L^2(\mathbb{R}, dx) \to L^2(\mathbb{R}, dx)$ with $(P\psi)(x) = -i\hbar \frac{d\psi(x)}{dx}$ and domain

$$\begin{aligned} \mathcal{D}(P) &= \{\psi, P\psi \in L^2(\mathbb{R}, dx) : \\ &\qquad \psi \textit{ abs. con. on every compact interval on } \mathbb{R}\} \end{aligned}$$

is also unbounded and self-adjoint.

Spectral Properties of Self-adjoint operators

Definition (Regular Value)

Let the normed space $(X(\mathbb{C}), \|\cdot\|)$ and the linear operator $T : \mathcal{D}(T) \to X$. A regular value λ of T is a complex number such that:

- $R_\lambda(T) := T_\lambda^{-1} = (T - \lambda I)^{-1}$ exists.
- $R_\lambda(T)$ is bounded.
- $R_\lambda(T)$ is defined on a dense set of X.

The resolvent set $\rho(T) = \{\text{regular values}\lambda\}$. The spectrum is $\sigma(T) = \rho^c(T)$ and $\sigma(T) = \sigma_p(T) \cup \sigma_c(T) \cup \sigma_r(T)$ which are pairwise disjoint.

Theorem (Regular values)

Let $T : \mathcal{D}(T) \to \mathcal{H}$ be a self-adjoint linear operator which is densely defined in a complex Hilbert space $\mathcal{H}$. Then a number λ belongs to the resolvent set $\rho(T)$ iff there exists $c > 0$ such that

$$\|T_\lambda x\| \geq c\,\|x\|\,,\ \forall x \in \mathcal{D}(T),\ \textit{where}\ T_\lambda = T - \lambda I.$$

Proposition (Spectrum)

Let $T : \mathcal{D}(T) \to \mathcal{H}$ be a self-adjoint linear operator which is densely defined in a complex Hilbert space $\mathcal{H}$. The spectrum $\sigma(T)$ is real and closed.

Exc.: Prove the closedness.

PART II

Warm up

The result of a measurement is a random variable and Q.M. deals with the probability distributions of such variables.

Physical quantities whose values (real numbers) can be determined experimentally are called *observables*.

(1) A single particle moving in $\mathbb{R}^3$ is described by a wave function $\psi : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{C}$.

(2) The quantity $\rho_t(x) = |\psi(x,t)|^2$ is interpreted as the probality density function of the particle at time t in the state ψ.

(3) The location x of a particle (which is an observable) due to the probabilistic interpretation it is also a random variable with expectation value given by $\mathbb{E}_\psi(X) = \int_{\mathbb{R}^3} x\,|\psi(x,t)|^2\, d^3x$. In real life $\mathbb{E}_\psi(\chi_\Omega) = \int_{\mathbb{R}^3} \chi_\Omega(x)\,|\psi(x,t)|^2\, d^3x = \int_\Omega |\psi(x,t)|^2\, d^3x$, $\Omega \subset \mathbb{R}^3$.

(4) The mean square deviation $\Delta_\psi(X) = \mathbb{E}_\psi(X^2) - (\mathbb{E}_\psi(X))^2 = \|(X - \mathbb{E}_\psi(X))\psi\|^2$ is always no zero in contradistinction to Classical Mechanics.

The Spectral Theorem for Unbounded Self-Adjoint Operators

Let A be an unbounded, densely defined and self-adjoint operator in a complex Hilbert space $\mathcal{H}$. Then there exists a family of orthogonal projections $\{E(\lambda)\}$, $-\infty < \lambda < \infty$ such that:

(1) $\lambda_1 \leq \lambda_2$ implies $E(\lambda_1) \leq E(\lambda_2)$ (monotonicity).

(2) For $\epsilon > 0$ $E(\lambda + \epsilon) \xrightarrow{s} E(\lambda)$ as $\epsilon \to 0$ (strong continuity from the right).

(3) $E(\lambda) \xrightarrow{s} 0$ as $\lambda \to -\infty$ and $E(\lambda) \xrightarrow{s} I$ as $\lambda \to +\infty$.

(4) A is recovered from the family $\{E(\lambda)\}$ by the formula

$$A = \int_{\mathbb{R}} \lambda dE(\lambda)$$

with domain

$$\mathcal{D}(A) = \left\{ f \in \mathcal{H} : \|Af\|^2 = \int_{\mathbb{R}} \lambda^2 d\, \|E(\lambda) f\|^2 < \infty \right\}.$$

(5) If $\{F(\lambda)\}$ is a generalised resolution of the identity (properties (1)-(3)) such that

$$A = \int_{\mathbb{R}} \lambda dF(\lambda)$$

then

$$E(\lambda) = F(\lambda), \forall \lambda.$$

Proof due to Riesz and Lorch or J. von Neumann.

J. von Neumann's Postulates

Post. 1 The states of a quantum mechanical system are described by non-zero vectors of a complex separable Hilbert space $\mathcal{H}$. Two vectors describe the same state iff they differ by a non-zero complex factor. Each observable corresponds to a certain (unique) linear self-adjoint operator in $\mathcal{H}$.

Post. 2 Observables are simultaneously measurable iff the corresponding self-adjoint operators commute. If observables s_j, $j = 1, \cdots, n$ are simultaneously measurable then, for a given ψ, their joint distribution function is of the form

$$\mathcal{P}_\psi(\lambda_1, \cdots, \lambda_n) = \left\| E^{(1)}_{\lambda_1} \cdots E^{(n)}_{\lambda_n} \psi \right\|^2$$

where $E^{(j)}_{\lambda_j}$ are the projection operators of the spectral families correspoding to operators S_j.

Continued

Post. 3 Let ψ_0 represents the state of a system at $t = 0$. Then the state of the system at any time t is represented by $\psi(t) = U_t \psi_0$ where $U_t = e^{-\frac{i}{\hbar}Ht}$ is a unitary operator called evolution operator. The vector $\psi(t)$ is differentiable if $\psi \in \mathcal{D}(H)$ and in this case satisfies the Schrödinger's equation

$$i\hbar \frac{d\psi(t)}{dt} = H\psi(t),\ \hbar = \frac{h}{2\pi}$$

where H is time-independent, h is Planck's constant and $i = \sqrt{-1}$.

Post. 4 Every non-zero vector of the state space $\mathcal{H}$ corresponds to a state of the system and every self-adjoint operator corresponds to an observable.

Theorems

Theorem

Let $\hat{A}$ be a self-adjoint operator and define $U(t) = e^{it\hat{A}}$. Then

(1) $\forall t \in \mathbb{R}$, $U(t)$ *is a unitary operator and* $U(t+s) = U(t)U(s)$, $\forall t, s \in \mathbb{R}$.

(2) *If* $\psi \in \mathcal{H}$ *then* $\lim_{t\to t_0} U(t)\psi = U(t_0)\psi$ *in the strong operator toplology. Exc.: Prove this.*

(3) *For* $\psi \in \mathcal{D}(\hat{A})$, $\lim_{t\to 0}(\frac{U(t)-I}{t})\psi = i\hat{A}\psi$.

(4) *If* $\lim_{t\to 0}(\frac{U(t)-I}{t})\psi$ *exists then* $\psi \in \mathcal{D}(\hat{A})$.

Theorem (Stone)

Let $U(t)$ be a strongly continuous one-parameter unitary group on a Hilbert space $\mathcal{H}$. Then, there is a self-adjoint operator $\hat{A}$ on $\mathcal{H}$ so that $U(t) = e^{it\hat{A}}$.

Corollaries

(1) If $\psi \in \mathcal{D}(\hat{A})$ then the mean value of the corresponding observable in the state ψ is given by $\mathbb{E}_\psi(A) = \langle \hat{A}\psi, \psi \rangle$.

(2) If $\psi \in \mathcal{D}(f(\hat{A}))$ then the mean value of the corresponding observable in the state ψ is given by $\mathbb{E}_\psi(f(A)) = \langle f(\hat{A})\psi, \psi \rangle$.

(3) The variance of an observable exists iff $\psi \in \mathcal{D}(\hat{A})$ and is given by $Var_\psi(A) = \left\| (\hat{A} - \mathbb{E}_\psi(A))\psi \right\|^2$.

(4) In a state ψ an observable A takes the value λ with certainty iff ψ is an eigenvector of the operator $\hat{A}$ with eigenvalue λ. Exc.: Prove this.

(5) The probability for the value of an observable measured in a state ψ to belong in Ω is $\|E(\Omega)\psi\|^2$.

Heisenberg's Uncertainty Principle

Theorem

Suppose $\hat{A}$ and $\hat{B}$ are two densely defined self-adjoint operators. Then for any $\psi \in \mathcal{D}(\hat{A}) \cap \mathcal{D}(\hat{B})$ such that $\hat{A}\psi, \hat{B}\psi \in \mathcal{D}(\hat{A}) \cap \mathcal{D}(\hat{B})$ we have

$$\Delta_\psi(A)\Delta_\psi(B) \geq \frac{1}{2}|\mathbb{E}_\psi(i[\hat{A}, \hat{B}])|$$

with equality if $(\hat{A} - \mathbb{E}_\psi(A)\hat{I})\psi = -i\lambda(\hat{B} - \mathbb{E}_\psi(B)\hat{I})\psi$, $\lambda \in \mathbb{R}/\{0\}$ or if ψ is an eigenstate of $\hat{A}$ or $\hat{B}$.

Exc.: Prove it.

Corollary

If two observables are canonically conjugate ($[\hat{A}, \hat{B}] = i\hbar\hat{I}$) then their mean-square deviations satisfy the inequality

$$\Delta_\psi(A)\Delta_\psi(B) \geq \frac{\hbar}{2}.$$

Continued

The equality (for $\hat{X}, \hat{P}$) is achieved by the Gaussian's wavepackets

$$\psi(x_1, x_2, x_3) = \prod_{j=1}^{3} \left(\frac{1}{2\pi(\Delta_\psi X_j)^2} \right)^{\frac{1}{4}} e^{-\left[\frac{(x_j - \mathbb{E}_\psi(X_j))}{2(\Delta_\psi X_j)} \right]^2} e^{\frac{i}{\hbar}(\mathbb{E}_\psi P_j) x_j}.$$

Exc.: Prove it in one-dimension.

Proposition (The “refined“ Heisenberg's Uncertainty Principle)

For $\psi \in C_0^\infty(\mathbb{R}^d)$ the following inequality holds

$$-\triangle \geq \frac{(d-2)^2}{4} \frac{1}{|X|^2}.$$

Theorem

Let $\psi \in \mathcal{D}(\hat{H}), \|\psi\| = 1$ be an eigenstate of the Schrödinger operator $\hat{H} = \hat{H}_0 + \hat{V}$ with homogeneous potential of degree ρ. Then

$$\mathbb{E}_\psi H_0 = \frac{\rho}{2} \mathbb{E}_\psi V.$$

Exc.: Apply it to the case of the one-dimensional quantum harmonic oscillator to find $\mathbb{E}_{\psi_n} V$ knowing $\mathbb{E}_{\psi_n} H$.

PART III

The classical harmonic oscillator

The equation of motion is

$$m\ddot{q}(t) + kq(t) = 0 \Rightarrow \ddot{q}(t) + \omega^2 q(t) = 0,\ \omega^2 = \frac{k}{m}$$

where ω is the angular frequency and the general solution is

$$q(t) = A\cos(\omega t + \phi)$$

The momentum and energy are given by

$$p(t) = m\dot{q}(t) = -Am\omega\sin(\omega t + \phi),\ E = \frac{1}{2}kA^2.$$

Using th initial conditions $p(0) = p_0$ and $q(0) = q_0$ we obtain

$$q(t) = q_0\cos(\omega t) + \frac{p_0}{m\omega}\sin(\omega t),\ p(t) = p_0\cos(\omega t) - q_0 m\omega\sin(\omega t).$$

Continued

The probability of finding the oscillating object in the interval $[x, x + dx]$ is

$$f_{cl}(x)dx = \frac{dt(x)}{T/2} = \frac{dx}{\pi\sqrt{A^2 - x^2}}$$

where $f_{cl}(x)$ is the classical probability density function.
Exc.: Show the second equality.

The quantum harmonic oscillator

The Schrödinger (or Hamiltonian) operator is

$$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{1}{2}k\hat{X}^2 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}k\hat{X}^2 = \hbar\omega(A^*A + \frac{1}{2})$$

where

$$A = \frac{1}{\sqrt{2}}(\xi + \frac{d}{d\xi}) = \frac{1}{\sqrt{2}}(aX + \frac{i}{\hbar a}P),\ A^* = \frac{1}{\sqrt{2}}(\xi - \frac{d}{d\xi})$$

A, A^* are the annihilation and creation operators correspondingly.
The domain of the Hamiltonian is the Schwartz space

$$\begin{aligned}\mathcal{D}(H) = S(\mathbb{R}) &= \{f \in C^\infty(\mathbb{R}) : sup_{x\in\mathbb{R}}|x^n(D^m f)(x)| < \infty, \forall m, n \in \mathbb{N}_0\} \\ &\subseteq L^2(\mathbb{R})\end{aligned}$$

Continued

The operators A, A^* satisfy the commutation relations

$$[A, A^*] = I,\ [N, A] = -A,\ [N, A^*] = A^*, N = A^*A$$

Note that If $N\psi = \lambda\psi$ with $\psi \neq 0$ then

- From $\|A\psi\|^2 \geq 0$ implies $\lambda \geq 0$ (boundedness from below).
- For $\lambda = 0$, $A\psi_0 = 0$ and for $\lambda > 0$, $A\psi \neq 0$ and $N(A\psi) = (\lambda - 1)A\psi$
- $A^*\psi \neq 0$ and $N(A^*\psi) = (\lambda + 1)A^*\psi$.
- $\sigma_p(N) = \mathbb{N}_0$.

Exc.: Show the second or third claim.

Continued

The eigenstates of the Hamiltonian are

$$\psi_n(x) = \frac{1}{\sqrt{n!}}(A^*)^n \psi_0(x),\ \psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}$$

the Hermite polynomials. They span the eigenspace with eigenvalues $E_n = \hbar\omega(n + \frac{1}{2})$, $n \in \mathbb{N}_0$. Using the isomorphism

$$L^2(\mathbb{R}, dq) \ni \psi = \sum_{n=0}^{\infty} c_n \psi_n \to c = \{c_n\}_{n\in\mathbb{N}} \in l^2$$

the annihilation and creation operators are represented by the semi-infinite matrices:

$$A = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & \cdots \\ 0 & 0 & 0 & \cdots & \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad A^* = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Correspondence with Classical Mechanics

Exc.: Justify the matrix representations of A and A^* from the previous transparency as well as those for X, P.

$$\begin{aligned} f_{qm}(x) &= |\psi_n(x)|^2 \overset{n>>1}{\sim} \frac{2\alpha}{\pi\sqrt{2n-\alpha^2x^2}} \cos^2\left[\left(2n+\frac{1}{2}\right)\frac{\alpha x}{\sqrt{2n}} - \frac{n\pi}{2}\right] \\ &\cong \frac{1}{\pi\sqrt{\frac{2n}{\alpha^2}-x^2}} = f_{cl}(x) \end{aligned}$$

Remark: Classically the particle is constrained into the interval $|x| \leq A = \sqrt{\frac{2E}{m\omega^2}}$ but quantum mechanically

$$\begin{aligned} P(X \in (-\infty, -\sqrt{\frac{\hbar}{m\omega}}] \cup [\sqrt{\frac{\hbar}{m\omega}}, \infty)) &= \int_{|x|\geq\sqrt{\frac{\hbar}{m\omega}}} |\psi_0(x)|^2 dx \\ &\simeq 0.1572992070 \end{aligned}$$

Thank you for your attention