QUANTUM MECHANICS NOTES

CARSON JAMES

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1. Hilbert Spaces

Note 1.1. In the notes we will consider a Hilbert Space \mathbb{H} with an inner product $\langle \cdot, \cdot \rangle$: $\mathbb{H} \times \mathbb{H} \to \mathbb{C}$ which is linear in the first argument and antilinear in the second argument.

Definition 1.2. Let \mathbb{H} be a Hilbert space and $A \in L(\mathbb{H})$. For each $x \in \mathbb{H}$, define $\phi_x \in \mathbb{H}^*$ by $\phi_x(y) = \langle Ay, x \rangle$. The Riesz representation theorem tells us that there exists $x' \in \mathbb{H}$ such that $\phi_x = \langle \cdot, x' \rangle$. Define $A^* \in L(\mathbb{H})$ by $A^*x = x'$. Thus for each $x, y \in \mathbb{H}$, we have that

$$\langle Ay, x \rangle = \langle y, A^*x \rangle$$

The linear operator A^* is called the **adjoint** of A.

Exercise 1.3. Let $A \in L(\mathbb{H})$. Then

- (1) for each $x, y \in \mathbb{H}$, $\langle x, Ay \rangle = \langle A^*x, y \rangle$.
- (2) $A^{**} = A$.

Proof.

(1) Let $x, y \in \mathbb{H}$. Then

$$\begin{split} \langle x, Ay \rangle &= \overline{\langle Ay, x \rangle} \\ &= \overline{\langle y, A^*x \rangle} \\ &= \langle A^*x, y \rangle \end{split}$$

(2) We have that for each $x, y \in \mathbb{H}$, $\langle Ay, x \rangle = \langle y, A^*x \rangle = \langle A^{**}y, x \rangle \rangle$. Hence for each $x, y \in \mathbb{H}$, $\langle (A - A^{**})y, x \rangle = 0$. This implies that $A - A^{**} = 0$ and thus $A = A^{**}$.

Definition 1.4. Let $A \in L(\mathbb{H})$. Then A is said to be **self-adjoint** if $A = A^*$.

Exercise 1.5. Let $A \in L(\mathbb{H})$. Suppose that A is self adjoint. Then

- (1) the eigenvalues of A are real.
- (2) the eigenvectors of distinct eigenvalues are orthogonal.

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Proof.

(1) Let $\lambda \in \mathbb{C}$, $x \in \mathbb{H}$. Suppose that $x \neq 0$ and $Ax = \lambda x$. Then

$$\lambda \langle x, x \rangle = \langle Ax, x \rangle$$

$$= \langle x, A^*x \rangle$$

$$= \langle x, Ax \rangle$$

$$= \overline{\langle Ax, x \rangle}$$

$$= \overline{\lambda \langle x, x \rangle}$$

$$= \overline{\lambda \langle x, x \rangle}$$

So $(\lambda - \overline{\lambda})\langle x, x \rangle = 0$. Since $x \neq 0$, $\langle x, x \rangle \neq 0$. Hence $\lambda = \overline{\lambda}$.

(2) Let $\lambda_1, \lambda_2 \in \mathbb{C}$ and $x_1, x_2 \in \mathbb{H}$. Suppose that $\lambda_1 \neq \lambda_2, x_1, x_2 \neq 0$, $Ax_1 = \lambda_1 x_1$ and $Ax_2 = \lambda_2 x_2$. Then

$$\lambda_{1}\langle x_{1}, x_{2}\rangle = \langle \lambda_{1}x_{1}, x_{2}\rangle$$

$$= \langle Ax_{1}, x_{2}\rangle$$

$$= \langle x_{1}, A^{*}x_{2}\rangle$$

$$= \langle x_{1}, Ax_{2}\rangle$$

$$= \langle x_{1}, \lambda_{2}x_{2}\rangle$$

$$= \overline{\lambda_{2}}\langle x_{1}, x_{2}\rangle$$

$$= \lambda_{2}\langle x_{1}, x_{2}\rangle \quad \text{by (1)}$$

So $(\lambda_1 - \lambda_2)\langle x_1, x_2 \rangle = 0$. Since $\lambda_1 \neq \lambda_2$, we have that $\langle x_1, x_2 \rangle = 0$.

Note 1.6. To show that $A \in L(\mathbb{H})$ is self-adjoint. It suffices to show that for each $x_1, x_2 \in \mathbb{H}$, $\langle Ax_1, x_2 \rangle = \langle x_1, Ax_2 \rangle$

2. Wave Mechanics

2.1. Schrodinger Equation.

Note 2.1. In what follows, we will take $\mathcal{R} = \mathbb{R}$ or $\mathcal{R} = \mathbb{R}^3$ and $\mathbb{H} = L^2(\mathcal{R}) \cap \mathcal{N}(\mathcal{R})$ where $\mathcal{N}(\mathcal{R})$ signifies the "nice" functions on \mathcal{R} . The inner product on \mathbb{H} is given by

$$\langle f, g \rangle = \int_{\mathcal{R}} f \overline{g} dm_{\mathcal{R}}$$

We will typically discuss functions (states of the system) $\psi \in \mathbb{H}$ given by $x \mapsto \psi(x)$. The evolution of the state of a system will be given by $\Psi : \mathcal{R} \times \mathbb{R} \to \mathbb{C}$ given by $(x,t) \mapsto \Psi(x,t)$ where for each $t \in \mathbb{R}$, $\Psi(\cdot,t) \in \mathbb{H}$. In these notes, the Laplace operator Δ is only spatial.

Exercise 2.2. Let $A \in L(\mathbb{H})$, $\lambda \in \mathbb{C}$ and $f = g + ih \in H \setminus \{0\}$. Suppose that $Af = \lambda f$. Then

(1)
$$Ag = \lambda g$$
 and $Ah = \lambda h$.

(2)
$$A\overline{f} = \lambda \overline{f}$$

Proof.

(1) Since A is linear,

$$Ag + iAh = Af$$

$$= \lambda f$$

$$= \lambda q + i\lambda h$$

Thus $Ag = \lambda g$ and $Ah = \lambda h$.

(2)

$$A\overline{f} = A(g - ih)$$

$$= Ag - iAh$$

$$= \lambda g - i\lambda h$$

$$= \lambda \overline{f}$$

Definition 2.3. For j = 1, 2, 3, define the j^{th} position operator $X_j \in L(\mathbb{H})$ by

 $[X_j f](x) = x_j f(x)$

.

Exercise 2.4. The j^{th} position operator X_j is self-adjoint.

Proof. Let $f, g \in \mathbb{H}$. Then and

$$\begin{split} \langle X_j f, g \rangle &= \int_{\mathcal{R}} x_j f(x) \overline{g(x)} dm_{\mathcal{R}}(x) \\ &= \int_{\mathcal{R}} f(x) x_j \overline{g(x)} dm_{\mathcal{R}}(x) \\ &= \int_{\mathcal{R}} f(x) \overline{x_j g(x)} dm_{\mathcal{R}}(x) \\ &= \langle f, X_j g \rangle \end{split}$$

Definition 2.5. For j = 1, 2, 3, define the j^{th} momentum operator $P_j \in L(\mathbb{H})$ by

$$P_j f = -i\hbar \frac{\partial f}{\partial x_j}$$

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Exercise 2.6. The j^{th} momentum operator P_j is self-adjoint.

Proof. We will assume the case $\mathcal{R} = \mathbb{R}^3$ since the case $\mathcal{R} = \mathbb{R}$ uses the same method. Let $f, g \in \mathbb{H}$. Then

$$\langle P_{j}f,g\rangle = \int_{\mathbb{R}^{3}} -i\hbar \frac{\partial f}{\partial x_{j}} \overline{g} dm^{3}$$

$$= \int_{\mathbb{R}^{2}} \int_{\mathbb{R}} -i\hbar \frac{\partial f}{\partial x_{j}}(x) \overline{g(x)} dm(x_{j}) dm^{2}(x_{j-})$$

$$= \int_{\mathbb{R}^{2}} \left(-i\hbar f(x) \overline{g(x)} \right]_{x_{j}=-\infty}^{x_{j}=\infty} - \int_{\mathbb{R}} -i\hbar f(x) \frac{\partial \overline{g}}{\partial x_{j}} dm(x_{j}) dm^{2}(x_{j-})$$

$$= \int_{\mathbb{R}^{2}} \int_{\mathbb{R}} f(x) i\hbar \frac{\partial \overline{g}}{\partial x_{j}} dm(x_{j}) dm^{2}(x_{j-})$$

$$= \int_{\mathbb{R}^{3}} f\left(-i\hbar \frac{\partial g}{\partial x_{j}} \right) dm^{3}$$

$$= \langle f, P_{j}g \rangle$$

Hence P_j is self-adjoint.

Note 2.7. Often instead of the operators X_1, X_2, X_3 and P_1, P_2, P_3 acting on functions f with $(x_1, x_2, x_3) \mapsto f(x_1, x_2, x_3)$ we write X, Y, Z and P_x, P_y, P_z acting on functions f with $(x, y, z) \mapsto f(x, y, z)$

Definition 2.8. Consider a particle of mass m with a "nice" potential energy $V : \mathcal{R} \to \mathbb{R}$ where V(x) signifies the potential energy of a particle at position x. We define the **Hamiltonian operator**, $H \in L(\mathbb{H})$, by

$$H = -\frac{\hbar^2}{2m}\Delta + VI$$

where I is the identity operator. Thus for each $x \in \mathcal{R}$,

$$[H\psi](x) = -\frac{\hbar^2}{2m}\Delta\psi(x) + V(x)\psi(x)$$

Exercise 2.9. The Hamiltonian operator H is self-adjoint. Hint: use Green's identity.

Proof. Let $f, g \in \mathbb{H}$. Then

$$\langle Hf, g \rangle = \int_{\mathcal{R}} \left[-\frac{\hbar^2}{2m} \Delta f(x) + V(x) f(x) \right] \overline{g}(x) dm_{\mathcal{R}}(x)$$

and

$$\langle f, Hg \rangle = \int_{\mathcal{R}} f(x) \left[-\frac{\hbar^2}{2m} \Delta \overline{g}(x) + V(x) \overline{g}(x) \right] dm_{\mathcal{R}}(x)$$

So

$$\langle Hf, g \rangle - \langle f, Hg \rangle = -\frac{\hbar^2}{2m} \int_{\mathcal{R}} \overline{g} \Delta f - f \Delta \overline{g} dm_{\mathcal{R}}$$

$$= -\frac{\hbar^2}{2m} \int_{\partial \mathcal{R}} \overline{g} \nabla_n f - f \nabla_n \overline{g} ds_{\mathcal{R}} \quad \text{(Green's identity)}$$

$$= 0$$

So $\langle Hf, g \rangle = \langle f, Hg \rangle$ and H is self-adjoint.

Definition 2.10. Suppose we have a system containing a particle with potential energy $V: \mathcal{R} \to \mathbb{R}$. Let $\psi \in \mathbb{H}$ and $\Psi: \mathcal{R} \times \mathbb{R} \to \mathbb{C}$. We say that ψ is a **state** (of the system) if

$$\langle \psi, \psi \rangle = \int_{\mathcal{R}} \psi(x) \overline{\psi(x)} dm_{\mathcal{R}}(x) = 1$$

We say that Ψ is a **wave function** (of the system) if for each $t \in \mathbb{R}$, $\Psi(\cdot, t) \in \mathbb{H}$ is a state of the system and for each $t \in \mathbb{R}$, Ψ satisfies the **Schrodinger equation**:

$$i\hbar \frac{\partial \Psi}{\partial t}(\cdot, t) = H\Psi(\cdot, t)$$

Note 2.11. Our interpretation of this model is the following: The wave function tells us the state of the system at each time $t \in \mathbb{R}$ and each state ψ of the system gives us the probability density of the position X of the particle via the relation:

$$\mathbb{P}(X \in A) = \int_{A} \psi \overline{\psi} dm_{\mathcal{R}}$$

The act of measuring a physical quantity of the state of the system, such as the energy, the momentum in the x direction, etc, correspond to applying a self-adjoint operator to the state. The eigenvalues of self-adjoint operators tell us the possible measurements of that physical quantity. We assume that the eigenvectors of our self-adjoint operator form an orthonormal basis for \mathbb{H} . If a system has a wavefunction Ψ and at time t, we measure a physical quantity corresponding to a self-adjoint operator A with distinct eigenvalues $(\lambda_j)_{j\in J}$ and corresponding eigen states (normalized eigenvectors) $(\psi_j)_{j\in J}$, then the probability of measuring the quantity λ_j , $\mathbb{P}(m(\Psi, A, t) = \lambda_j)$ is given by

$$\mathbb{P}(m(\Psi, A, t) = \lambda_j) = |\langle \Psi(\cdot, t), \psi_j \rangle|^2 = \left| \int_{\mathcal{R}} \Psi(x, t) \overline{\psi_j(x)} dm_{\mathcal{R}}(x) \right|^2$$

If for $j \in J$, we define $c_j : \mathbb{R} \to \mathbb{C}$ by

$$c_j(t) = \int_{\mathcal{R}} \Psi(x, t) \overline{\psi_j(x)} dm_{\mathcal{R}}(x)$$

then the expected value of the measurement at time t, $\langle A \rangle_t$, is given by

$$\langle A \rangle_t = \sum_{j \in J} \lambda_j |c_j(t)|^2$$