QUANTUM MECHANICS NOTES

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Contents

1. Introduction

1.1. Schrödinger Equation.

Definition 1.1. *A particle with potential energy $V(r,t)$ is completely decribed by its* ***position wavefunction*** $\Psi(r,t)$*, which satisfies the* ***Schrödinger equation****:*

$$i\hbar\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\Delta\Psi + V\Psi$$

Interpretation 1.2. *We interpret $|\Psi(r,t)|^2$ to be the* ***probability density*** *for the position, r, of the particle at time t. Therefore, we require that for each $t \in \mathbb{R}$,*

$$\int_{\mathbb{R}^n} \Psi(r,t)^*\Psi(r,t)dr = 1$$

1.2. Operators.

Definition 1.3. *We define the jth* ***position*** *and* ***momentum*** *coordinate operators X_j, P_j, (in position space) by*

$$X_j\Psi(r,t) = x_j\Psi(r,t)$$

and

$$P_j\Psi(r,t) = -i\hbar\frac{\partial}{\partial x_j}\Psi(r,t)$$

If the partical has potential energy $V(r,t)$, we define the ***Hamiltonian*** *operator, H, by*

$$H = \frac{P^2}{2m} + V$$

Thus the Schrödinger equation reads

$$i\hbar\frac{\partial}{\partial t}\Psi = H\Psi$$

Note 1.4. *If the potential energy doesn't depend on time, we may write*

$$H = \frac{P^2}{2m} + V(X)$$

meaning Hamiltonian only depends on the position and momentum operators, X and P. For the rest of these notes, we assume that the potential energy V does not depend on time.

Definition 1.5. *Let A and B be operators. Then B is said to be the **adjoint** of A if for each Ψ_1, Ψ_2,*

$$\langle \Psi_1 | A\Psi_2 \rangle = \langle B\Psi_1 | \Psi_2 \rangle$$

i.e.

$$\int_{\mathbb{R}^n} \Psi_1^*(A\Psi_2)dr = \int_{\mathbb{R}^n} (B\Psi_1)^*\Psi_2 dr$$

If B is the adjoint of A, we write

$$B = A^\dagger$$

Exercise 1.6. *Let A be an operator, then*

1. *for each Ψ_1, Ψ_2, $\langle A\Psi_1 | \Psi_2 \rangle = \langle \Psi_1 | A^\dagger \Psi_2 \rangle$*
2. *$(A^\dagger)^\dagger = A$*

Proof. (1) For wavefunctions Ψ_1, Ψ_2, we have

$$\begin{aligned}\langle A\Psi_1 | \Psi_2 \rangle &= \langle \Psi_2 | A\Psi_1 \rangle^* \\ &= \langle A^\dagger \Psi_2 | \Psi_1 \rangle^* \quad \text{(by definition)} \\ &= \langle \Psi_1 | A^\dagger \Psi_2 \rangle\end{aligned}$$

(2) For each Ψ_1, Ψ_2, we have that

$$\begin{aligned}\langle A\Psi_1 | \Psi_2 \rangle &= \langle \Psi_1 | A^\dagger \Psi_2 \rangle \\ &= \langle (A^\dagger)^\dagger \Psi_1 | \Psi_2 \rangle\end{aligned}$$

This implies that for each Ψ_1, Ψ_2,

$$\left\langle \left[A - (A^\dagger)^\dagger\right]\Psi_1, \Psi_2 \right\rangle = 0$$

Therefore for each Ψ_1,

$$\left[A - (A^\dagger)^\dagger\right]\Psi_1 = 0$$

Hence $\langle A - (A^\dagger)^\dagger = 0$ and $A = (A^\dagger)^\dagger$.

□

Definition 1.7. *An linear operator Q is **self-adjoint** if*

$$Q = Q^\dagger$$

Interpretation 1.8. *For each measurable, observable quantity $\hat{Q}$, there is a self-adjoint operator Q whose eigenvalues are the possible measurment values and whose eigenfunctions are the possible states of the system at measurment.*

Exercise 1.9. *The operators X_j, P_j and H are self adjoint.*

Proof. Since x_j is real, clearly

$$\langle \Psi_1 | X_j \Psi_2 \rangle = \langle X_j \Psi_1 | \Psi_2 \rangle$$

Similarly, we have that

$$\begin{aligned}
\langle \Psi_1 | P_j \Psi_2 \rangle &= \int_{\mathbb{R}^n} \Psi_1^* \Big(-i\hbar \frac{\partial}{\partial x_j} \Psi_2 \Big) dr \\
&= -i\hbar \int_{\mathbb{R}^n} \Psi_1^* \Big(\frac{\partial}{\partial x_j} \Psi_2 \Big) dr \\
&= i\hbar \int_{\mathbb{R}_n} \Big(\frac{\partial}{\partial x_j} \Psi_1^* \Big) \Psi_2 dr \qquad \text{(integration by parts)} \\
&= \int_{\mathbb{R}^n} \Big(-i\hbar \frac{\partial}{\partial x_j} \Psi_1 \Big)^* \Psi_2 dr \\
&= \langle P \Psi_1 | \Psi_2 \rangle
\end{aligned}$$

Finally

$$\begin{aligned}
\langle \Psi_1 | H \Psi_2 \rangle - \langle H \Psi_1 | \Psi_2 \rangle &= \int_{\mathbb{R}^n} \Psi_1^* \Big(-\frac{\hbar^2}{2m} \Delta \Psi_2 + V \Psi_2 \Big) dr - \int_{\mathbb{R}^n} \Big(-\frac{\hbar^2}{2m} \Delta \Psi_1 + V \Psi_1 \Big)^* \Psi_2 dr \\
&= \frac{\hbar^2}{2m} \int_{\mathbb{R}^n} (\Delta \Psi_1^*) \Psi_2 - \Psi_1^* (\Delta \Psi_2) dr \\
&= 0 \qquad \text{(Green's second identity)}
\end{aligned}$$

□

Exercise 1.10. *Let Q be a self-adjoint operator. Then*

1. *the eigenvalues of Q are real.*
2. *the eigenfunctions of Q corresponding to distinct eigenvalues are orthogonal.*

Proof.

1. Let λ be an eigenvalue of Q with corresponding eigenfunction Ψ. Then

$$\begin{aligned}
\lambda \langle \Psi | \Psi \rangle &= \langle \Psi | Q \Psi \rangle \\
&= \langle Q \Psi | \Psi \rangle \\
&= \lambda^* \langle \Psi | \Psi \rangle
\end{aligned}$$

Thus $\lambda = \lambda^*$ and is real

2. Let λ_1 and λ_2 be eigenvalues of Q with corresponding eigenfunctions Ψ_1 and Ψ_2. Suppose that $\lambda_1 \neq \lambda_2$. Then

$$\begin{aligned}
\lambda_2 \langle \Psi_1 | \Psi_2 \rangle &= \langle \Psi_1 | Q \Psi_2 \rangle \\
&= \langle Q \Psi_1 | \Psi_2 \rangle \\
&= \lambda_1 \langle \Psi_1 | \Psi_2 \rangle
\end{aligned}$$

So $(\lambda_2 - \lambda_1) \langle \Psi_1 | \Psi_2 \rangle = 0$. Which implies that $\langle \Psi_1 | \Psi_2 \rangle = 0$

□

Definition 1.11. *Let A and B be operators. The* ***commutator*** *of A and B, $[A, B]$, is defined by*

$$[A, B] = AB - BA$$

Exercise 1.12. *We have* $[X_j, P_j] = i\hbar$.

Proof. For a position wave function Ψ,

$$\begin{aligned}
[X_j, P_j]\Psi(r,t) &= [x_j, -i\hbar\frac{\partial}{\partial x_j}]\Psi(r,t) \\
&= (-i\hbar)\left[x_j\frac{\partial}{\partial x_j}\Psi(r,t) - \frac{\partial}{\partial x_j}x_j\Psi(r,t)\right] \\
&= (-i\hbar)\left[x_j\frac{\partial}{\partial x_j}\Psi(r,t) - \Psi(r,t) - x_j\frac{\partial}{\partial x_j}\Psi(r,t)\right] \\
&= i\hbar\Psi(r,t)
\end{aligned}$$

Hence $[X_j, P_j] = i\hbar$ □

1.3. **Continuity Equation.**

Exercise 1.13. *If* V *is real and* Ψ *satisfies the Schrödinger equation, then*

$$i\hbar\frac{\partial}{\partial t}\Psi^* = -H\Psi^*$$

Proof. We have that

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}\Psi^* &= \left(-i\hbar\frac{\partial}{\partial t}\Psi\right)^* \\
&= \left(-\left[-\frac{\hbar^2}{2m}\Delta\Psi + V\Psi\right]\right)^* \\
&= -\left[-\frac{\hbar^2}{2m}\Delta\Psi^* + V\Psi^*\right] \\
&= -H\Psi^*
\end{aligned}$$

□

Exercise 1.14. *We have that*

$$\frac{\partial}{\partial t}(\Psi^*\Psi) + \frac{\hbar}{2mi}\nabla\cdot\left[\Psi^*(\nabla\Psi) - (\nabla\Psi^*)\Psi\right] = 0$$

Proof.

$$\begin{aligned}
\frac{\partial}{\partial t}(\Psi^*\Psi) &= \left(\frac{\partial}{\partial t}\Psi^*\right)\Psi + \Psi^*\left(\frac{\partial}{\partial t}\Psi\right) \\
&= \left(\frac{\hbar}{2mi}(\Delta\Psi^*)\Psi - \frac{1}{i\hbar}V\Psi^*\Psi\right) + \left(-\frac{\hbar}{2mi}\Psi^*(\Delta\Psi) + \frac{1}{i\hbar}V\Psi^*\Psi\right) \\
&= \frac{\hbar}{2mi}\left[(\Delta\Psi^*)\Psi - \Psi^*(\Delta\Psi)\right] \\
&= -\frac{\hbar}{2mi}\left[\Psi^*(\Delta\Psi) - (\Delta\Psi^*)\Psi\right] \\
&= -\frac{\hbar}{2mi}\nabla\cdot\left[\Psi^*(\nabla\Psi) - (\nabla\Psi^*)\Psi\right]
\end{aligned}$$

Therefore
$$\frac{\partial}{\partial t}(\Psi^*\Psi) + \frac{\hbar}{2mi}\nabla \cdot \left[\Psi^*(\nabla\Psi) - (\nabla\Psi^*)\Psi\right] = 0$$
□

Definition 1.15. *We define the* ***probability current density****, j, of the particle to be*
$$j = \frac{\hbar}{2mi}\left[\Psi^*(\nabla\Psi) - (\nabla\Psi^*)\Psi\right]$$

1.4. Position and Momentum Space.

Definition 1.16. *We define the* ***momemtum wavefunction****, Φ, of the particle to be the Fourier transform of the position wavefunction:*
$$\begin{aligned}\Phi(p,t) &= F[\Psi](p,t) \\ &= \frac{1}{(2\pi\hbar)^{n/2}}\int_{\mathbb{R}^n}\Psi(r,t)e^{-i\frac{p\cdot r}{\hbar}}\,dr\end{aligned}$$

Note 1.17. *We recall the following facts about Fourier transforms:*

(1)
$$\Phi(p,t) = \frac{1}{(2\pi\hbar)^{n/2}}\int_{\mathbb{R}^n}\Psi(r,t)e^{-i\frac{p\cdot r}{\hbar}}\,dr$$
and
$$\Psi(r,t) = \frac{1}{(2\pi\hbar)^{n/2}}\int_{\mathbb{R}^n}\Phi(p,t)e^{i\frac{p\cdot r}{\hbar}}\,dp$$

(2)
$$F\left[\frac{\partial}{\partial x_j}\Psi\right] = \frac{ip_j}{\hbar}F[\Psi]$$
and
$$F^{-1}\left[\frac{\partial}{\partial p_j}\Phi\right] = -\frac{ix_j}{\hbar}F[\Psi]$$

(3)
$$\int_{\mathbb{R}^n}\Psi_1^*\Psi_2 dr = \int_{\mathbb{R}^n}F[\Psi_1]^*F[\Psi_2]dr$$

Note 1.18. *Let $Q(X,P)$ be a self-adjoint operator. Then the properties of the Fourier transform inmply that:*
$$Q(X,P) = \begin{cases} Q(x, -i\hbar\nabla) & \textit{(position space)} \\ Q(i\hbar\nabla, p) & \textit{(momentum space)}\end{cases}$$

Exercise 1.19. *If Ψ satisfies the Schrödinger equation, then Φ satisfies*
$$i\hbar\frac{\partial}{\partial t}\Phi = \frac{p^2}{2m}\Phi + V(i\hbar\nabla)\Phi$$

Proof. Starting with the Schrödinger equation, we have

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\Psi &= \left[\frac{P^2}{2m} + V(X)\right]\Psi \\ &= \left[\frac{-\hbar^2}{2m}\Delta + V(r)\right]\Psi \qquad \text{(position space)} \end{aligned}$$

Taking Fourier transforms of both sides, we see that

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\Phi &= \left[\frac{P^2}{2m} + V(X)\right]\Phi \\ &= \left[\frac{p^2}{2m} + V(i\hbar\nabla)\right]\Phi \qquad \text{(position space)} \end{aligned}$$

□

Interpretation 1.20. *We interpret $|\Phi(p,t)|^2$ to be the probability density for the momentum, p, of the particle at time t.*

Note 1.21. *For a self-adjoint operator $Q(X,P)$, the expected value of Q, is given by*

$$\langle Q\rangle = \begin{cases} \langle \Psi(r,t)|Q(r,-i\hbar\nabla)\Psi(r,t)\rangle & \textit{(position space)} \\ \langle \Phi(p,t)|Q(i\hbar\nabla,p)\Phi(p,t)\rangle & \textit{(momentum space)} \end{cases}$$

1.5. **Stationary States.**

Definition 1.22. *When the potential energy V doesn't depend on time, we look for solutions to the Schrödinger equation of the form*

$$\Psi(r,t) = \psi(r)\varphi(t)$$

With a closer look, we find that

(1) $H\psi = E\psi$
(2) $\varphi(t) = e^{-i\frac{E}{\hbar}t}$

*Eigenfuntions of the Hamiltonian operator are called **stationary states**. If the possible eigenvalues for the Hamiltonian operator are discreet $(E_n)_{n\in\mathbb{N}}$ with stationary states $(\psi_n)_{n\in\mathbb{N}}$, then the general solution to the Schrödinger equation is*

$$\Psi(r,t) = \sum_{n\in\mathbb{N}} c_n\psi_n(r)e^{-i\frac{E_n}{\hbar}t}$$

where

$$c_n = \int_{\mathbb{R}^n} \psi_n^*(r)\Psi(r,0)dr$$

Definition 1.23. *If the spectrum of the Hamiltonian is discreet, the stationary state with the least energy is called the **ground state**. The stationary states that are not the ground state are called **excited states**.*

2. Fundamental Examples in One Dimension

2.1. The Harmonic Oscillator.

Definition 2.1. *The **harmonic oscillator** in one dimension is defined by the potential energy:*

$$V(x) = \frac{1}{2}m\omega^2 x^2$$

*We define the **lowering operator**, a, by*

$$a = \frac{1}{\sqrt{2\hbar m\omega}}\Big(m\omega X + iP\Big)$$

Exercise 2.2. *The adjoint of the lowering operator is*

$$a^\dagger = \frac{1}{\sqrt{2\hbar m\omega}}\Big(m\omega X - iP\Big)$$

Proof. For a wave functions Ψ_1, Ψ_2,

$$\begin{aligned}\int_{\mathbb{R}}\left[\frac{1}{\sqrt{2\hbar m\omega}}\Big(m\omega X - iP\Big)\Psi_1\right]^*\Psi_2 dx &= \frac{1}{\sqrt{2\hbar m\omega}}\int_{\mathbb{R}}(m\omega x\Psi_1(x,t)^*\Psi_2(x,t) - \hbar\left(\frac{\partial}{\partial x}\Psi_1(x,t)^*\right)\Psi_2(x,t)dx \\ &= \frac{1}{\sqrt{2\hbar m\omega}}\int_{\mathbb{R}}(m\omega x\Psi_1(x,t)^*\Psi_2(x,t) + \hbar\Psi_1(x,t)^*\left(\frac{\partial}{\partial x}\Psi_2(x,t)\right)dx \\ &= \int_{\mathbb{R}}\Psi_1^*\left[\frac{1}{\sqrt{2\hbar m\omega}}\Big(m\omega X + iP\Big)\Psi_2\right]dx\end{aligned}$$

□

Definition 2.3. *We call $a^\dagger$ the **raising operator** and together, a and $a^\dagger$ are called the ladder operators.*

Exercise 2.4. *We have that*

(1) $aa^\dagger = \frac{1}{\hbar\omega}H + \frac{1}{2}$
(2) $a^\dagger a = \frac{1}{\hbar\omega}H - \frac{1}{2}$
(3) $[a, a^\dagger] = 1$

Proof. (1)

$$\begin{aligned}aa^\dagger &= \frac{1}{2\hbar m\omega}\big(m\omega X + iP\big)\big(m\omega X - iP\big) \\ &= \frac{1}{2\hbar m\omega}\Big[\big(m^2\omega^2X^2 + P^2\big) - m\omega i\big(XP - PX\big)\Big] \\ &= \frac{1}{\hbar\omega}\big(\frac{1}{2m}P^2 + \frac{1}{2}m\omega^2X^2\big) - \frac{i}{2\hbar}[X, P] \\ &= \frac{1}{\hbar\omega}H + \frac{1}{2}\end{aligned}$$

(2) Similar
(3) Trivial

□

Exercise 2.5. *If $H\psi = E\psi$, then*

(1) $Ha\psi = (E - \hbar\omega)a\psi$
(2) $Ha^\dagger\psi = (E + \hbar\omega)a^\dagger\psi$

Proof.

(1)

$$\begin{aligned} Ha\psi &= \hbar\omega\left(aa^\dagger - \frac{1}{2}\right)a\psi \\ &= \hbar\omega\left(aa^\dagger a - \frac{1}{2}a\right)\psi \\ &= \hbar\omega a\left(a^\dagger a - \frac{1}{2}\right)\psi \\ &= \hbar\omega a\left(a^\dagger a + \frac{1}{2} - 1\right)\psi \\ &= \hbar\omega a\left(\frac{1}{\hbar\omega}H - 1\right)\psi \\ &= aH\psi - \hbar\omega a\psi \\ &= (E - \hbar\omega)a\psi \end{aligned}$$

(2) Similar

$\square$

Interpretation 2.6. *The lowering operator "lowers" a stationary state ψ with energy E to a stationary state $a\psi$ with energy $E - \hbar\omega$ and the raising operator "raises" a stationary state ψ with energy E to a stationary state $a^\dagger\psi$ with energy $E + \hbar\omega$.*

Definition 2.7. *Since the zero function is a solution to the time-independent Schrödinger equation, we define the ground state, ψ_0 of the harmonic oscillator to be the stationary state that satisfies $a\psi_0 = 0$. The excited states ψ_n, for $n \geq 1$, are obtained by applying the rasing operator n times and then normalizing.*

Exercise 2.8. *We have that*

(1) $\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}$
(2) $E_0 = \frac{1}{2}\hbar\omega$
(3) $\psi_n = c_n(a^\dagger)^n\psi_0$ *(for some constant c_n)*
(4) $E_n = \hbar\omega(n + \frac{1}{2})$

Proof.

(1) The simple differential equation $a\psi_0 = 0$ has the solution

$$\psi_0 = Ae^{-\frac{m\omega}{2\hbar}x^2}$$

Thus

$$|\psi_0|^2 = |A|^2 e^{-\frac{m\omega}{\hbar}x^2}$$

If we normalize this function, we obtain

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

(2) It is tedious but straightforward to show that

$$H\psi_0 = \frac{1}{2}\hbar\omega\psi_0$$

(3) Clear by definition.
(4) Clear by previous exercise.

□

Exercise 2.9.
(1) $\psi_{n+1} = \frac{1}{\sqrt{n+1}} a^\dagger \psi_n$
(2) $\psi_{n-1} = \frac{1}{\sqrt{n}} a\psi_n$
Hint: use the adjoint-ness of a and $a^\dagger$

Proof.
(1)

$$\begin{aligned} aa^\dagger\psi_n &= \left(\frac{1}{\hbar\omega}H + \frac{1}{2}\right)\psi_n \\ &= \frac{1}{\hbar\omega}E_n\psi_n + \frac{1}{2}\psi_n \\ &= (n+1)\psi_n \end{aligned}$$

Since $\psi_{n+1} = ca^\dagger\psi_n$, we have that

$$\begin{aligned} 1 &= \langle\psi_{n+1}|\psi_{n+1}\rangle \\ &= \langle ca^\dagger\psi_n|ca^\dagger\psi_n\rangle \\ &= |c|^2\langle a^\dagger\psi_n|a^\dagger\psi_n\rangle \\ &= |c|^2\langle aa^\dagger\psi_n|\psi_n\rangle \\ &= |c|^2\langle (n+1)\psi_n|\psi_n\rangle \\ &= |c|^2(n+1)\langle\psi_n|\psi_n\rangle \\ &= |c|^2(n+1) \end{aligned}$$

So $c = \frac{1}{\sqrt{n+1}}$
(2) Similar to (1).

□

Exercise 2.10. *The n^{th} stationary state is given by* $\psi_n = \frac{1}{\sqrt{n!}}(a^\dagger)^n\psi_0$

Proof. Clear by induction. □

Exercise 2.11. *Show that*
(1) $\psi_1(x) = \left(\frac{4m^3\omega^3}{\hbar^3\pi}\right)xe^{-\frac{m\omega}{2\hbar}x^2}$
(2) $E_1 = \frac{3}{2}\hbar\omega$

Proof. Straightforward. □

Exercise 2.12. *If particle one is in state ψ_0 at time $t = 0$, then the momentum wave function is*

$$\Phi(p,t) = \left(\frac{1}{m\omega\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{1}{2m\omega\hbar}p^2} e^{-i\frac{\omega}{2}t}$$

Proof. By assumption

$$\Psi(x,t) = \psi_0(x)e^{-i\frac{\omega}{2}t}$$

Thus

$$\Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{\mathbb{R}} \Psi(x,t)e^{-i\frac{px}{\hbar}}\, dx$$

The rest is straightforward. □

3. Fundamental Examples in Three Dimensions