QUANTUM MECHANICS NOTES

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1. Introduction

1.1. Schrödinger Equation.

Definition 1.1. *A particle with potential energy $V(x,t)$ is completely decribed by its* ***position wavefunction*** *$\Psi(x,t)$, 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 $|\Psi(x,t)|^2$ to be the* ***probability density*** *for the position, x, of the particle at time t. Therefore, we require that for each $t \in \mathbb{R}$,*

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

1.2. Operators.

Definition 1.3. *We define the j^{th}* ***position*** *and* ***momentum coordinate operators*** *X_j, P_j, (in position space) by*

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

and

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

We define the ***position*** *and* ***momentum*** *operators, X and P, by*

$$X = (X_1, X_2, \cdots, X_n)$$

and

$$P = (P_1, P_2, \cdots, P_n)$$

We denote $P \cdot P$ by P^2. Note that

$$P^2 = -\hbar^2\Delta$$

If the partical has potential energy $V(x,t)$, 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.

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

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.*
Hint: for H, use Green's second identity.

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

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

Finally

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

□

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,

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

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*

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

Proof.

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

Therefore

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

□

Definition 1.15. *We define the **probability current density**, j, of the particle to be*

$$j = \frac{\hbar}{2mi}\Big[\Psi^*(\nabla\Psi) - (\nabla\Psi^*)\Psi\Big]$$

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:*

$$\begin{aligned}
\Phi(p,t) &= F[\Psi](p,t) \\
&= \frac{1}{(2\pi\hbar)^{n/2}}\int_{\mathbb{R}^n} \Psi(x,t)e^{-i\frac{p\cdot x}{\hbar}}\,dx
\end{aligned}$$

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

(1)

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

and

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

(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)

$$\int_{\mathbb{R}^n} \Psi_1^* \Psi_2 dx = \int_{\mathbb{R}^n} F[\Psi_1]^* F[\Psi_2] dx$$

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

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

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*

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

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*

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

With a closer look, we find that

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

Statement (1) *is referred to as the* ***time-independent Schrödinger equation****. 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*

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

where

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

Definition 1.23. *An energy eiganvalue E_n of H is said to have a* ***degeneracy of degree*** *k if it corresponds to k orthonomal stationary states.*

Note 1.24. *If the energy eigenvalues $(E_n)_{n\in\mathbb{N}}$ have degeneracies of degrees $(k_n)_{n\in\mathbb{N}}$ with corresponding orthonormal stationary states $(\psi_{n,j})_{j=1}^{k_n}$ and*

$$\Psi(x,t) = \sum_{n\in\mathbb{N}} \sum_{j=1}^{k_n} c_{n,j}\psi_{n,j}(x) e^{-i\frac{E_n}{\hbar}t}$$

Then the probability of measuring the energy E_n is

$$\mathbb{P}(E_n) = \sum_{j=1}^{k_n} |c_{n,j}|^2$$

Definition 1.25. *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 Infinite Square Well.**

Definition 2.1. *The infinite square well is defined by the potential*

$$V(x) = \begin{cases} \infty & x \in I_1 = (-\infty, a] \\ 0 & x \in I_2 = (0,a) \\ \infty & x \in I_3 = [a, \infty) \end{cases}$$

Exercise 2.2. *By starting with a finite potental well and letting the height of the well go to infinity, show that the stationary states and their energies are given by*

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right) & x \in (0,a) \\ 0 & x \notin (0,a) \end{cases}$$

and

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

Proof. Define

$$V_\alpha(x) = \begin{cases} \alpha & x \in I_1 \\ 0 & x \in I_2 \\ \alpha & x \in I_3 \end{cases}$$

For the potential energy V_α, in sections I_1, I_3 the Schrödinger equation may be written as

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = \frac{2m}{\hbar^2}(\alpha - E)\psi$$

Assuming $\alpha > E$, we may write $l = \frac{\sqrt{2m(\alpha-E)}}{\hbar}$ and substitute to get

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = l^2\psi$$

Thus in region I_1, $\psi_1(x) = Ae^{lx} + Be^{-lx}$ and in region I_3, $\psi_3(x) = Fe^{lx} + Ge^{-lx}$. Since e^{-lx} blows up as $x \to -\infty$, $B = 0$. Since e^{lx} blows up as $x \to \infty$, $F = 0$.

In section I_2, the Schrödinger equation may be written as

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -\frac{2mE}{\hbar^2}\psi$$

We write $k = \frac{\sqrt{2mE}}{\hbar}$ and substitute to get

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -k^2\psi$$

Hence in region I_2, $\psi_2(x) = C\sin(kx) + D\cos(kx)$.

So far we have

$$\psi_\alpha(x) = \begin{cases} Ae^{lx} & x \in I_1 \\ C\sin(kx) + D\cos(kx) & x \in I_2 \\ Ge^{-lx} & x \in I_3 \end{cases}$$

To find possible wavefunctions ψ for the infinite potential, we let $\alpha \to \infty$. As $\alpha \to \infty$, we have that $l \to \infty$. Hence $\psi_1 \to 0$ and $\psi_3 \to 0$. So for the infinite potential,

$$\psi(x) = \begin{cases} C\sin(kx) + D\cos(kx) & x \in (0, a) \\ 0 & x \notin (0, a) \end{cases}$$

By continuity at the points $x = 0$ and $x = a$, we see that $0 = C\sin(0) + D\cos(0)$ which imples that $D = 0$ and $0 = C\sin(ka)$ which yields various solutions

$$k_n = \frac{n\pi}{a} \qquad n \in \mathbb{Z}$$

To avoid non-normalizable solutions or linearly dependent solutions, we restrict $n \in \mathbb{N}$. Our energies are then

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2ma^2} \qquad n \in \mathbb{N}$$

and (after normalizing) our stationary states are

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right) & x \in (0, a) \\ 0 & x \notin (0, a) \end{cases}$$

$\square$

2.2. **The Harmonic Oscillator.**

Definition 2.3. *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 2.4. *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,

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

∎

Definition 2.5. *We call $a^\dagger$ the* ***raising operator*** *and together, a and $a^\dagger$ are called the ladder operators.*

Exercise 2.6. *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 2.7. *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

□

Interpretation 2.8. *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 2.9. *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 2.10. *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)
$$\psi_n = c_n(a^\dagger)^n\psi_0 \quad (\textit{for some constant } c_n)$$

(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 2.11.
(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 2.12. *The n^{th} stationary state is given by $\psi_n = \frac{1}{\sqrt{n!}}(a^\dagger)^n\psi_0$*

Proof. Clear by induction. □

Exercise 2.13. *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 2.14. *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

3.1. **Spherical Coordinates.**

Definition 3.1. *We now set $n = 3$, and work with spherical coordinates (r, θ, ϕ) where r is the distance in from the origin, $0 \le \theta \le \pi$ is the angle with initial side on the positive z-axis, and $0 \le \phi < 2\pi$ is the angle in the x-y plane with initial side on the positive x-axis going towards the positive y-axis.*

Proposition 3.2. *In spherical coordinates, the time independent Schrödinger equation becomes*

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi + V\psi = E\psi$$

Definition 3.3. *If the potential energy V only depends on r, then we can solve for stationary solutions of the form $\psi(r,\theta,\phi) = R(r), Y(\theta,\phi)$. It results that there is some constant l such that*

(1)
$$\frac{1}{R}\frac{d}{dr}r^2\frac{dR}{dr} - \frac{2m}{\hbar^2}r^2(V - E) = l(l+1)$$

(2)
$$\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right] = -l(l+1)$$

The number l is called the ***azimuthal quantum number****, equation* (1) *is called the* ***radial equation*** *and equation* (2) *is called the* ***angular equation****.*

Definition 3.4. *We can look for solutions to the angular equation of the form $Y(\theta,\phi) = \Theta(\theta)\Phi(\phi)$. It results that there is some constant m such that*

(1)
$$\frac{1}{\Theta}\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + l(l+1)\sin^2\theta = m^2$$

(2)
$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2$$

Equation (2) has the solution

$$\Phi(\phi) = e^{im\phi}$$

Since (r, θ, ϕ) is the same point in space as $(r, \theta, \phi + 2\pi)$, we require that $\Phi(\phi) = \Phi(\phi + 2\pi)$. This implies that $m \in \mathbb{Z}$. The integer m is called the ***magnetic quantum number****.*

If $l \in \mathbb{N}_0$ and $m \leq l$, then equation (1) has the solution

$$\Theta(\theta) = AP_l^m(\cos\theta)$$

where P_l^m is the ***associated Legendre*** *function given by*

$$P_l^m(x) = (1 - x^2)^{\frac{|m|}{2}} \left(\frac{d}{dx}\right)^{|m|} P_l(x)$$

and $P_l(x)$ is the l^{th} ***Legendre polynomial*** *defined by*

$$P_l(x) = \frac{1}{2^l l!} \left(\frac{d}{dx}\right)^l (x^2 - 1)^l$$

The angular function $Y_l^m(\theta, \phi) = A_l^m P_l^m(\cos\theta)e^{im\phi}$ may be normalized by setting

$$A_l^m = \epsilon \sqrt{\frac{(2l+1)}{4\pi} \frac{(l - |m|)!}{(l + |m|)!}}$$

where

$$\epsilon = \begin{cases} (-1)^m & m \geq 0 \\ 1 & m < 0 \end{cases}$$

The normalized angular functions are called ***spherical harmonics****.*

Exercise 3.5. *Compute some spherical harmonics.*

Definition 3.6. *If we make the substitution $u(r) = rR(r)$, we may rewrite the radial equation as*

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu$$

which looks like the one dimensional Schrödinger equation. The function

$$V + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}$$

is called the ***effective potential****.*

3.2. **Spherical Harmonic Oscillator (Cartesian Coordinates).**

Definition 3.7. *The spherical harmonic oscillator (in cartesian coordinates) is defined by the potential energy*

$$V(x, y, z) = x^2 + y^2 + z^2$$

Exercise 3.8. *In cartesian coordinates, the the stationary states of the harmonic oscillator are given by*

$$\psi_{n_x,n_y,n_z}(x, y, z) = \psi_{n_x}(x)\psi_{n_y}(y)\psi_{n_z}(z)$$

with energies

$$E_{n_x,n_y,n_z} = \hbar\omega\left(n_x + n_y + n_z + \frac{3}{2}\right)$$

where $\psi_{n_x}, \psi_{n_y}, \psi_{n_z}$ are stationary states for the one dimensional harmonic oscillator.

Proof. We look for solutions of the form $\psi(x,y,z) = \psi_x(x)\psi_y(y)\psi_z(z)$. Plugging this into the time-independent Schrödinger equation, we get

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi_x}{\partial x^2}\psi_y\psi_z + \psi_x\frac{\partial^2\psi_y}{\partial y^2}\psi_z + \psi_x\psi_y\frac{\partial^2\psi_z}{\partial z^2}\right] + \frac{1}{2}m\omega^2(x^2+y^2+x^2)\psi = E\psi$$

Dividing both sides by ψ and rearranging, we obtain

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi_x}{\partial x^2}\frac{1}{\psi_x}+\frac{1}{2}m\omega^2x^2\right)+\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi_y}{\partial y^2}\frac{1}{\psi_y}+\frac{1}{2}m\omega^2y^2\right)+\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi_z}{\partial z^2}\frac{1}{\psi_z}+\frac{1}{2}m\omega^2z^2\right) = E$$

Thus each part is constant and we may write

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_x}{\partial x^2} + \frac{1}{2}m\omega^2x^2\psi_x = E_x\psi_x$$
$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_y}{\partial y^2} + \frac{1}{2}m\omega^2y^2\psi_y = E_y\psi_y$$
$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_z}{\partial z^2} + \frac{1}{2}m\omega^2z^2\psi_z = E_z\psi_z$$

So we have three one-dimensional harmonic oscillators and we have

$$\psi_x = \psi_{n_x} = \frac{1}{\sqrt{n_x!}}(a^\dagger)^{n_x}\psi_0 \text{ and } E_x = E_{n_x} = \hbar\omega\left(n_x+\frac{1}{2}\right)$$
$$\psi_y = \psi_{n_y} = \frac{1}{\sqrt{n_y!}}(a^\dagger)^{n_y}\psi_0 \text{ and } E_y = E_{n_y} = \hbar\omega\left(n_y+\frac{1}{2}\right)$$
$$\psi_z = \psi_{n_z} = \frac{1}{\sqrt{n_z!}}(a^\dagger)^{n_z}\psi_0 \text{ and } E_z = E_{n_z} = \hbar\omega\left(n_z+\frac{1}{2}\right)$$

Thus

$$\psi = \psi_{n_x,n_y,n_z}(x,y,z) = \psi_{n_x}(x)\psi_{n_y}(y)\psi_{n_z}(z)$$

with energy

$$E = E_{n_x,n_y,n_z} = \hbar\omega\left(n_x+n_y+n_z+\frac{3}{2}\right)$$

□

Exercise 3.9. *Show that the degeneracy of E_n is*

$$deg(E_n) = \binom{n+2}{2}$$

Proof. Stars and bars □

Interpretation 3.10. *The energies of the three-dimensional harmonic oscillator are given by $E_n = \hbar\omega\left(n+\frac{3}{2}\right)$ which correspond to $\binom{n+2}{2}$ stationary states.*

3.3. **Spherical Harmonic Oscillator (Spherical Coordinates).**

Definition 3.11. *The spherical harmonic oscillator (in spherical coordinates) is defined by the potential energy*

$$V(r) = r^2$$

Exercise 3.12. *Making the substitution $\kappa = \frac{\sqrt{2mE}}{\hbar}$, we can rewrite the radial equation for the harmonic oscillator as*

$$\frac{1}{\kappa^2}\frac{\mathrm{d}^2 u}{\mathrm{d}r^2} = \left[\frac{\hbar^2\omega^2(\kappa r)^2}{2^2 E^2} + \frac{l(l+1)}{(\kappa r)^2} - 1\right]u$$

Proof. Straightforward ∎

Exercise 3.13. *Making the substitution $\rho = \kappa r$ and $\rho_0 = \frac{\hbar\omega}{2E}$, we can rewrite the radial equation as*

$$\frac{1}{\kappa^2}\frac{\mathrm{d}^2 u}{\mathrm{d}r^2} = \left[\rho_0^2\rho^2 + \frac{l(l+1)}{\rho^2} - 1\right]u$$

Proof. Straightforward. ∎

Exercise 3.14. *We have*

$$\frac{\mathrm{d}^2 u}{\mathrm{d}\rho^2} = \frac{1}{\kappa^2}\frac{\mathrm{d}^2 u}{\mathrm{d}r^2}$$

and thus we may rewrite the radial equation as

$$\frac{\mathrm{d}^2 u}{\mathrm{d}\rho^2} = \left[\rho_0^2\rho^2 + \frac{l(l+1)}{\rho^2} - 1\right]u$$

Proof. Straightforward by chain-rule. ∎

Exercise 3.15. *As $\rho \to \infty$, $u \approx e^{-\frac{\rho_0}{2}\rho^2}$*

Proof. As $\rho \to \infty$,

$$\frac{\mathrm{d}^2 u}{\mathrm{d}\rho^2} \approx \rho_0^2\rho^2 u$$

Trying the function $u(\rho) = e^{-\frac{\rho_0}{2}\rho^2}$, we see that

$$\begin{aligned}\frac{\mathrm{d}^2 u}{\mathrm{d}\rho^2} &= (\rho_0^2\rho^2 - \rho_0)e^{-\frac{\rho_0}{2}\rho^2} \\ &\approx \rho_0^2\rho^2 e^{-\frac{\rho_0}{2}\rho^2} \qquad (\text{as } \rho \to \infty) \\ &= \rho_0^2\rho^2 u\end{aligned}$$

∎

Exercise 3.16. *As $\rho \to 0$, $u \approx \rho^{l+1}$*

Proof. As $\rho \to 0$,

$$\frac{\mathrm{d}^2 u}{\mathrm{d}\rho^2} \approx \frac{l(l+1)}{\rho^2}u$$

Trying the function $u(\rho) = \rho^{l+1}$, we see that

$$\begin{aligned}\frac{\mathrm{d}^2 u}{\mathrm{d}\rho^2} &= l(l+1)\rho^{l-1} \\ &= \frac{l(l+1)}{\rho^2} u\end{aligned}$$

□

Note 3.17. *We can now, "glue" these functions together with a third unknown function $v(\rho)$ to obtain the prototype solution*

$$u(\rho) = \rho^{l+1} e^{-\frac{\rho_0}{2}\rho^2} v(\rho)$$

Exercise 3.18. *Suppose that for some nice function $v(\rho)$,*

$$u(\rho) = \rho^{l+1} e^{-\frac{\rho_0}{2}\rho^2} v(\rho)$$

Then computing $\frac{\mathrm{d}^2 u}{\mathrm{d}\rho^2}$ and plugging into the radial equation and simplifying, we obtain the relation

$$\rho \frac{\mathrm{d}^2 v}{\mathrm{d}\rho^2} + 2(l + 1 - \rho_0 \rho^2) \frac{\mathrm{d}v}{\mathrm{d}\rho} + \rho(1 - \rho_0(2l+3))v = 0$$

Proof. Very tedious but straightforward. □

Exercise 3.19. *If $v(\rho)$ can be represented by a power series*

$$v(\rho) = \sum_{j=0}^{\infty} c_j \rho^j$$

then plugging in $v(\rho)$ into the previous relation combining like terms and solving for the coefficients yields the relations

$$c_1 = 0$$

and

$$c_{j+2} = \left[\frac{\rho_0(2j + 2l + 3) - 1}{(j+2)(j+2l+3)}\right] c_j \quad j \geq 0$$

This implies that for each odd j, $c_j = 0$.

Proof. Tedious but straightforward. □

Exercise 3.20. *If for each $j \geq 0$, $c_{2j} \neq 0$, then v behaves asymptotically like $e^{\rho_0 \rho^2}$. Thus $u(\rho)$ behaves asymptotically like $\rho^{l+1} e^{\frac{\rho_0}{2}\rho^2}$. This implies that $R(r)$ is not normalizable. Therefore there exists $j_{max} \geq 0$ such that $c_{2j+2} = 0$ and $v(\rho)$ is a polynomial of degree $2j_{max}$ and consists of only even powers of ρ.*

Proof. As $j \to \infty$, $c_{j+2} \approx \frac{2\rho_0}{j} c_j$. Hence $v(\rho)$ behaves asymptotically like

$$\begin{aligned}\sum_{j=0}^{\infty} \frac{2^j \rho_0^j}{\prod_{k=1}^{j} 2k} \rho^{2j} &= \sum_{j=0}^{\infty} \frac{(\sqrt{\rho_0}\rho)^{2j}}{j!} \\ &= e^{(\sqrt{\rho_0}\rho)^2} \\ &= e^{\rho_0 \rho^2}\end{aligned}$$

□

3.4. **The Infinite Spherical Box.**

3.5. **The Hydrogen Atom.**

3.6. **Orbital Angular Momentum.**