

QUANTUM MECHANICS NOTES

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1. MATHEMATICAL BACKGROUND

1.1. Hilbert Spaces.

Definition 1.1. Let H be a vector space and $\langle \cdot | \cdot \rangle : H \times H \rightarrow \mathbb{C}$. Then H is said to be an **inner product space** with inner product $\langle \cdot | \cdot \rangle$ if for each $\Psi_1, \Psi_2, \Psi_3 \in H$ and $c \in \mathbb{C}$

- (1) $\langle \Psi_1 | \Psi_2 + c\Psi_3 \rangle = \langle \Psi_1 | \Psi_2 \rangle + c\langle \Psi_1 | \Psi_3 \rangle$
- (2) $\langle \Psi_1 | \Psi_2 \rangle = \langle \Psi_2 | \Psi_1 \rangle^*$

- (3) $\langle \Psi_1 | \Psi_1 \rangle \geq 0$
 (4) if $\langle \Psi_1 | \Psi_1 \rangle = 0$, then $\Psi_1 = 0$.

Note 1.2. For the rest of this section, we assume that H is an inner product space with inner product $\langle \cdot | \cdot \rangle$.

Exercise 1.3. Let $(\Psi_j)_{j=1}^n \subset H$. Then

$$\left\langle \sum_{i=1}^n \Psi_i \middle| \sum_{j=1}^n \Psi_j \right\rangle = \sum_{i=1}^n \sum_{j=1}^n \langle \Psi_i | \Psi_j \rangle$$

Definition 1.4. Let $\Psi_1, \Psi_2 \in H$ and $S \subset H$. Then Ψ_1 and Ψ_2 are said to be **orthogonal** if $\langle \Psi_1 | \Psi_2 \rangle = 0$ and S is said to be **orthogonal** if for each $\Psi_1, \Psi_2 \in S$, Ψ_1, Ψ_2 are orthogonal.

Exercise 1.5. Let $S \subset H$. Suppose that $0 \notin S$. If S is orthogonal, then S is linearly independent.

Proof. Let $\Psi_1, \dots, \Psi_n \in S$ and $c_1, \dots, c_n \in \mathbb{C}$. Suppose that $\sum_{j=1}^n c_j \Psi_j = 0$. Then

$$\begin{aligned} 0 &= \left\langle \sum_{i=1}^n c_i \Psi_i \middle| \sum_{j=1}^n c_j \Psi_j \right\rangle \\ &= \sum_{i=1}^n \sum_{j=1}^n c_i \overline{c_j} \langle \Psi_i | \Psi_j \rangle \\ &= \sum_{j=1}^n |c_j|^2 \langle \Psi_j | \Psi_j \rangle \end{aligned}$$

So for $j = 1, \dots, n$, $c_j = 0$ and S is linearly independent. □

Proof. Clear. □

Theorem 1.6. (Cauchy-Schwarz Inequality):

Let $\Psi_1, \Psi_2 \in H$. Then $\langle \Psi_1 | \Psi_2 \rangle^2 \leq \langle \Psi_1 | \Psi_1 \rangle \langle \Psi_2 | \Psi_2 \rangle$

Exercise 1.7. Define $\| \cdot \| : H \rightarrow \mathbb{R}_{\geq 0}$ by

$$\| \Psi_1 \| = \langle \Psi_1 | \Psi_1 \rangle^{1/2}$$

Then $\| \cdot \|$ is a norm on H .

Proof. The only nontriviality needed to be shown is the triangle inequality. To see this, we observe that

$$\begin{aligned} \| \Psi_1 + \Psi_2 \|^2 &= \langle \Psi_1 + \Psi_2 | \Psi_1 + \Psi_2 \rangle \\ &= \langle \Psi_1 | \Psi_1 \rangle + \langle \Psi_1 | \Psi_2 \rangle + \langle \Psi_2 | \Psi_1 \rangle + \langle \Psi_2 | \Psi_2 \rangle \\ &= \| \Psi_1 \|^2 + \| \Psi_2 \|^2 + 2 \operatorname{Re}(\langle \Psi_1 | \Psi_2 \rangle) \\ &\leq \| \Psi_1 \|^2 + \| \Psi_2 \|^2 + 2 \| \Psi_1 \| \| \Psi_2 \| \\ &\leq (\| \Psi_1 \| + \| \Psi_2 \|)^2 \end{aligned}$$

Hence

$$\|\Psi_1 + \Psi_2\| \leq \|\Psi_1\| + \|\Psi_2\|$$

□

Definition 1.8. A set $S \subset H$ is said to be **orthonormal** if S is orthogonal and for each $\Psi_1 \in S$, $\|\Psi_1\| = 1$.

Definition 1.9. Let H be a vector space and $\langle \cdot | \cdot \rangle : G \times H \rightarrow \mathbb{C}$. Then H is said to be a **Hilbert space** if H is complete with respect to the norm on H induced by $\langle \cdot | \cdot \rangle$.

Note 1.10. For the rest of this section, we assume that H is a Hilbert space.

Exercise 1.11. (Pythagorean theorem):

Let $(\Psi_j)_{j \in \mathbb{N}} \subset H$ be an orthogonal set. Suppose that $\sum_{j \in \mathbb{N}} \Psi_j$ converges, then

$$\left\| \sum_{j \in \mathbb{N}} \Psi_j \right\|^2 = \sum_{j \in \mathbb{N}} \|\Psi_j\|^2$$

Proof. Let $n \in \mathbb{N}$. Then

$$\begin{aligned} \left\| \sum_{j=1}^n \Psi_j \right\|^2 &= \left\langle \sum_{i=1}^n \Psi_i \left| \sum_{j=1}^n \Psi_j \right. \right\rangle \\ &= \sum_{i=1}^n \sum_{j=1}^n \langle \Psi_i | \Psi_j \rangle \\ &= \sum_{j=1}^n \langle \Psi_j | \Psi_j \rangle \\ &= \sum_{j=1}^n \|\Psi_j\|^2 \end{aligned}$$

Since $\|\cdot\|$ is continuous on H , we have that

$$\begin{aligned} \left\| \sum_{j \in \mathbb{N}} \Psi_j \right\|^2 &= \lim_{n \rightarrow \infty} \left\| \sum_{j=1}^n \Psi_j \right\|^2 \\ &= \lim_{n \rightarrow \infty} \sum_{j=1}^n \|\Psi_j\|^2 \\ &= \sum_{j \in \mathbb{N}} \|\Psi_j\|^2 \end{aligned}$$

□

Definition 1.12. Let $S \subset H$. Then S is said to **span** H if $\text{span } S$ is dense in H and S is said to be a **basis** for H if S spans H and S linearly independent.

Definition 1.13. Let $A : H \rightarrow H$. Then A is said to be an **operator** on H .

Definition 1.14. Let A, B be operators on H . Then B is said to be the **adjoint** of A if for each $\Psi_1, \Psi_2 \in H$,

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

If B is the adjoint of A , we write

$$B = A^\dagger$$

Exercise 1.15. Let A be an operator on H , 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 ,

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

Therefore for each Ψ_1 ,

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

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

□

Definition 1.16. An linear operator Q on H is said to be **self-adjoint** if

$$Q = Q^\dagger$$

Exercise 1.17. Let Q be a self-adjoint operator on H . Then

- (1) the eigenvalues of Q are real.
- (2) the eigenvectors 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 1.18. Let A and B be operators. The **commutator** of A and B , $[A, B]$, is defined by

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

Exercise 1.19. Let A, B and C be operators, then $[AB, C] = A[B, C] + [A, C]B$

Proof. We have

$$\begin{aligned} [AB, C] &= ABC - CAB \\ &= ABC - ACB + ACB - CAB \\ &= A(BC - CB) + (AC - CA)B \\ &= A[B, C] + [A, C]B \end{aligned}$$

□

Definition 1.20. (Tensor Product):

Let H_1, H_2 be Hilbert spaces. Denote the free vector space over $H_1 \times H_2$ by $F(H_1 \times H_2)$. Define the relation \sim on $F(H_1 \times H_2)$ by

- (1) $(\Psi, \Phi) \sim (\Phi, \Psi)$ (reflexive)
- (2) if $(\Psi_1, \Phi_1) \sim (\Psi_2, \Phi_2)$, then $(\Psi_2, \Phi_2) \sim (\Psi_1, \Phi_1)$ (symmetric)
- (3) if $(\Psi_1, \Phi_1) \sim (\Psi_2, \Phi_2)$ and $(\Psi_2, \Phi_2) \sim (\Psi_3, \Phi_3)$, then $(\Psi_1, \Phi_1) \sim (\Psi_3, \Phi_3)$ (transitive)
- (4) $(\Psi + \lambda\Phi, \Xi) \sim (\Psi, \Xi) + \lambda(\Phi, \Xi)$ and $(\Psi, \Phi + \lambda\Xi) \sim (\Psi, \Phi) + \lambda(\Psi, \Xi)$ (bilinear)

We define the **tensor product** of H_1 with H_2 , denoted $H_1 \otimes H_2$ to be

$$H_1 \otimes H_2 = F(H_1 \times H_2) / \sim$$

We denote the equivalence class of (Ψ, Φ) in $H_1 \otimes H_2$ by $\Psi \otimes \Phi$. We define $\otimes : H_1 \times H_2 \rightarrow H_1 \otimes H_2$ by $(\Psi, \Phi) \mapsto \Psi \otimes \Phi$.

In summary

$$H_1 \otimes H_2 = \text{span}\{\Psi \otimes \Phi : \Psi \in H_1, \Phi \in H_2\}$$

where $\otimes : H_1 \times H_2 \rightarrow H_1 \otimes H_2$ is bilinear.

We define the inner product $\langle \cdot | \cdot \rangle$ on $H_1 \otimes H_2$ by setting

$$\langle \Psi_1 \otimes \Phi_1 | \Psi_2 \otimes \Phi_2 \rangle = \langle \Psi_1 | \Psi_2 \rangle_{H_1} \langle \Phi_1 | \Phi_2 \rangle_{H_2}$$

and extending linearly in the second argument.

Note 1.21. Typically, unless H_1 and H_2 are finite dimensional, $H_1 \otimes H_2$ is not complete. For the remainder of these notes, we assume we are working in the completion of $H_1 \otimes H_2$.

Exercise 1.22. Let H_1, H_2 be Hilbert spaces. If $(\Psi_j)_{j \in \mathbb{N}}$ is an orthonormal basis for H_1 and $(\Phi_j)_{j \in \mathbb{N}}$ is an orthonormal basis for H_2 , then $(\Psi_i \otimes \Phi_j)_{i,j \in \mathbb{N}}$ is an orthonormal basis for $H_1 \otimes H_2$.

Proof. Clear.

□

Note 1.23. If H_1 and H_2 are function spaces over sets S_1 and S_2 respectively, then $H_1 \otimes H_2$ is a function space over $S_1 \times S_2$ with $f_1 \otimes f_2(s_1, s_2) = f_1(s_1)f_2(s_2)$.

1.2. Permutation Groups.

2. POSTULATES OF QUANTUM MECHANICS

2.1. First Postulate.

Postulate 1. *Associated to any isolated physical system is a Hilbert space. The state space of the system is a subset of the unit sphere in the corresponding Hilbert space. All states which are unit modulus scalar multiples (rotations) of each other are identified.*

Definition 2.1. *We will typically denote the state of a system containing N particles at any given time by a **position wavefunction** $\Psi : \mathbb{R}^{3N+1} \rightarrow \mathbb{C}$.*

Interpretation 2.2. *Writing $r_i = (x_i, y_i, z_i)$ and $r = (r_1, \dots, r_N)$, we interpret $|\Psi(r_1, \dots, r_N, t)|^2$ to be the **joint probability density** for the positions r_1, \dots, r_N , of the particles at time t . Therefore, we require that for each $t \in \mathbb{R}$,*

$$\int_{\mathbb{R}^{3N}} \Psi(r, t)^* \Psi(r, t) dr = 1$$

We assume that $\Psi \in C^1$ with existing second partials and for each $t \in \mathbb{R}$, $\Psi(r, t) \rightarrow 0$ as $\|r\| \rightarrow \infty$.

2.2. Second Postulate.

Postulate 2. *For each observable quantity of an isolated system, there exists a corresponding self-adjoint operator whose eigenstates span the Hilbert space and whose eigenvalues consist of all possible measurements of the observable quantity. If two operators commute, there exists a set of simultaneous eigenstates of the two operators that span the Hilbert space.*

Definition 2.3. *The **x -component position operator of the j th particle**, denoted X_j , is defined by*

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

(we define the y -component and z -component position operators of the j th particle similarly)

Definition 2.4. *The **x -component momentum operator of the j th particle**, denoted P_{x_j} , is defined by*

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

(we define the y -component and z -component momentum operators of the j th particle similarly)

Definition 2.5. *For a system of N particles with masses m_1, \dots, m_N and potential energy $V(r_1, \dots, r_N, t)$ we define the **Hamiltonian** operator, denoted H , by*

$$H = \sum_{j=1}^N -\frac{\hbar^2}{2m_j} \Delta_j + V$$

where

$$\Delta_j = \frac{\partial^2}{\partial x_j^2} + \frac{\partial^2}{\partial y_j^2} + \frac{\partial^2}{\partial z_j^2}$$

Exercise 2.6. *We have that*

- (1) X_j is self-adjoint
- (2) P_{x_j} is self-adjoint

(3) H is self-adjoint (Hint: use [Green's second identity](#))

Proof.

- (1) Clear since x_j is real.
- (2) We have that

$$\begin{aligned}
 \langle \Psi_1 | P_{x_j} \Psi_2 \rangle &= \int_{\mathbb{R}^{3N}} \Psi_1^* \left(-i\hbar \frac{\partial}{\partial x_j} \Psi_2 \right) dx \\
 &= -i\hbar \int_{\mathbb{R}^{3N}} \Psi_1^* \left(\frac{\partial}{\partial x_j} \Psi_2 \right) dx \\
 &= i\hbar \int_{\mathbb{R}^n} \left(\frac{\partial}{\partial x_j} \Psi_1^* \right) \Psi_2 dx \quad (\text{integration by parts}) \\
 &= \int_{\mathbb{R}^{3N}} \left(-i\hbar \frac{\partial}{\partial x_j} \Psi_1 \right)^* \Psi_2 dx \\
 &= \langle P_{x_j} \Psi_1 | \Psi_2 \rangle
 \end{aligned}$$

(3) Finally, we have that

$$\begin{aligned}
 \langle \Psi_1 | H \Psi_2 \rangle - \langle H \Psi_1 | \Psi_2 \rangle &= \int_{\mathbb{R}^{3N}} \Psi_1^* (H \Psi_2) dx - \int_{\mathbb{R}^{3N}} (H \Psi_1)^* \Psi_2 dx \\
 &= \int_{\mathbb{R}^{3N}} \Psi_1^* \left(\sum_{j=1}^N -\frac{\hbar^2}{2m_j} \Delta_j \Psi_2 \right) - \left(\sum_{j=1}^N -\frac{\hbar^2}{2m_j} \Delta_j \Psi_1 \right)^* \Psi_2 dx \\
 &= \sum_{j=1}^N \frac{\hbar^2}{2m_j} \int_{\mathbb{R}^{3N}} (\Delta \Psi_1^*) \Psi_2 - \Psi_1^* (\Delta \Psi_2) dx \\
 &= 0 \quad (\text{Green's second identity})
 \end{aligned}$$

□

Exercise 2.7. We have that

- (1) $[X_i, P_{x_j}] = \delta_{i,j} i\hbar$
- (2) $[Y_i, P_{x_j}] = 0$ (and similar for any other mix of x, y and z)

Proof.

- (1) For a position wave function Ψ ,

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

Hence $[X_j, P_{x_j}] = i\hbar$

For $i \neq j$,

$$\begin{aligned} X_i P_{x_j} \Psi(r, t) &= \frac{\partial}{\partial x_j} x_i \Psi(r, t) \\ &= -i\hbar x_i \frac{\partial}{\partial x_j} \Psi(r, t) \\ &= P_{x_j} X_i \Psi(r, t) \end{aligned}$$

So

$$[X_i, P_{x_j}] = 0$$

(2) For a position wave function Ψ ,

$$\begin{aligned} [Y_i, P_{x_j}] \Psi(r, t) &= \left[y_i, -i\hbar \frac{\partial}{\partial x_j} \right] \Psi(r, t) \\ &= (-i\hbar) \left[y_i \frac{\partial}{\partial x_j} \Psi(r, t) - \frac{\partial}{\partial x_j} y_i \Psi(r, t) \right] \\ &= (-i\hbar) \left[y_i \frac{\partial}{\partial x_j} \Psi(r, t) - y_i \frac{\partial}{\partial x_j} \Psi(r, t) \right] \\ &= 0 \end{aligned}$$

□

2.3. Third Postulate.

Note 2.8. Let A be a self-adjoint operator corresponding to an observable quantity of the system with eigenvalues $(\lambda_n)_{n \in \mathbb{N}}$ of degeneracy $(k_n)_{n \in \mathbb{N}}$. The second postulate tells us that we are given a spanning set $(\Psi_{n,j})_{n \in \mathbb{N}, j \leq k_n}$ of eigenstates with $(\Psi_{n,j})_{j=1}^{k_n}$ a basis for the eigenspace of λ_n . Using the Gram-Schmidt process within each eigenspace of λ_n , we may assume that $(\Psi_{n,j})_{n \in \mathbb{N}, j \leq k_n}$ is an orthonormal basis for the Hilbert space. In these notes, we assume that our spanning set of eigenstates is orthonormal (this happens often in practice).

Postulate 3. Let A be a self-adjoint operator corresponding to an observable quantity of the system with eigenvalues $(\lambda_n)_{n \in \mathbb{N}}$ of degeneracy $(k_n)_{n \in \mathbb{N}}$ and an orthonormal basis of eigenstates $(\Psi_{n,j})_{n \in \mathbb{N}, j \leq k_n}$ for the Hilbert space with $(\Psi_{n,j})_{j=1}^{k_n}$ a basis for the eigenspace of λ_n and $\Psi = \sum_{n \in \mathbb{N}} \sum_{j=1}^{k_n} c_{n,j} \Psi_{n,j}$ the state of the system. Then upon measurement,

(1) the probability of measuring λ_n , denoted $P(\lambda_n)$, is given by

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

(2) if λ_n is measured, then the state of the system collapses to the state

$$\left(\frac{1}{\sum_{j=1}^{k_n} |c_{n,j}|^2} \right)^{1/2} \sum_{j=1}^{k_n} c_{n,j} \Psi_{n,j}$$

2.4. Fourth Postulate.

Postulate 4. If the state space for system S_1 is a subset of the hilbert space H_1 and the state space for system S_2 is a subset of the hilbert space H_2 , then the state space for the composite system of S_1 with S_2 is a subset of the tensor product $H_1 \otimes H_2$. The state $\Psi_1 \otimes \Psi_2$ corresponds to the first system being in state Ψ_1 and the second system being in state Ψ_2 .

Exercise 2.9. Let A be an operator corresponding to an observable quantity of the first component system with an orthonormal basis of eigenstates $(\Psi_j)_{j \in \mathbb{N}}$, B an operator corresponding to an observable quantity of the first component system with an orthonormal basis of eigenstates $(\Phi_k)_{k \in \mathbb{N}}$. Then $A \otimes B$ corresponds to an observable quantity of the composite system with an orthonormal basis of eigenstates $(\Psi_k \otimes \Phi_k)_{j,k \in \mathbb{N}}$. Let $\Xi = \sum_{j \in \mathbb{N}} \sum_{k \in \mathbb{N}} c_{j,k} \Psi_j \otimes \Phi_k$, be the state of the composite system. Upon measurement of the observable quantity of the composite system corresponding to $A \otimes B$. Then

Definition 2.10. Consider two systems, S_1 and S_2 with each consisting of a single particle where the statespaces of S_1 and S_2 are a subset of Hilbert spaces H_1 and H_2 respectively. The state of the composite system is said to be an **entangled state** if it cannot be expressed in the form $\Psi_1 \otimes \Psi_2$ for any $\Psi_1 \in H_1$ or $\Psi_2 \in H_2$. In this case, the two particles are said to be **entangled**.

Exercise 2.11. Suppose we have a composite system of two identical particles whose component systems are each contained in a 2 dimensional hilbert space with orthonormal basis $\{|0\rangle, |1\rangle\}$. Then the state

$$\frac{1}{\sqrt{2}}|0\rangle \otimes |0\rangle + \frac{1}{\sqrt{2}}|1\rangle \otimes |1\rangle$$

is an entangled state.

Proof. Suppose there exist $c_1, \dots, c_4 \in \mathbb{C}$ such that

$$\frac{1}{\sqrt{2}}|0\rangle \otimes |0\rangle + \frac{1}{\sqrt{2}}|1\rangle \otimes |1\rangle = (c_1|0\rangle + c_2|1\rangle) \otimes (c_3|0\rangle + c_4|1\rangle)$$

Since

$(c_1|0\rangle + c_2|1\rangle) \otimes (c_3|0\rangle + c_4|1\rangle) = c_1c_3|0\rangle \otimes |0\rangle + c_1c_4|0\rangle \otimes |1\rangle + c_2c_3|1\rangle \otimes |0\rangle + c_2c_4|1\rangle \otimes |1\rangle$
we know that $c_1c_4 = 0$. So $c_1 = 0$ or $c_4 = 0$. This is a contradiction. \square

Exercise 2.12.

2.5. Fifth Postulate.

Definition 2.13. The **Schrödinger equation** is the linear partial differential equation given by

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

Postulate 5. The time evolution of an isolated system is described by the Schrödinger equation.

Exercise 2.14. Suppose that the potential energy V doesn't depend on time. Let Ψ be a solution to the Schrödinger equation. If there exist ψ, φ such that

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

Then Ψ is an eigenstate of H and there exists $E \in \mathbb{R}$ such that $H\psi = E\psi$ and $\varphi(t) = e^{-i\frac{E}{\hbar}t}$.

Proof. Plugging $\Psi = \psi\varphi$ into the Schrödinger equation, we get that

$$i\hbar\psi\frac{d}{dt}\varphi = \varphi H\psi$$

So

$$i\hbar\frac{1}{\varphi}\frac{d}{dt}\varphi = \frac{1}{\psi}H\psi$$

Since the left side only depends on time and the right side does not depend on time, both sides are constant functions. So there exists $E \in \mathbb{C}$ such that

$$(1) \quad H\psi = E\psi$$

and

$$(2) \quad \frac{1}{\varphi}\frac{d}{dt}\varphi = -i\frac{E}{\hbar}$$

Equation (1) implies that

$$\begin{aligned} H\Psi &= H(\psi\varphi) \\ &= \varphi H\psi \\ &= \varphi E\psi \\ &= E\Psi \end{aligned}$$

So that Ψ is an eigenstate of H . Since H is self-adjoint, $E \in \mathbb{R}$. Equation (2) then implies that $\varphi(t) = e^{-i\frac{E}{\hbar}t}$ □

Note 2.15. For the remainder of these notes, we assume that the potential energy V of the system is independent of time.

Definition 2.16. In the situation of the previous exercise, since we identify states that are rotations of each other, the the state is not changing over time. Thus we call Ψ a **stationary state** of H .

Note 2.17. By the [Sturm-Liouville theory](#), the stationary states form an orthonormal basis, so in practice, we can solve the time-independent Schrödinger equation, append the time dependencies to obtain the stationary states and then use those to represent a general state of the system.

Definition 2.18. A stationary state of the system is called a **ground state** if the corresponding energy eigenvalue is minimal. All other stationary states are called **excited states**.

Exercise 2.19. If V is real and Ψ satisfies the Schrödinger equation, then

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

Proof. We have that

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\Psi^* &= \left(-i\hbar\frac{\partial}{\partial t}\Psi\right)^* \\ &= (-H\Psi)^* \\ &= -H\Psi^* \end{aligned}$$

□

Definition 2.20. Consider a system consisting of one particle with mass m with a potential energy V . We define the **probability current density**, j , of the particle to be

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

Exercise 2.21. (Continuity Equation):

We have that

$$\frac{\partial}{\partial t}(\Psi^*\Psi) + \nabla \cdot j = 0$$

Proof.

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

Therefore

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

□

3. FUNDAMENTAL EXAMPLES IN ONE DIMENSION

3.1. The Infinite Square Well.

Definition 3.1. *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 3.2. *By starting with a finite potential 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

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

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

$$\frac{d^2\psi}{dx^2} = l^2\psi$$

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 $x \rightarrow -\infty$, $B = 0$. Since e^{lx} blows up as $x \rightarrow \infty$, $F = 0$.

In section I_2 , the Schrödinger equation may be written as

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

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

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

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 $\alpha \rightarrow \infty$. As $\alpha \rightarrow \infty$, we have that $l \rightarrow \infty$. Hence $\psi_1 \rightarrow 0$ and $\psi_3 \rightarrow 0$. 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 implies that $D = 0$ and $0 = C \sin(ka)$ which yields various solutions

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

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

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

and (after normalizing) our stationary states are

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

□

3.2. The Harmonic Oscillator.

Definition 3.3. 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

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

and we define the **raising operator**, a_+ , by

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

Exercise 3.4. The adjoint of the lowering operator is the raising operator:

$$(a_-)^\dagger = a_+$$

Proof. Let Ψ_1, Ψ_2 be wavefunctions. Since X, P are self-adjoint, we have that

$$\begin{aligned} \langle \Psi_1 | a_- \Psi_2 \rangle &= \frac{1}{\sqrt{2\hbar m\omega}} \langle \Psi_1 | (m\omega X + iP) \Psi_2 \rangle \\ &= \frac{1}{\sqrt{2\hbar m\omega}} \left[m\omega \langle \Psi_1 | X \Psi_2 \rangle + i \langle \Psi_1 | P \Psi_2 \rangle \right] \\ &= \frac{1}{\sqrt{2\hbar m\omega}} \left[\langle m\omega X \Psi_1 | \Psi_2 \rangle + \langle -iP \Psi_1 | \Psi_2 \rangle \right] \\ &= \frac{1}{\sqrt{2\hbar m\omega}} \langle (m\omega X - iP) \Psi_1 | \Psi_2 \rangle \\ &= \langle a_+ \Psi_1 | \Psi_2 \rangle \end{aligned}$$

□

Exercise 3.5. *We have that*

- (1) $a_-a_+ = \frac{1}{\hbar\omega}H + \frac{1}{2}$
- (2) $a_+a_- = \frac{1}{\hbar\omega}H - \frac{1}{2}$
- (3) $[a_-, a_+] = 1$

Proof. (1)

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

- (2) Similar
- (3) Trivial

□

Exercise 3.6. *If $H\psi = E\psi$, then*

- (1) $Ha_-\psi = (E - \hbar\omega)a_-\psi$
- (2) $Ha_+\psi = (E + \hbar\omega)a_+\psi$

Proof.

(1)

$$\begin{aligned}
 Ha_-\psi &= \hbar\omega\left(a_-a_+ - \frac{1}{2}\right)a\psi \\
 &= \hbar\omega\left(a_-a_+a_- - \frac{1}{2}a_-\right)\psi \\
 &= \hbar\omega a_-\left(a_+a_- - \frac{1}{2}\right)\psi \\
 &= \hbar\omega a_-\left(a_+a_- + \frac{1}{2} - 1\right)\psi \\
 &= \hbar\omega a_-\left(\frac{1}{\hbar\omega}H - 1\right)\psi \\
 &= a_-H\psi - \hbar\omega a_-\psi \\
 &= (E - \hbar\omega)a_-\psi
 \end{aligned}$$

(2) Similar

□

Interpretation 3.7. *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 $a_+\psi$ with energy $E + \hbar\omega$.*

Definition 3.8. 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 raising operator n times and then normalizing.

Exercise 3.9. We have that

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

$$(2) \quad E_0 = \frac{1}{2}\hbar\omega$$

$$(3) \quad \psi_n = c_n(a_+)^n\psi_0 \quad (\text{for some constant } c_n)$$

$$(4) \quad E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

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 3.10.

$$(1) \quad \psi_{n+1} = \frac{1}{\sqrt{n+1}}a_+\psi_n$$

$$(2) \quad \psi_{n-1} = \frac{1}{\sqrt{n}}a_-\psi_n$$

Hint: use the adjoint-ness of a_- and a_+

Proof.

(1)

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

Since $\psi_{n+1} = ca_+\psi_n$, we have that

$$\begin{aligned}
 1 &= \langle \psi_{n+1} | \psi_{n+1} \rangle \\
 &= \langle ca_+\psi_n | ca_+\psi_n \rangle \\
 &= |c|^2 \langle a_+\psi_n | a_+\psi_n \rangle \\
 &= |c|^2 \langle a_-a_+\psi_n | \psi_n \rangle \\
 &= |c|^2 \langle (n+1)\psi_n | \psi_n \rangle \\
 &= |c|^2 (n+1) \langle \psi_n | \psi_n \rangle \\
 &= |c|^2 (n+1)
 \end{aligned}$$

So $c = \frac{1}{\sqrt{n+1}}$

(2) Similar to (1). □

Exercise 3.11. The n^{th} stationary state is given by $\psi_n = \frac{1}{\sqrt{n!}}(a_+)^n\psi_0$

Proof. Clear by induction. □

Exercise 3.12. Show that

$$\begin{aligned}
 (1) \quad \psi_1(x) &= \left(\frac{4m^3\omega^3}{\hbar^3\pi}\right)xe^{-\frac{m\omega}{2\hbar}x^2} \\
 (2) \quad E_1 &= \frac{3}{2}\hbar\omega
 \end{aligned}$$

Proof. Straightforward. □

Exercise 3.13. 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. □

4. SPHERICAL COORDINATES AND ORBITAL ANGULAR MOMENTUM

Note 4.1. In the rest of the notes we will be working in three dimensions. In this section, we develop a method to solve the time independent Schrödinger equation when the potential energy is spherically symmetric. We also develop a theory of orbital angular momentum and see how it relates to the time independent Schrödinger equation.

4.1. The Time Independent Schrödinger Equation in Spherical Coordinates.

Definition 4.2. We will now work with spherical coordinates (r, θ, ϕ) where r is the distance from the origin, $0 \leq \theta \leq \pi$ is the angle with initial side on the positive z -axis, and $0 \leq \phi < 2\pi$ is the angle in the x - y plane with initial side on the positive x -axis going towards the positive y -axis.

Proposition 4.3. 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 4.4. 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

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

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

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

Definition 4.5. 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

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

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

This equation is called the **azimuthal equation** and 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 4.6. Compute some spherical harmonics.

Definition 4.7. If we make the substitution $u(r) = rR(r)$, we may rewrite the radial equation as

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

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**.

4.2. Orbital Angular Momentum.

Definition 4.8. *Extrapolating from the classical formula for angular momentum, we define the **orbital angular momentum operator** L , of a particle by*

$$L = R \times P$$

so that

$$\begin{aligned} L_x &= YP_z - ZP_y \\ L_y &= ZP_x - XP_z \\ L_z &= XP_y - YP_x \end{aligned}$$

and

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

Exercise 4.9. *We have that*

- (1) $[L_x, L_y] = i\hbar L_z$
- (2) $[L_y, L_z] = i\hbar L_x$
- (3) $[L_z, L_x] = i\hbar L_y$

Proof.

(1)

$$\begin{aligned} [L_x, L_y] &= (YP_z - ZP_y)(ZP_x - XP_z) - (ZP_x - XP_z)(YP_z - ZP_y) \\ &= YP_x(P_z Z - ZP_z) + XP_y(ZP_z - P_z Z) \\ &= (XP_y - YP_x)[Z.P_z] \\ &= i\hbar L_z \end{aligned}$$

(2) Similar

(3) Similar

□

Exercise 4.10.

- (1) $[L^2, L_x] = 0$
- (2) $[L^2, L_y] = 0$
- (3) $[L^2, L_z] = 0$

Proof.

(1)

$$\begin{aligned} [L^2, L_x] &= [L_x^2, L_x] + [L_y^2, L_x] + [L_z^2, L_x] \\ &= (L_y[L_y, L_x] + [L_y, L_x]L_y) + (L_z[L_z, L_x] + [L_z, L_x]L_z) \\ &= -i\hbar(L_y L_z + L_z L_y) + i\hbar(L_z L_y + L_y L_z) \\ &= 0 \end{aligned}$$

(2) Similar.

(3) Similar.

□

Exercise 4.11. *The operators L_x, L_y and L_z are self-adjoint.*

Proof. Let Ψ_1, Ψ_2 be wave functions. Since X_i and P_j are self-adjoint and commute for $i \neq j$, we have that

$$\begin{aligned}\langle \Psi_1 | L_x \Psi_2 \rangle &= \langle \Psi_1 | Y P_z \Psi_2 \rangle - \langle \Psi_1 | Z P_y \Psi_2 \rangle \\ &= \langle P_z Y \Psi_1 | \Psi_2 \rangle - \langle P_y Z \Psi_1 | \Psi_2 \rangle \\ &= \langle Y P_z \Psi_1 | \Psi_2 \rangle - \langle Z P_y \Psi_1 | \Psi_2 \rangle \\ &= \langle L_x \Psi_1 | \Psi_2 \rangle\end{aligned}$$

So L_x is self-adjoint. The case is similar for L_y and L_z □

Definition 4.12. We define the **raising operator** L_+ and **lowering operator** L_- by

$$L_+ = L_x + iL_y \quad \text{and} \quad L_- = L_x - iL_y$$

Exercise 4.13.

$$[L^2, L_+] = [L^2, L_-] = 0$$

Proof. Trivial. □

Exercise 4.14. The lowering operator is the adjoint of the raising operator:

$$L_- = (L_+)^{\dagger}$$

Proof. Let Ψ_1, Ψ_2 be wavefunctions. Then

$$\begin{aligned}\langle \Psi_1 | L_+ \Psi_2 \rangle &= \langle \Psi_1 | L_x \Psi_2 \rangle + i \langle \Psi_1 | L_y \Psi_2 \rangle \\ &= \langle L_x \Psi_1 | \Psi_2 \rangle + i \langle L_y \Psi_1 | \Psi_2 \rangle \\ &= \langle L_x \Psi_1 | \Psi_2 \rangle + \langle -iL_y \Psi_1 | \Psi_2 \rangle \\ &= \langle (L_x - iL_y) \Psi_1 | \Psi_2 \rangle \\ &= \langle L_- \Psi_1 | \Psi_2 \rangle\end{aligned}$$

Hence $L_- = (L_+)^{\dagger}$. □

Exercise 4.15. We have

- (1) $[L_z, L_+] = \hbar L_+$
- (2) $[L_z, L_-] = -\hbar L_-$

Proof.

(1)

$$\begin{aligned}[L_z, L_+] &= [L_z, L_x] + i[L_z, L_y] \\ &= i\hbar L_y + \hbar L_x \\ &= \hbar L_+\end{aligned}$$

(2) Similar. □

Exercise 4.16. We have

- (1) $L^2 = L_+ L_- + L_z^2 - \hbar L_z$
- (2) $L^2 = L_- L_+ + L_z^2 + \hbar L_z$

Proof.

(1)

$$\begin{aligned}
L_+L_- &= (L_x + iL_y)(L_x - iL_y) \\
&= L_x^2 - i(L_xL_y - L_yL_x) + L_y^2 \\
&= L_x^2 + L_y^2 - i[L_x, L_y] \\
&= L^2 - L_z^2 + \hbar L_z
\end{aligned}$$

Therefore

$$L^2 = L_+L_- + L_z^2 - \hbar L_z$$

(2) Similar

□

Exercise 4.17. Suppose that f is simultaneously an eigenfunction of L^2 with eigenvalue λ and an eigenfunction of L_z with eigenvalue μ . Then

- (1) L_+f is simultaneously an eigenfunction of L^2 with eigenvalue λ and an eigenfunction of L_z with eigenvalue $\mu + \hbar$
- (2) L_-f is simultaneously an eigenfunction of L^2 with eigenvalue λ and an eigenfunction of L_z with eigenvalue $\mu - \hbar$

Proof.

(1) First we have

$$\begin{aligned}
L^2L_+f &= L_+L^2f \\
&= L_+\lambda f \\
&= \lambda L_+f
\end{aligned}$$

Second we see that

$$\begin{aligned}
L_zL_+f &= \left[L_+L_z + (L_zL_+ - L_+L_z) \right] f \\
&= (L_+L_z + [L_z, L_+])f \\
&= (\mu L_+ + \hbar L_+)f \\
&= (\mu + \hbar)L_+f
\end{aligned}$$

(2) Similar.

□

Interpretation 4.18. The raising/lowering operators change the state of a particle from simultaneous eigenstate to simultaneous eigenstate and increase/decrease the z -component of the orbital angular momentum of a particle by \hbar , but does not change the total orbital angular momentum of the particle.

Note 4.19. If we repeatedly applied the increasing/decreasing operator to a simultaneous eigenstate of a particle, we would arrive at a top/bottom eigenstate since there is a finite amount of total angular momentum.

Definition 4.20. We define the **top state** f_t to be the simultaneous eigenstate of L^2 and L_z such that

$$L_+f_t = 0$$

and we define the **bottom state** f_b to be the simultaneous eigenstate of L^2 and L_z such that

$$L_- f_b = 0$$

Exercise 4.21. Let $\hbar l$ and $\hbar l'$ be the eigenvalues of L_z for f_t and f_b respectively. Then

- (1) $\hbar^2 l(l+1)$ and $\hbar^2 l'(l'-1)$ are the eigenvalue of L^2 for f_t and f_b respectively
- (2) $l' = -l$
- (3) $l \in \frac{1}{2}\mathbb{N}_0$

Proof.

(1)

$$\begin{aligned} L^2 f_t &= (L_- L_+ + L_z^2 + \hbar L_z) f_t \\ &= \hbar^2 l^2 f_t + \hbar^2 l f_t \\ &= \hbar^2 l(l+1) f_t \end{aligned}$$

The case is similar for l' .

(2) For some $N \in \mathbb{N}_0$ and constant C , we have $f_b = CL_-^N f_t$. Thus

$$\begin{aligned} \hbar^2 l'(l'-1) f_b &= L^2 f_b \\ &= L^2 CL_-^N f_t \\ &= CL_-^N L^2 f_t \\ &= CL_-^N \hbar^2 l(l+1) f_t \\ &= \hbar^2 l(l+1) f_b \end{aligned}$$

So $l'(l'-1) = l(l+1)$. By completing the square, we see that the only two ways that this equation is satisfied is if $l' = l+1$ or $l' = -l$. The first case is not possible since it would imply that the orbital angular momentum for a particle is greater in the state f_b than in the state f_t . So $l' = -l$.

(3) Since for some $N \in \mathbb{N}_0$ and constant C , $L_b = CL_-^N f_t$, a previous exercise implies that

$$\begin{aligned} -\hbar l f_b &= L_z f_b \\ &= L_z CL_-^N f_t \\ &= \hbar(l-N) CL_-^N f_t \\ &= \hbar(l-N) f_b \end{aligned}$$

So $-l = l - N$ and $l = \frac{N}{2}$. Thus $l \in \frac{1}{2}\mathbb{N}_0$. □

Definition 4.22. For $m = -l, -l+1, \dots, l-1, l$ define f_l^m to be the simultaneous eigenstate of L^2 and L_z given by

$$f_l^m = \langle L_-^{l-m} f_t | L_-^{l-m} f_t \rangle^{-\frac{1}{2}} L_-^{l-m} f_t$$

Exercise 4.23. We have that

- (1) the eigenvalue of L^2 corresponding to f_l^m is $\hbar^2 l(l+1)$
- (2) the eigenvalue of L_z corresponding to f_l^m is $\hbar m$.

Proof. Straightforward (and kind of already did it in the last exercise). □

Exercise 4.24. For $l \in \mathbb{N}_0$ and $m \in \{-l, -l+1, \dots, l\}$ we have that

$$(1) L_+ f_l^m = \hbar \sqrt{l(l+1) - m(m+1)} f_l^{m+1}$$

$$(2) L_- f_l^m = \hbar \sqrt{l(l+1) - m(m-1)} f_l^{m-1}$$

Proof. (1) By definition, there exists $c \in \mathbb{C}$ such that $L_+ f_l^m = c f_l^{m+1}$. Since $L_- = (L_+)^{\dagger}$ and $L_- L_+ = L^2 - L_z^2 - \hbar L_z$, we have that

$$\begin{aligned} |c|^2 &= \langle L_+ f_l^m | L_+ f_l^m \rangle \\ &= \langle f_l^m | L_- L_+ f_l^m \rangle \\ &= \langle f_l^m | (L^2 - L_z^2 - \hbar L_z) f_l^m \rangle \\ &= [\hbar^2 l(l+1) - \hbar^2 m^2 - \hbar^2 m] \langle f_l^m | f_l^m \rangle \\ &= \hbar^2 [l(l+1) - m(m+1)] \end{aligned}$$

So $c = \hbar \sqrt{l(l+1) - m(m+1)}$.

(2) Similar to (1). □

Proposition 4.25. *In spherical coordinates, we may write*

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

and

$$L_z = -i\hbar \frac{\partial}{\partial \phi}$$

Note 4.26. *Using the relations given above we see that simultaneous eigenstates f_l^m of L^2 and L_z satisfy*

$$\begin{aligned} \hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] f_l^m &= L^2 f_l^m \\ &= \hbar^2 l(l+1) f_l^m \end{aligned}$$

and

$$\begin{aligned} -i\hbar \frac{\partial}{\partial \phi} f_l^m &= L_z f_l^m \\ &= \hbar m f_l^m \end{aligned}$$

which implies that

$$-\hbar^2 \frac{\partial^2}{\partial \phi^2} f_l^m = \hbar^2 m^2 f_l^m$$

If we recall from earlier, these are just the angular and azimuthal equations respectively. Thus the simultaneous eigenstates of L^2 and L_z are $f_l^m = Y_l^m$. Therefore, if $R(r)$ solves the radial equation and is normalized, then the states $R(r)Y_l^m(\theta, \phi)$ are simultaneous eigenstates of H, L^2 and L_z .

Note 4.27. *the quantum number m is dependent on the quantum number l . Later we will write m_l to emphasize this, as well as to avoid confusion with mass or other quantum numbers.*

5. FUNDAMENTAL EXAMPLES IN THREE DIMENSIONS

Note 5.1. *In this section we will introduce discuss the 3D harmonic oscillator and the hydrogen atom.*

5.1. Spherical Harmonic Oscillator (Cartesian Coordinates).

Definition 5.2. *The spherical harmonic oscillator (in cartesian coordinates) is defined by the potential energy*

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

Exercise 5.3. *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

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

Dividing both sides by ψ and rearranging, we obtain

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

Thus each part is constant and we may write

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

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

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

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 5.4. Show that the degree of degeneracy of E_n is

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

Proof. Stars and bars

□

Interpretation 5.5. 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.

5.2. The Hydrogen Atom.

Definition 5.6. We will consider a hydrogen atom consisting of one proton and one electron. We will fix the proton at the origin and investigate the electron. This model is defined by the potential energy of the electron given by

$$V(r) = -\frac{e^2}{4\pi\epsilon_0} \frac{1}{r}$$

Note 5.7. We will walk through the solution to the radial equation. The goal will be to find the asymptotic behavior of $R(r)$ as $r \rightarrow 0$ and $r \rightarrow \infty$ and then glue this behavior together. This is a clever and useful technique that can be utilized in various situations.

Exercise 5.8. Since $\sup_{r \in \mathbb{R}} V(r) = 0$, we know that for the bound states of the electron, the energy must satisfy $E < 0$. Making the substitution

$$\kappa = \frac{\sqrt{-2mE}}{\hbar}$$

we can rewrite the radial equation as

$$\frac{1}{\kappa^2} \frac{d^2 u}{dr^2} = \left[1 - \frac{me^2}{2\pi\epsilon_0 \hbar^2 \kappa} \frac{1}{(\kappa r)} + \frac{l(l+1)}{(\kappa r)^2} \right] u$$

Then making the substitutions

$$\rho = \kappa r \text{ and } \rho_0 = \frac{me^2}{2\pi\epsilon_0 \hbar^2 \kappa}$$

, we can further simplify the radial equation as

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

Proof. Straightforward using chain rule.

□

Exercise 5.9. As $\rho \rightarrow \infty$, $u \approx e^{-\rho}$.

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

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

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

$$\begin{aligned}\frac{d^2u}{d\rho^2} &= e^{-\rho} \\ &= u\end{aligned}$$

□

Exercise 5.10. As $\rho \rightarrow 0$, $u \approx \rho^{l+1}$.

Proof. As $\rho \rightarrow 0$,

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

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

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

□

Note 5.11. We can now, “glue” these functions together with a third unknown function $v(\rho)$ to obtain the prototype solution

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

Exercise 5.12. Suppose that for some nice function $v(\rho)$,

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

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

$$\rho \frac{d^2v}{d\rho^2} + 2(l+1-\rho) \frac{dv}{d\rho} + [\rho_0 - 2(l+1)]v = 0$$

Proof. Very tedious but straightforward. □

Exercise 5.13. 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 relation

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

Proof. Tedious but straightforward. □

Exercise 5.14. If for each $j \geq 0$, $c_j \neq 0$, then v behaves asymptotically like e^ρ . Thus $u(\rho)$ behaves asymptotically like $\rho^{l+1}e^\rho$. This implies that $R(r)$ is not normalizable. Therefore there exists $j_{\max} \geq 0$ such that $c_{j_{\max}+1} = 0$ and $v(\rho)$ is a polynomial of degree j_{\max} .

Proof. Suppose that for each $j \geq 0$, $c_j \neq 0$. Then as $j \rightarrow \infty$,

$$c_{j+1} \approx \frac{2}{j+1} c_j$$

Thus asymptotically,

$$\begin{aligned} v(\rho) &\approx c_0 \sum_{j=0}^{\infty} \frac{(2\rho)^j}{j!} \\ &= c_0 e^{2\rho} \end{aligned}$$

This implies that asymptotically,

$$\begin{aligned} u(\rho) &\approx \rho^{l+1} e^{-\rho} e^{2\rho} \\ &= \rho^{l+1} e^{\rho} \end{aligned}$$

Therefore asymptotically,

$$R(r) = \frac{1}{r} (r\kappa)^{l+1} e^{r\kappa}$$

which blows up as $r \rightarrow \infty$. □

Exercise 5.15. *The allowed energies of the electron are given by*

$$E_n = - \left[\frac{m}{2\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0} \right)^2 \right] \frac{1}{n^2} = \frac{E_1}{n^2}, \quad n \in \mathbb{N}$$

Proof. Starting with the relation

$$0 = \left[\frac{2(j_{\max} + l + 1) - \rho_0}{(j_{\max} + 1)(j_{\max} + 2l + 2)} \right] c_{j_{\max}}$$

we can see that

$$\rho_0 = 2(j_{\max} + l + 1)$$

Since j_{\max} and l may be any nonnegative integers, we introduce a positive integer $n = j_{\max} + l + 1$. If we know n and l , then we know j_{\max} and l and vice versa, so it is the same information, but it will help us more neatly index the energies. So we put $\rho_0 = 2n$ and using the fact that

$$\kappa^2 = -\frac{2mE}{\hbar^2} \text{ and } \rho_0 = \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa}$$

we solve for E to get that

$$\begin{aligned} E_n &= -\frac{me^4}{8\pi^2\epsilon_0^2\hbar^2\rho_0^2} \\ &= -\left[\frac{m}{2\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0} \right)^2 \right] \frac{1}{n^2} \end{aligned}$$

□

Note 5.16. *Since $n = j_{\max} + l + 1$, $j_{\max} \geq 0$ and $n \geq 1$ we know that $l = n - j_{\max} - 1 \leq n - 1$. Thus the simultaneous eigenstates of H, L^2, L_z are $\psi_{n,l,m}(r, \theta, \phi) R_n(r) Y_l^m$ with $1 \leq n$, $0 \leq l \leq n - 1$ and $-l \leq m \leq l$.*

5.3. Spherical Harmonic Oscillator (Spherical Coordinates).

Definition 5.17. *The spherical harmonic oscillator (in spherical coordinates) is defined by the potential energy*

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

Exercise 5.18. *Making the substitution $\kappa = \frac{\sqrt{2mE}}{\hbar}$, we can rewrite the radial equation for the harmonic oscillator as*

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

Proof. Straightforward □

Exercise 5.19. *Making the substitution $\rho = \kappa r$ and $\rho_0 = \frac{\hbar \omega}{2E}$, we can rewrite the radial equation as*

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

Proof. Straightforward. □

Exercise 5.20. *We have*

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

and thus we may rewrite the radial equation as

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

Proof. Straightforward by chain-rule. □

Exercise 5.21. *As $\rho \rightarrow \infty$, $u \approx e^{-\frac{\rho_0}{2}\rho^2}$*

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

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

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

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

□

Exercise 5.22. *As $\rho \rightarrow 0$, $u \approx \rho^{l+1}$*

Proof. Same as in the case of the hydrogen atom. □

Note 5.23. *Just like in the case of the hydrogen atom, we can “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 5.24. Suppose that for some nice function $v(\rho)$,

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

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

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

Proof. Very tedious but straightforward. □

Exercise 5.25. 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 5.26. 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 $c_{j_{max}+2} = 0$ and $v(\rho)$ is a polynomial of degree j_{max} and consists of only even powers of ρ .

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

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

□

Exercise 5.27. The energies allowed for this system are

$$E_n = \hbar \omega \left(n + \frac{3}{2} \right) \quad n \in \mathbb{N}_0$$

Proof. Using the recursion relation found earlier, we have that

$$0 = \left[\frac{\rho_0(2j_{max} + 2l + 3) - 1}{(j_{max} + 2)(j_{max} + 2l + 3)} \right] c_{j_{max}}$$

This implies that

$$0 = \rho_0(2j_{max} + 2l + 3) - 1$$

and so

$$\frac{1}{\rho_0} = 2j_{max} + 2l + 3$$

Using the fact that $\rho_0 = \frac{\hbar\omega}{2E}$, we solve for E to obtain

$$E = \hbar\omega \left(j_{max} + l + \frac{3}{2} \right)$$

Since j_{max} and l may be any non-negative integers, we introduce a non-negative integer $n = j_{max} + l$ and index the allowed energies as

$$E_n = \hbar\omega \left(n + \frac{3}{2} \right) \quad n \in \mathbb{N}_0$$

□

6. SPIN

6.1. Introduction.

Definition 6.1. It turns out that there is another inherent quality which all things have which was revealed by experiment. We call this inherent quality **spin**. In these notes we take as given that the spin of a particle in the x, y and z directions is a measurable quantity which corresponds to self adjoint operators S_x, S_y, S_z that satisfy the commutation relations:

- (1) $[S_x, S_y] = i\hbar S_z$
- (2) $[S_y, S_z] = i\hbar S_x$
- (3) $[S_z, S_x] = i\hbar S_y$

With this assumption we can follow the exact same procedure as we did with the orbital angular momentum to obtain for each $s \geq 0$, a set of simultaneous eigenstates of S^2 and S_z called **spin states** given by $(|s, m\rangle)_{m=-s}^s$ such that

- (1) $S^2|s, m\rangle = \hbar^2 s(s+1)|s, m\rangle$
- (2) $S_z|s, m\rangle = \hbar m|s, m\rangle$
- (3) $S_{\pm}|s, m\rangle = \hbar\sqrt{s(s+1) - m(m \pm 1)}|s, m \pm 1\rangle$

The nonnegative integer s is called the **spin quantum number**. The difference between the simultaneous eigenstates in the spin case and in the orbital case is that in the spin case, the eigenstates are not functions of position, they are simply a basis of a $2s+1$ dimensional vector space. The quantum number s is inherent to the type of particle. For example, electrons have spin $s = \frac{1}{2}$, photons have spin $s = 1$.

Definition 6.2. Consider a particle with spin eigenstates $(|s, m_s\rangle)_{m_s=-s}^s$ and energy eigenstate $|\psi_n\rangle_{n=1}^{\infty}$ can be fully described by the tensor product of these two spaces. That

 6.2. Spin $\frac{1}{2}$ Particles.

Definition 6.3. In the case $s = \frac{1}{2}$, it is easier on the eyes to denote the states $|\frac{1}{2}, \frac{1}{2}\rangle$ and $|\frac{1}{2}, -\frac{1}{2}\rangle$ as $|\uparrow\rangle$ and $|\downarrow\rangle$ respectively. We now fix the ordered basis $(|\uparrow\rangle, |\downarrow\rangle)$ and define $\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

Exercise 6.4. If we identify the operators in definition 5.1, then we have that

- (1) $S^2 = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
- (2) $S_z = \frac{1}{2}\hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
- (3) $S_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$
- (4) $S_- = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$
- (5) $S_x = \frac{1}{2}\hbar \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
- (6) $S_y = \frac{1}{2}\hbar \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

Proof. Parts (1) through (4) are straight forward using the properties given in definition 5.1. For parts (5) and (6), we observe that $S_x = \frac{1}{2}(S_+ + S_-)$ and $S_y = -\frac{i}{2}(S_+ - S_-)$ \square

Definition 6.5. We define the **Pauli spin matrices** to be

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

So that $S_x = \frac{1}{2}\hbar\sigma_x$, $S_y = \frac{1}{2}\hbar\sigma_y$ and $S_z = \frac{1}{2}\hbar\sigma_z$

7. PERTURBATION THEORY

8. MULTIPLE IDENTICAL PARTICLES

Note 8.1. For the remainder of this section, we consider a system of N identical particles and we assume that the potential energy of the system, $V(r_1, \dots, r_N)$, is symmetric in r_1, \dots, r_N .

8.1. Bosons and Fermions.

Theorem 8.2. The wave function $\Psi(r_1, \dots, r_N)$ of a system is either symmetric or alternating in r_1, \dots, r_N and whether it is symmetric or alternating depends only on the type of particle that populates the system.

Definition 8.3. The particles in a system are called **bosons** if the wave function is symmetric and the particles are called **fermions** if the wave function is alternating.

Definition 8.4. Let $(\Psi_j)_{j \in \mathbb{N}}$ be an orthonormal basis of stationary states for a single-particle component system. For $k = 1, \dots, N$, let $\Psi_{j_k} \in (\Psi_j)_{j \in \mathbb{N}}$ (not necessarily distinct) be the state that particle k . For $j \in \mathbb{N}$, define n_j to be the number of particles in state Ψ_j .

Proof.

□

Exercise 8.5. Show that

Definition 8.6.

9. EXTRA

9.1. Position and Momentum Space.

Definition 9.1. We define the **momentum 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 9.2. 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 9.3. Let $Q(X, P)$ be a self-adjoint operator. Then the properties of the Fourier transform imply that:

$$Q(X, P) = \begin{cases} Q(x, -i\hbar\nabla) & (\text{position space}) \\ Q(i\hbar\nabla, p) & (\text{momentum space}) \end{cases}$$

Exercise 9.4. 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

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

Taking Fourier transforms of both sides, we see that

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

□

Interpretation 9.5. *We interpret $|\Phi(p, t)|^2$ to be the probability density for the momentum, p , of the particle at time t .*

Note 9.6. *For a self-adjoint operator $Q(X, P)$, the expected value of Q , is given by*

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