Notes of Introduction to Quantum Mechanics

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Contents

Chapter 1

The Wave Function

1.1 The Schrodinger Equation

Looking for Particle's wave function

$$\Psi(x,t)$$

by solving the Schrodinger equation

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

Planck's constant

$$\hbar = \frac{h}{2\pi} = 1.054573 \times 10^{-34}\mathrm{Js}$$

1.2 The Statistical Interpretation

Born's statistical interpretation

$$\int_a^b |\Psi(x,t)|^2 \,\mathrm{d}x = \text{probability of finding the particle between a and b}$$

- All quantum mechanics has to offer is statistical information about the possible results.

1.3 Probability

1.3.1 Discrete Variables

The average value of some *function* of *j* is given by

$$\langle f(j)\rangle = \sum_{j=0}^{\infty} f(j)P(j)$$

The **variance** of the distribution

$$\sigma^2 \equiv \langle(\Delta j)^2\rangle$$

The **standard deviation**

$$\sigma = \sqrt{\langle j^2\rangle - \langle j\rangle^2}$$

1.3.2 Continuous Variables

$\rho(x)$: **probability density**

$$P_{ab} = \int_a^b \rho(x)\,\mathrm{d}x$$

Rules:

$$\int_{-\infty}^{\infty} \rho(x)\,\mathrm{d}x = 1$$
$$\langle x\rangle = \int_{-\infty}^{\infty} x\rho(x)\,\mathrm{d}x$$
$$\langle f(x)\rangle = \int_{-\infty}^{\infty} f(x)\rho(x)\,\mathrm{d}x$$
$$\sigma^2 \equiv \langle(\Delta x)^2\rangle = \langle x^2\rangle - \langle x\rangle^2$$

1.4 Normalization

Normalizing the wave function (square-integrable)

$$\int_{-\infty}^{\infty} |\Psi(x)|^2\,\mathrm{d}x = 1$$

Proof the Schrodinger equation automatically preserves the normalization of the wave function:

$$\frac{\partial\Psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} - \frac{i}{\hbar}V\Psi, \quad \frac{\partial\Psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + \frac{i}{\hbar}V\Psi^*$$
$$\downarrow$$
$$\frac{\partial}{\partial t}|\Psi|^2 = \frac{\partial}{\partial t}(\Psi^*\Psi) = \Psi^*\frac{\partial\Psi}{\partial t} + \frac{\partial\Psi^*}{\partial t}\Psi$$
$$\downarrow$$
$$\frac{d}{dt}\int_{-\infty}^{\infty} |\Psi(x)|^2\,\mathrm{d}x = \int_{-\infty}^{\infty} \frac{\partial}{\partial t}|\Psi(x)|^2\,\mathrm{d}x = 0 \qquad \text{QED}$$

1.5 Momentum

For a particle in state Ψ, the expectation value of x is

$$\langle x\rangle = \int_{-\infty}^{\infty} x|\Psi(x)|^2\,\mathrm{d}x = \int \Psi^*\,[x]\,\Psi\,\mathrm{d}x$$

the expectation value of **momentum** is

$$\frac{d\langle x\rangle}{dt} = \frac{i\hbar}{2m}\int x\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\mathrm{d}x = -\frac{i\hbar}{m}\int \Psi^*\frac{\partial\Psi}{\partial x}\mathrm{d}x \quad \Rightarrow$$
$$\langle p\rangle = m\frac{d\langle x\rangle}{dt} = -i\hbar\int\left(\Psi^*\frac{\partial\Psi}{\partial x}\right)\mathrm{d}x = \int \Psi^*\,[-i\hbar(\partial/\partial x)]\,\Psi\,\mathrm{d}x$$

- operator: $x \to$ position; $-i\hbar(\partial/\partial x) \to$ momentum

  the expectation of any $Q(x,p)$ is

$$\langle Q(x,p)\rangle = \int \Psi^*[Q(x, -i\hbar\partial/\partial x)]\Psi\,\mathrm{d}x$$

- **Ehrenfest's theorem**

$$\frac{d\langle p\rangle}{dt} = \left\langle \frac{\partial V}{\partial x} \right\rangle$$

proof: $\displaystyle \frac{d\langle p\rangle}{dt} = -i\hbar \int \frac{\partial}{\partial t}\left(\Psi^* \frac{\partial \Psi}{\partial x}\right) \mathrm{d}x = -i\hbar \left(\frac{i}{\hbar}\right) \int -|\Psi|^2 \frac{\partial V}{\partial x} \mathrm{d}x$

1.6 The Uncertainty Principle

- **de Broglie formula**

$$p = \frac{h}{\lambda} = \frac{2\pi\hbar}{\lambda}$$

- Heisenberg's **uncertainty principle**

$$\sigma_x \sigma_p \geqslant \frac{\hbar}{2}$$

Chapter 2

Time-Independent Schrodinger Equation

2.1 Stationary States

Separation of variables $\Psi(x,t) = \psi(x)\varphi((t)$

$$\frac{d\varphi}{dt} = -\frac{iE}{\hbar}\varphi \qquad \rightarrow \qquad \varphi(t) = e^{-iEt/\hbar}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi \qquad \text{time-independent Schrodinger equation}$$

Three Answers:

- stationary states

$$\Psi(x,t) = \psi(x)\mathrm{e}^{-iEt/\hbar}$$

- states of definite total energy
  - Hamiltonain: $H(x,p) = \frac{p^2}{2m} + V(x)$
  - Hamiltonain operator:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

  - Rewrite time-independent Schrodinger Equation:

$$\hat{H}\psi = E\psi$$

  - expectation value of the total energy: $\langle H \rangle = E \qquad \langle H^2 \rangle = E^2$
  - variance: $\sigma_H = 0$

- linear combination of separable solutions

$$\Psi(x,t) = \sum_{n=1}^{\infty} \psi(x)\mathrm{e}^{-iE_nt/\hbar} = \sum_{n=1}^{\infty} c_n\Psi_n(x,t)$$

  - stationary states:$\Psi_n(x,t)$

- $|c_n|^2$: probability that a measurement of the energy would return the valur E_n

$$\sum_{n=1}^{\infty} |c_n|^2 = 1$$

$$\langle H \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n$$

Four therom

- For normalizable solutions, the separation constant E must be *real*
- $\psi(x)$ can always be taken to *real*; from any complex solution, we can

$$\psi = \frac{1}{2}[(\psi + \psi^*) - i(i(\psi - \psi^*))]$$

- If $V(-x) = V(x)$ then $\psi(x)$ can always be taken to be either even or odd
- E must $> V_{min}$

2.2 The Infinite Square Well

$$V(x) = \begin{cases} 0 & 0 \leqslant x \leqslant a \\ \infty & otherwise \end{cases}$$

Outside the well, $\psi(x) = 0$ Inside the well (**simple harmonic oscillator** equation)

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \qquad \text{where}\, k \equiv \frac{\sqrt{2mE}}{\hbar}$$

- $E \geqslant 0$
- general solution: $\psi(x) = A\sin(kx) + B\cos(kx)$
- **boundary conditions**: $\psi(0) = \psi(a) = 0$
- *distinct* solutions and normalize

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right), \qquad \text{with}\, E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad (n = 1, 2, 3, ...)$$

- **ground state**: ψ_1
- propeties for ψ_n
  - alternately **even** or **odd**
  - each successive state has one more **node**(zero-crossing)
  - matually **orthogonal**

$$\int \psi_m(x)^* \psi_n(x)\, \mathrm{d}x = \delta_{mn}$$

– **complete**

$$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

$$\int \psi_m(x)^* f(x) \mathrm{d}x = \sum_{n=1}^{\infty} c_n \int \psi_m(x)^* \psi_n(x) \mathrm{d}x = \sum_{n=1}^{\infty} c_n \delta_{mn} = c_m$$

$$\Rightarrow \qquad c_n = \int \psi_n(x)^* f(x)\, \mathrm{d}x$$

- ★

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-i(n^2\pi^2\hbar/2ma^2)t}$$

$$c_n = \sqrt{\frac{2}{a}} \int_0^a \sin\left(\frac{n\pi}{a}x\right) \Psi(x,0)\, \mathrm{d}x$$

-

$$\hat{H}\psi_n = E_n\psi_n \quad \rightarrow \quad \langle H \rangle = \int \Psi^* \hat{H} \Psi \mathrm{d}x = \sum |c_n|^2 E_n$$

2.3 The Harmonic Oscillator

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

$$\hat{H} = \frac{1}{2m}\left[\hat{p}^2 + (m\omega x)^2\right]$$

2.3.1 Algebratic Method

$$\left[\hat{A}, \hat{B}\right] \equiv \hat{A}\hat{B} - \hat{B}\hat{A} \rightarrow [x, \hat{p}] = i\hbar$$

$$\hat{a}_\pm \equiv \frac{1}{\sqrt{2\hbar m\omega}}(\mp i\hat{p} + m\omega x) \rightarrow \begin{cases} x = \sqrt{\dfrac{\hbar}{2m\omega}}(\hat{a}_+ + \hat{a}_-) \\ \hat{p} = i\sqrt{\dfrac{\hbar m\omega}{2}}(\hat{a}_+ - \hat{a}_-) \end{cases}$$

$$\downarrow$$

$$\begin{cases} \hat{a}_+\hat{a}_- = \dfrac{1}{\hbar\omega}\hat{H} - \dfrac{1}{2} \\ \hat{a}_-\hat{a}_+ = \dfrac{1}{\hbar\omega}\hat{H} + \dfrac{1}{2} \end{cases} \qquad \rightarrow \qquad \begin{array}{l} \star \quad \hbar\omega\left(\hat{a}_\pm\hat{a}_\mp \pm \dfrac{1}{2}\right)\psi = E\psi \\ \quad\;\; [\hat{a}_-, \hat{a}_+] = 1 \end{array}$$

$$\downarrow$$

$$\hat{H}(\hat{a}_+\psi) = (E + \hbar\omega)(\hat{a}_+\psi)$$

$$\hat{H}(\hat{a}_-\psi) = (E - \hbar\omega)(\hat{a}_-\psi)$$

There occurs a "lowest rung" : $\hat{a}_-\psi_0 = 0 \rightarrow \hbar\omega(\hat{a}_+\hat{a}_- + 1/2)\psi_0 = E_0\psi_0 \rightarrow$

$$\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}, \qquad \text{with} \qquad E_0 = \frac{1}{2}\hbar\omega$$

Exited states, increasing the energy by $\hbar\omega$ with each step:

$$\psi_n = A_n(\hat{a}_+)^n \psi_0(x), \qquad \text{with} \qquad E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

Normalization algebraically

- $\hat{a}_+\psi_n = c_n\psi_{n+1}, \qquad \hat{a}_-\psi_n = d_n\psi_{n-1}$

$$\int_{-\infty}^{\infty} f^*(\hat{a}_\pm g)\,\mathrm{d}x = \int_{-\infty}^{\infty} (\hat{a}_\mp f)^* g\,\mathrm{d}x$$

$$\downarrow$$

$$\begin{cases} c_n = \sqrt{n+1} \\ d_n = \sqrt{n} \end{cases} \qquad \leftarrow \begin{cases} \int_{-\infty}^{\infty} (\hat{a}_\pm\psi_n)^*(\hat{a}_\pm\psi_n)\,\mathrm{d}x = \int_{-\infty}^{\infty} (\hat{a}_\mp\hat{a}_\pm\psi_n)^*\psi_n\,\mathrm{d}x \\ \hat{a}_+\hat{a}_-\psi_n = n\psi_n, \qquad \hat{a}_-\hat{a}_+\psi_n = (n+1)\psi_n \end{cases}$$

$$\Downarrow$$

$$\star \quad \psi_n = \frac{1}{\sqrt{n!}}(\hat{a}_+)^n\psi_0(x)$$

2.3.2 Analytic Method

$$\frac{d^2\psi}{d\xi^2} = (\xi^2 - K)\psi \qquad \xi \equiv \sqrt{\frac{m\omega}{\hbar}}x \quad K \equiv \frac{2E}{\hbar\omega}$$

To begin with at very large ξ

$$\frac{d^2\psi}{d\xi^2} \approx \xi^2\psi \quad \xrightarrow{|x|\to\infty \qquad \text{asymptotic form}} \quad \psi(\xi) = h(\xi)e^{-\xi^2/2}$$

$$\xrightarrow{\frac{d\psi}{d\xi},\,\frac{d^2\psi}{d\xi^2}} \qquad \frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (K-1)h = 0$$

In the form of *power serires* in ξ

$$h(\xi) = \sum_{j=0}^{\infty} a_j\xi^j \quad \xrightarrow{\frac{dh}{d\xi},\,\frac{d^2h}{d\xi^2}}$$

$$\sum_{j=0}^{\infty}[(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j]\xi^j = 0$$

$$\Downarrow$$

$$a_{j+2} = \frac{(2j+1-K)}{(jh+1)(j+2)}a_j \quad \rightarrow \quad h(\xi) = h_{\text{even}}(\xi) + h_{\text{odd}}(\xi)$$

For physically acceptable solutions:

$$K = 2n+1 \Rightarrow E = (n+1/2)\hbar\omega \quad ,\text{for } n = 0, 1, 2, \ldots$$

$$\downarrow$$

$$a_{j+2} = \frac{-2(n-j)}{(jh+1)(j+2)}a_j$$

Nomalized stationary state

$$\star \qquad \psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}H_n(\xi)e^{-\xi^2/2}$$

- The first few of $H_n(\xi)$
  - $H_0 = 1$
  - $H_1 = 2\xi$
  - $H_2 = 4\xi^2 - 2$
  - $H_3 = 8\xi^3 - 12\xi$

2.4 The Free Particle

$$V(x) = 0$$

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \quad \text{where} \quad k \equiv \frac{\sqrt{2mE}}{\hbar}$$

$$\downarrow$$

$$\Psi(x,t) = Ae^{ik\left(x-\frac{\hbar k^2}{2m}t\right)} + Be^{-ik\left(x-\frac{\hbar k^2}{2m}t\right)}$$

Represents a wave traveling to *right* and another going to *left*, as well write

$$\Psi_k(x,t) = Ae^{i\left(kx-\frac{\hbar k^2}{2m}t\right)}$$

$$k \equiv \pm\frac{\sqrt{2mE}}{\hbar}, \quad \text{with} \quad \begin{cases} k > 0 \Rightarrow \text{traveling to the right} \\ k < 0 \Rightarrow \text{traveling to the left} \end{cases}$$

This wave function is not normalizable

$$\int_{-\infty}^{+\infty} \Psi_k^* \Psi_k \mathrm{d}x = |A|^2 \int_{-\infty}^{+\infty} \mathrm{d}x = |A|^2(\infty)$$

- **Plancherel's therem**

  $$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k)e^{ikx}\mathrm{d}k \leftrightarrow F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x)e^{-ikx}\mathrm{d}x$$

  Now *this* can be normalized

  $$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)e^{i\left(kx-\frac{\hbar k^2}{2m}t\right)}\mathrm{d}k$$

  $$\begin{cases} \Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)e^{ikx}\mathrm{d}k \\ \phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x,0)e^{-ikx}\mathrm{d}x \end{cases}$$

- $v_{\text{classical}} = v_{\text{group}} = 2v_{\text{phase}}$

2.5 The Delta-Function Potential

2.5.1 Bound States and Scattering States

$$\begin{cases} E < V(\infty) \Rightarrow \text{bound state} \\ E > V(\infty) \Rightarrow \text{scattering state} \end{cases}$$

2.5.2 The Delta-Fuction Well

$$V(x) = -\alpha\delta(x)$$

(1) bound state $E < 0$

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi, \quad \text{where} \quad \kappa \equiv \frac{\sqrt{-2mE}}{\hbar}$$

$$\Downarrow$$

$$\psi(x) = \begin{cases} Be^{\kappa x}, & (x < 0) \\ Fe^{-\kappa x}, & (x > 0) \end{cases}$$

- boundary conditions at $x = 0$:
  - ψ is always continuous; $\Rightarrow F = B$
  - $d\psi/dx$ is continuous except at points where the potential is infinite.

$$\kappa = \frac{m\alpha}{\hbar^2}$$

Proof: $(\epsilon \to 0)$

$$-\frac{\hbar^2}{2m}\int_{-\epsilon}^{+\epsilon}\frac{d^2\psi}{d^2x}dx + \int_{-\epsilon}^{+\epsilon}V(x)\psi(z)dx = E\int_{-\epsilon}^{+\epsilon}\psi(x)dx = 0$$

$$\Rightarrow \Delta\left(\frac{d\psi}{dx}\right) = \frac{2m}{\hbar^2}\lim_{\epsilon\to 0}\int_{-\epsilon}^{+\epsilon} -\alpha\delta(x)\psi(z)dx = -\frac{2m\alpha}{\hbar^2}\psi(0) = -\frac{2m\alpha}{\hbar^2}B_\kappa$$

$$\begin{cases} d\psi/dx|_+ = -B\kappa \\ d\psi/dx|_- = +B\kappa \end{cases} \quad \Rightarrow \quad \Delta\left(\frac{d\psi}{dx}\right) = -2B\kappa \quad \Rightarrow$$

Norminized $\to B = \sqrt{\kappa}$

$$\star \quad \psi(x) = \frac{\sqrt{m\alpha}}{\hbar}e^{-m\alpha|x|/\hbar^2}; \qquad E = -\frac{m\alpha^2}{2\hbar^2}$$

(2) scattering state $E > 0$

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \quad \text{where} \quad k \equiv \frac{\sqrt{2mE}}{\hbar}$$

$$\Downarrow$$

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & (x < 0) \\ Fe^{ikx} + Ge^{-ikx}, & (x > 0) \end{cases}$$

- Boundary conditions

$$F + G = A + B$$

$$\begin{cases} \Delta(d\psi/dx) = ik(F - G - A + B) \\ \psi(0) = (A + B) \end{cases} \quad \Rightarrow$$

$$ik(F - G - A + B) = -\frac{2m\alpha}{\hbar^2}(A + B)$$

$$F - G = A(1 + 2i\beta) - B(1 - 2i\beta), \qquad \text{where } \beta \equiv \frac{m\alpha}{\hbar^2 k}$$

When wave come from left:

- A: amplitude of the incident wave
- B: amplitude of the reflected wave
- F: amplitude of the transmitted wave

$$B = \frac{i\beta}{1-i\beta}A, \qquad F = \frac{1}{1-i\beta}A, \qquad G = 0$$

The *relative* probability of reflection and transmission:

$$\star \quad \begin{aligned} R &\equiv \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1+\beta} = \frac{1}{1+(2\hbar^2 E/m\alpha^2)} \\ T &\equiv \frac{|F|^2}{|A|^2} = \frac{1}{1+\beta} = \frac{1}{1+(m\alpha^2/2\hbar^2 E)} \end{aligned}$$

Discussion:

- If $E > V_{\max}$, then $T = 1$ and $R = 0$
- If $E < V_{\max}$, then $T = 0$ and $R = 1$
  - if $T \neq 0$, **tunneling**

Fourier transform of $\delta(x)$

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{ikx}\,dk \qquad \leftrightarrow \qquad F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\delta(x)e^{-ikx}dx = \frac{1}{\sqrt{2\pi}}$$

2.6 The Finite Square Well

$$V(x) = \begin{cases} -V_0, & -a \leqslant x \leqslant a \\ 0, & |x| > a \end{cases}$$

(1) bound state $E < 0$

1. $x < -a, V(x) = 0$

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi, \quad \text{where} \quad \kappa \equiv \frac{\sqrt{-2mE}}{\hbar}$$

$$\Rightarrow \qquad \psi(x) = Be^{\kappa x}$$

2. $-a < x < a, V(x) = -V_0$

$$\frac{d^2\psi}{dx^2} = -l^2\psi, \quad \text{where} \quad l \equiv \frac{\sqrt{2m(E+V_0)}}{\hbar}$$

$$\Rightarrow \qquad \psi(x) = C\sin(lx) + D\cos(lx)$$

3. $x > a, V(x) = 0$

$$\psi(x) = Fe^{-\kappa x}$$

- even solutions

$$\psi(x) = \begin{cases} Fe^{-\kappa x}, & (x > a) \\ D\cos(lx), & (0 < x < a) \\ \psi(-x), & (x < 0) \end{cases}$$

- boundary condition at $x = a$

$$\begin{cases} Fe^{-\kappa a} = D\cos(la) \\ -\kappa Fe^{-\kappa a} = -lD\sin(la) \end{cases} \Rightarrow \qquad \kappa = l\tan(la)$$

$$\begin{cases} z \equiv la \qquad z_0 \equiv \dfrac{a}{\hbar}\sqrt{2mV_0} \\ \kappa^2 + l^2 = 2mV_0/\hbar^2 \end{cases} \Rightarrow \qquad \boxed{\tan z = \sqrt{(z_0/z)^2 - 1}}$$

Discussion:

- Wide, deep well

$$z_0 \to \infty \qquad \Rightarrow z_n = n\pi/2 \qquad \Rightarrow$$

$$E_n + V_0 \approx \frac{n^2\pi^2\hbar^2}{2m(2a)^2} \qquad (n = 1, 3, 5, \cdots)$$

- Shallow, narrow well
  - for $z_0 < \pi/2$, only one remains

(2) scattering state $E > 0$ When wave come from left

$$\psi(x) = \begin{cases} Ae^{ikx} + B^{-ikx}, & x < -a \\ C\sin(lx) + D\cos(lx) & -a < x < a \\ Fe^{ikx} & x > a \end{cases}$$

Boundary conditions

$$\begin{aligned} Ae^{-ika} + B^{ika} &= -C\sin(la) + D\cos(la) \\ ik[Ae^{-ika} - B^{ika}] &= l[C\cos(la) + D\sin(la)] \\ C\sin(la) + D\cos(la) &+ Fe^{ika} \\ l[C\cos(la) - D\sin(la)] &= ikFe^{ika} \end{aligned} \Rightarrow$$

Eliminate

$$\begin{aligned} B &= i\frac{\sin(2la)}{2kl}(l^2 - k^2)F \\ F &= \frac{e^{-2ika}A}{\cos(2la) - i\frac{(k^2+l^2)}{2kl}\sin(2la)} \end{aligned} \Rightarrow$$

Transmission coefficient

$$T^{-1} = 1 + \frac{V_0^2}{4E(E+V_0)}\sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)$$

when $T = 1$

$$\frac{2a}{\hbar}\sqrt{2m(E+V_0)} = n\pi \qquad \Rightarrow E_n + V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}$$

Chapter 3

Formalism

3.1 Hilbert Space

Contructs:

- state: wave function
- observables: operators
- vectors: defining conditions
- linear transformation: the operators act on vectors
- linear algebra: the natural language of Quantum Mechanics

Properties:

1. wave function live in
2. complete inner product space
3. squre-integrable

Definition 1 *Inner product of two function*

$$\langle f|g\rangle \equiv \int_a^b f(x)^* g(x)\mathrm{d}x$$

Discussion:

- Schwarz inequality:

$$\left|\int_a^b f(x)^* g(x)\mathrm{d}x\right| \leqslant \sqrt{\int_a^b |f(x)|^2\mathrm{d}x \int_a^b |g(x)|^2\mathrm{d}x}$$

- $\langle g|f\rangle = \langle f|g\rangle^*$
- normalized $\langle f|f\rangle = 1$
- orthonormal $\langle f_m|f_n\rangle = \delta_{mn}$
- complete and orthonormal $f(x) = \sum_{n=1}^{\infty} c_n f_n(x), c_n = \langle f_n|f\rangle$

3.2 Observables

3.2.1 Hermitian Operators

Definition 2 *Hermitian Operators*

$$\langle f|\hat{Q}g\rangle = \langle \hat{Q}f|g\rangle \qquad \textit{for all } f(x) \textit{ and } g(x)$$

Discussion:

- Observables are represented by hermitian operators
- hermitian transformation $\hat{Q}^\dagger = \hat{Q}$
- momentum operator is hermitian

$$\langle f|\hat{p}g\rangle = \int_{-\infty}^{\infty} f^*(-i\hbar)\frac{\mathrm{d}g}{\mathrm{d}x}\mathrm{d}x = -i\hbar f^* g\bigg|_{-\infty}^{\infty} + \int_{-\infty}^{\infty}\left(-i\hbar\frac{\mathrm{d}f}{\mathrm{d}x}\right)^* g\mathrm{d}x = \langle \hat{p}f|g\rangle$$

Definition 3 *Hermitian conjugate of a matrix*

$$\mathsf{T}^\dagger = \tilde{\mathsf{T}}^*$$

$$\left\langle \alpha \middle| \hat{T}\beta \right\rangle = \mathsf{a}^\dagger \mathsf{T} \mathsf{b} = \left(\mathsf{T}^\dagger \mathsf{a}\right)^\dagger \mathsf{b} = \left\langle \hat{T}^\dagger \alpha \middle| \beta \right\rangle$$

Discussion:

- The eigenvalues of a hermitian transformation are real
  Proof: Let $\hat{T}\,|\alpha\rangle = \lambda\,|\alpha\rangle$, with $|\alpha\rangle \neq |0\rangle$. Then
  $$\left\langle \alpha \middle| \hat{T}\alpha \right\rangle = \langle \alpha|\lambda\alpha\rangle = \lambda\,\langle a|a\rangle$$
  Meanwhile, if $\hat{T}$ is hermitian, Then
  $$\left\langle \alpha \middle| \hat{T}\alpha \right\rangle = \left\langle \hat{T}\alpha \middle| \alpha \right\rangle = \langle \lambda\alpha|\alpha\rangle = \lambda^*\,\langle a|a\rangle$$
  But $\langle \alpha|\alpha\rangle \neq 0$, so $\lambda = \lambda^*$ QED
- The eigenvectors of a hermitian transformation belonging to distinct eigenvalues are orthognal
- The eigenvectors of a hermitian transformation span the space

3.2.2 Determinate State

$$\sigma^2 = \left\langle (Q - \langle Q\rangle)^2 \right\rangle = \left\langle \Psi|(\hat{Q}-q)^2\Psi \right\rangle = \left\langle (\hat{Q}-q)\Psi|(\hat{Q}-q)\Psi \right\rangle = 0$$
$$\Downarrow$$
$$\hat{Q}\Psi = q\Psi$$

Discussion:

- This is eigenvalue equation for $\hat{Q}$
- Ψ if an eigenfuction of $\hat{Q}$, and q is the corresponding eigenvalue
- Determinate state of Q are eigenfuction of $\hat{Q}$
- spectrum: the collection of all the eigenvalues of an operator
- degenerate: linearly independent eigenfuctions share the same eigenvalue

3.3 Eigenfuctions of a Hermitain Operator

3.3.1 Discrete Spectra

- the eigenvalues are separated from another
- the eigenfuctions lie in Hilbert space and constitute physically realizable states

Properties of normalizable eigenfuctions of a hermitian operator:

1. Their eigenvalues are *real*
2. Eigenfuctions belonging to distinct eigenvalues are *orthognal*

3.3.2 Continuous Spectra

- the eigenvalues fill out an entire range
- the eigenfuctions are not normalizable and do not represent possible wave functions

The eigenfuctions and eigenvalues of the momentum operator (on the interval $(-\infty < x < \infty)$:

$$-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}f_p(x) = pf_p(x) \quad \Rightarrow \quad f_p(x) = Ae^{ipx/\hbar}$$

$$\downarrow$$

$$\int_{-\infty}^{\infty} f_{p'}^*(x)f_p(x)\mathrm{d}x = |A|^2\int_{-\infty}^{\infty} e^{i(p-p')x/\hbar}\mathrm{d}x = |A|^2 2\pi\hbar\delta(p-p')$$

$$\Downarrow$$

$$f_p(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}$$

- Dirac orthonormality: $\langle f_{p'}|f_p\rangle = \delta(p-p')$
- Complete:

$$f(x) = \int_{-\infty}^{\infty} c(p)f_p(x)dp = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} c(p)e^{ipx/\hbar}\mathrm{d}p$$
$$\langle f_{p'}|f\rangle = \int_{-\infty}^{\infty} c(p)\langle f_{p'}|f_p\rangle\mathrm{d}p = \int_{-\infty}^{\infty} c(p)\delta(p-p')\mathrm{d}p = c(p')$$

The eigenfuctions and eigenvalues of the positoin operator:

$$\hat{x}g_y(x) = xg_y(x) = yg_y(y) \quad \Rightarrow \quad g_y(x) = A\delta(x-y)$$

$$\downarrow$$

$$\int_{-\infty}^{\infty} g_{y'}^* g_y(x)\mathrm{d}x = |A|^2\int_{-\infty}^{\infty} \delta(x-y')\delta(x-y)\mathrm{d}x = |A|^2\delta(y-y')$$

$$\Downarrow$$

$$g_y(x) = \delta(x-y)$$

3.4 Generalized Statistical Interpretation

Observable: $Q(x,p)$
State: $\Psi(x,t)$
One of eigenvalues: $\hat{Q}(x - i\hbar d/dx)$
The probablility of getting eigenvalues(orthonormal):

1. Discrete spectrum

   - probablility of getting q_n

   $$|c_n|^2, \qquad \text{where} \quad c_n = \langle f_n|\Psi\rangle$$

   - Complete:

   $$\Psi(x,t) = \sum_n c_n(t) f_n(x)$$
   $$c_n(t) = \langle f_n|\Psi\rangle = \int f_n(x)^*\Psi(x,t)\mathrm{d}x$$
   $$\sum_n |c_n|^2 = 1$$

   - The expectation value of Q:

   $$\langle Q\rangle = \left\langle \Psi|\hat{Q}\Psi\right\rangle = \sum_n\sum_{n'} c_{n'}^* c_n q_n \langle f_{n'}|f_n\rangle = \sum_n q_n|c_n|^2$$

2. Continuous spectrum

   - probablility of getting a result in the range dz

   $$|c(z)|^2\mathrm{d}z, \qquad \text{where} \quad c(z) = \langle f_z|\Psi\rangle$$

   - For positoin measurements:

   $$c(y) = \langle g_y|\Psi\rangle = \int_{-\infty}^{\infty} \delta(x-y)\Psi(x,t)\mathrm{d}x = \Psi(y,t)$$

   - For momentum measurements:

   $$c(p) = \langle f_p|\Psi\rangle = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\Psi(x,t)\mathrm{d}x$$

   - Fourier transformation:

   $$\Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\Psi(x,t)\mathrm{d}x$$
   $$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{ipx/\hbar}\Phi(p,t)\mathrm{d}p$$

   - Expectation:

   $$\langle Q(x,p,t)\rangle = \begin{cases} \int \Psi^*\hat{Q}\left(x, -i\hbar\dfrac{\partial}{\partial x}, t\right)\Psi\,\mathrm{d}x, & \text{in position space} \\ \int \Phi^*\hat{Q}\left(i\hbar\dfrac{\partial}{\partial p}, p, t\right)\Phi\,\mathrm{d}p, & \text{in momentum space} \end{cases}$$

3.5 The Uncertainty Principle

3.5.1 Proof of the Generalized Uncertainty Principle

$$f \equiv \left(\hat{A} - \langle A \rangle\right)\Psi \quad \rightarrow \quad \sigma_A^2 \sigma_B^2 = \langle f|f\rangle\langle g|g\rangle \geqslant |\langle f|g\rangle|^2$$

$$|z|^2 \geqslant [\mathrm{Im}(z)]^2 = \left[\frac{1}{2i}(z - z^*)\right]^2 \quad \Rightarrow \quad \sigma_A^2 \sigma_B^2 \geqslant \left(\frac{1}{2i}\left[\langle f|g\rangle - \langle g|f\rangle\right]\right)^2$$

$$\langle f|g\rangle - \langle g|f\rangle = \left\langle \hat{A}\hat{B} \right\rangle - \langle A\rangle\langle B\rangle - \left(\left\langle \hat{B}\hat{A} \right\rangle - \langle A\rangle\langle B\rangle\right) = \left\langle \left[\hat{A}, \hat{B}\right] \right\rangle$$

$$\Downarrow$$

$$\boxed{\sigma_A^2 \sigma_B^2 \geqslant \left(\frac{1}{2i}\left\langle \left[\hat{A}, \hat{B}\right] \right\rangle\right)^2}$$

3.5.2 The Minimum-Uncertainty Wave Packet

$$g(x) = iaf(x), \qquad \text{where } a \text{ is real}$$

$$\Rightarrow \left(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x} - \langle p\rangle\right)\Psi = ia(x - \langle x\rangle)\Psi$$

$$\Rightarrow \Psi(x) = Ae^{-a(x-\langle x\rangle)^2/2\hbar}e^{i\langle p\rangle/\hbar}$$

3.5.3 The Energy-Time Uncertainty Principle

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}\langle Q\rangle = \dfrac{\mathrm{d}}{\mathrm{d}t}\left\langle \Psi|\hat{Q}\Psi \right\rangle \\ i\hbar\dfrac{\partial \Psi}{\partial t} = \hat{H}\Psi, \quad \text{where} \qquad H = \dfrac{p^2}{2m} + V \\ \left\langle \hat{H}\Phi \middle| \hat{Q}\Phi \right\rangle = \left\langle \Phi \middle| \hat{H}\hat{Q}\Phi \right\rangle \end{cases} \qquad \Rightarrow$$

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\langle Q\rangle = \frac{i}{\hbar}\left\langle \left[\hat{H}, \hat{Q}\right] \right\rangle + \left\langle \frac{\partial \hat{Q}}{\partial t} \right\rangle}$$

Assume that Q does not depend explicity on t:

$$\sigma_H^2 \sigma_Q^2 \geqslant \left(\frac{1}{2i}\left\langle \left[\hat{H}, \hat{Q}\right] \right\rangle\right)^2 = \left(\frac{\hbar}{2}\right)^2 \left(\frac{d\langle Q\rangle}{dt}\right)^2$$

$$\begin{matrix} \Delta E \equiv \sigma_H \\ \Delta t \equiv \dfrac{\sigma_Q}{|d\langle Q\rangle/dt|} \end{matrix} \qquad \Rightarrow \qquad \Delta t \Delta E \geqslant \frac{\hbar}{2}$$

3.6 Vectors and Operators

3.6.1 Bases in Hillbert Space

$$\begin{aligned}
\Psi(x,t) &= \langle x|\mathcal{S}(t)\rangle \\
\Phi(p,t) &= \langle p|\mathcal{S}(t)\rangle \\
c_n(t) &= \langle n|\mathcal{S}(t)\rangle
\end{aligned}$$

$$\begin{aligned}
|\mathcal{S}(t)\rangle \to \int \Psi(y,t)\delta(x-y)\,\mathrm{d}y &= \int \Phi(p,t)\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}\,\mathrm{d}p \\
&= \sum c_n e^{-iE_nt/\hbar}\psi_n(x)
\end{aligned}$$

Operator "Trandform"

$$|\beta\rangle = \hat{Q}\,|\alpha\rangle\,, \quad \text{components} \begin{cases} |\alpha\rangle = \sum\limits_n a_n\,|e_n\rangle & a_n = \langle e_n|\alpha\rangle \\ |\beta\rangle = \sum\limits_n b_n\,|e_n\rangle & b_n = \langle e_n|\beta\rangle \end{cases}$$

$$\Rightarrow \qquad \sum_n b_n\,\langle e_m|e_n\rangle = \sum_n a_n\,\langle e_m|\hat{Q}|e_n\rangle \qquad \to \langle e_m|\hat{Q}|e_n\rangle \equiv Q_{mn}$$

$$\Rightarrow \qquad b_m = \sum_n Q_{mn}a_n$$

Schrodinger equation:

$$\begin{aligned}
i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\mathcal{S}(t)\rangle = \hat{H}|\mathcal{S}(t)\rangle, &\qquad \text{Time-dependent} \\
\hat{H}|s\rangle = E|s\rangle, &\qquad \text{Time-independent}
\end{aligned}$$

Particular example of vectors:

$$\hat{x}\,\text{(the position operator)} \to \begin{cases} x & \text{(in positoin space)} \\ i\hbar\partial/\partial p & \text{(in momentum space)} \end{cases}$$

$$\hat{p}\,\text{(the momentum operator)} \to \begin{cases} -i\hbar\partial/\partial x & \text{(in positoin space)} \\ p & \text{(in momentum space)} \end{cases}$$

3.6.2 Dirac Notation

bra: $\langle\alpha|$
ket: $|\beta\rangle$
Orthonormal basis (complete):

- Discrete

$$\langle e_m|e_n\rangle = \delta_{mn} \qquad \to \qquad \sum_n |e_n\rangle\langle e_n| = 1$$

- Continuous

$$\langle e_z|e_{z'}\rangle = \delta(z-z') \qquad \to \qquad \int |e_z\rangle\langle e_{z'}|\,\mathrm{d}z = 1$$

Baker-Campbell-Hausdrff formula:

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{-\hat{C}/2}, \qquad \text{where} \qquad \hat{C} = \left[\hat{A},\hat{B}\right]$$

3.6.3 Changing Bases in Dirac Notation

$$\text{the positoin eigenstats : } |x\rangle \qquad 1 = \int dx\, |x\rangle\langle x|$$
$$\rightarrow \quad |\mathcal{S}(t)\rangle = \int dx\, |x\rangle\langle x|\mathcal{S}(t)\rangle \equiv \int \Psi(x,t)\, |x\rangle\, \mathrm{d}x$$
$$\text{the momentum eigenstats : } |p\rangle \qquad 1 = \int dp\, |p\rangle\langle p|$$
$$\rightarrow \quad |\mathcal{S}(t)\rangle = \int dp\, |p\rangle\langle p|\mathcal{S}(t)\rangle \equiv \int \Phi(p,t)\, |p\rangle\, \mathrm{d}p$$
$$\text{the energy eigenstats : } |n\rangle \qquad 1 = \sum |n\rangle\langle n|$$
$$\rightarrow \quad |\mathcal{S}(t)\rangle = \sum_n |n\rangle\langle n|\mathcal{S}(t)\rangle \equiv \sum c_n(t)\, |n\rangle$$

Operators act on kets

$$\langle x|\hat{x}|\mathcal{S}(t)\rangle = \text{action of position operator in } x \text{ basis} = x\Psi(x,t)$$
$$\langle p|\hat{x}|\mathcal{S}(t)\rangle = \text{action of position operator in } p \text{ basis} = i\hbar\frac{\partial \Phi}{\partial p}$$

Proof:

$$\langle p|\hat{x}|\mathcal{S}(t)\rangle = \left\langle p \left| \hat{x} \int dx |x\rangle\langle x| \right| \mathcal{S}(t) \right\rangle = \int \langle p|x|x\rangle\langle x|\mathcal{S}(t)\rangle dx = i\hbar\frac{\partial}{\partial p}\langle p|\mathcal{S}(t)\rangle$$

3.7 Wave Functions in Position and Momentum Space(Additic

NOTE: x,$f(x)$,p are operators, different form all above

3.7.1 Position-Space Wave Function

The base ket used are the position kets satisfying

$$x|x'\rangle = x'|x'\rangle \qquad \langle x''|x'\rangle = \delta(x'' - x')$$

A physical state can be expanded in terms of x'

$$|\alpha\rangle = \int dx' |x'\rangle\langle x'|\alpha\rangle$$
$$|\langle x'|\alpha\rangle|^2 dx' \qquad \text{probablility}$$
$$\langle x'|\alpha\rangle \equiv \psi_\alpha(x') \qquad \text{wave function}$$

Using the completness of $|x'\rangle$, we have

$$\langle \beta|\alpha\rangle = \int dx'\, \langle \beta|x'\rangle\langle x'|\alpha\rangle = \int dx' \psi^*_\beta(x')\psi^*_\alpha(x')$$

the probablility amplitude for state $|\alpha\rangle$ to be found in state $|\beta\rangle$

$f(x)$ is a function of x

$$\langle x'|f(x)|x''\rangle = (\langle x'|) \cdot (f(x'')|x'') = f(x')\delta(x' - x'')$$
$$\langle \beta|f(x)|\alpha\rangle = \int dx' \int dx''\, \langle \beta|x'\rangle\langle x'|f(x)|x''\rangle\langle x''|\alpha\rangle$$
$$= \int dx'\, \psi^*_\beta(x')f(x')\psi_\alpha(x')$$

3.7.2 Momentum Operator in the Position Basis

$$p|\alpha\rangle = \int dx'|x'\rangle \left(-i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle\right)$$
$$\Rightarrow \langle x'|p|\alpha\rangle = -i\hbar\frac{\partial}{\partial x'}\langle x'|\alpha\rangle$$

Properties:

$$\langle x'|p^n|x''\rangle = (-i\hbar)^n\frac{\partial^n}{\partial x'^n}\delta(x'-x'')$$
$$\langle\beta|p^n|\alpha\rangle = \int dx'\,\psi^*_\beta(x')\left((-i\hbar)^n\frac{\partial^n}{\partial x'^n}\right)\psi_\alpha(x')$$

3.7.3 Momentum-Space Wave Function

The base eigenkets in the p-basis specify

$$p|p'\rangle = p'|p'\rangle \qquad \langle p'|p''\rangle = \delta(p'-p'')$$

Same way as $|x'\rangle$

$$|\alpha\rangle = \int dp'|p'\rangle\langle p'|\alpha\rangle$$
$$|\langle p'|\alpha\rangle|^2 dp' \qquad \text{probablility}$$
$$\langle p'|\alpha\rangle \equiv \phi_\alpha(p') \qquad \text{momentum-space wave function}$$

Transformation function from x to p: $\langle x'|p'\rangle$

$$\langle x'|p|p'\rangle = -i\hbar\frac{\partial}{\partial x'}\langle x'|p'\rangle = p'\langle x'|p'\rangle$$
$$\Rightarrow \langle x'|p'\rangle = N\exp\left(\frac{ip'x'}{\hbar}\right)$$

Discussion:

- the probablility amplitude for $|p'\rangle$ specified by p' to be found at positoin x'
- the wave function for $|p'\rangle$, referred to as the momentum eigenfuction (still in the x-space)
- Nomalization: $N = \dfrac{1}{\sqrt{2\pi\hbar}}$

$$\langle x'|x''\rangle = \int \mathrm{d}p'\,\langle x'|p'\rangle\langle p'|x''\rangle$$
$$\delta(x'-x'') = |N|^2\int \mathrm{d}p'\exp\left[\frac{ip'(x'-x'')}{\hbar}\right]$$
$$= 2\pi\hbar\delta(x'-x'')$$

Rewrite:

$$\begin{cases}\langle x'|\alpha\rangle = \int dp'\langle x'|p'\rangle\langle p'|\alpha\rangle \\ \langle p'|\alpha\rangle = \int dx'\langle p'|x'\rangle\langle x'|\alpha\rangle\end{cases} \Leftrightarrow \begin{aligned}\psi_\alpha(x') &= \left[\frac{1}{\sqrt{2\pi\hbar}}\right]\int dp'\exp\left(\frac{ip'x'}{\hbar}\right)\phi_\alpha(p') \\ \phi_\alpha(p') &= \left[\frac{1}{\sqrt{2\pi\hbar}}\right]\int dx'\exp\left(\frac{-ip'x'}{\hbar}\right)\psi_\alpha(x')\end{aligned}$$

Chapter 4

Quantum Mechanics in Three Dimensionss

4.1 The Schroding Equation

4.1.1 Cartesian Coordinates

Laplacian

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Schroding's Equation

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

Canonical commutation relations

$$[r_i, p_j] = i\hbar\delta_{ij} \qquad [r_i, r_j] = [p_i, p_j] = 0$$

Three-Dimensional of Ehrenfest's theorem

$$\frac{\mathrm{d}}{\mathrm{d}r}\langle \mathbf{r} \rangle = \frac{1}{m}\langle \mathbf{p} \rangle, \qquad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}t}\langle \mathbf{p} \rangle = \langle -\nabla V \rangle$$

Heisenberg's uncertainty principle

$$\sigma_{x,y,z}\sigma_{p_x,p_y,p_z} \geqslant \hbar/2$$

4.1.2 Spherical Coordinates

Time-independent Schrodinger equation

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

$$\Downarrow$$

$$\psi(r,\theta,\phi) = R(r)Y(\theta,\phi) \qquad \Rightarrow \qquad \begin{aligned} &\frac{1}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) - \frac{2mr^2}{\hbar^2}[V(r) - E] = \ell(\ell+1) \\ &\frac{1}{Y}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right\} = -\ell(\ell+1) \end{aligned}$$

4.1.3 The Angular Equation

$$Y(\theta,\phi)=\Theta(\theta)\Phi(\phi) \qquad \Rightarrow \qquad \begin{aligned} &\frac{1}{\Theta}\left[\sin\theta\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right)\right]+\ell(\ell+1)\sin^2\theta=m^2 \\ &\frac{1}{\Phi}\frac{\mathrm{d}^2\Theta}{\mathrm{d}\theta^2}=-m^2 \end{aligned}$$

Associated Legendre function

$$P_\ell^m(x)\equiv(-1)^m\left(1-x^2\right)^{m/2}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^m P_\ell(x)$$

Legendre polynomial

$$P_\ell(x)\equiv\frac{1}{2^\ell\ell!}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^\ell\left(x^2-1\right)^\ell$$

Spherical harmonics

$$\boxed{Y_\ell^m(\theta,\phi)=\sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}e^{im\phi}P_\ell^m(\cos\theta)}$$

- $\ell=0,1,2\cdots$
- $m=-\ell,-\ell+1,\cdots,-1,0,1,\cdots,\ell-1,\ell$

Nomalization

$$\int_0^\infty|R|^2r^2\mathrm{d}r=1 \qquad \int_0^\pi\int_0^{2\pi}|Y|^2\sin\theta\mathrm{d}\theta\mathrm{d}\phi=1$$

orthognal

$$\int_0^\pi\int_0^{2\pi}\left[Y_\ell^m(\theta,\phi)\right]^*\left[Y_{\ell'}^{m'}(\theta,\phi)\right]\sin\theta\mathrm{d}\theta\mathrm{d}\phi=\delta_{\ell\ell'}\delta_{mm'}$$

4.1.4 The Radial Equation

$$u(r)\equiv rR(r)$$

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

Effective potential

$$V_{\text{eff}}=V+\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}$$

Nomalization

$$\int_0^\infty|u|^2\mathrm{d}r=1$$

4.2 The Hydrogen Atom

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

4.2.1 The Radial Wave Function

Let

$$\kappa \equiv \frac{\sqrt{-2m_e E}}{\hbar} \qquad \rho \equiv \kappa r \qquad \rho_0 \equiv \frac{m_e e^2}{2\pi\epsilon_0 \hbar^2 \kappa}$$

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

Asymptitic behavior

- As $\rho \to \infty$

$$u(\rho) \sim Ae^{-\rho}$$

- As $\rho \to 0$

$$u(\rho) = C\rho^{\ell+1}$$

Peel off Asymptitic behavior

$$u(\rho) = \rho^{\ell+1} e^{\rho} v(\rho) \quad \to \quad v(\rho) = \sum_{j=0}^{\infty} c_j \rho^j \quad \to \quad c_{j+1} = \left\{\frac{2(j+\ell+1) - \rho_0}{(j+1)(j+2\ell+2)}\right\} c_j$$

For large j

$$c_j \approx \frac{2^j}{j!} c_0$$

Then

$$v(\rho) = c_0 e^{2\rho} \quad \to \quad u(\rho) = c_0 \rho^{\ell+1} e^{\rho}$$

The series must terminate

$$c_{N-1} \neq 0 \quad \text{but} \quad c_N = 0$$

$$\begin{cases} 2(N+\ell) - \rho_0 = 0 \\ n \equiv N + \ell \end{cases} \quad \Rightarrow \quad \rho_0 = 2n \qquad \Rightarrow$$

Bohr formula

$$\boxed{E_n = -\left[\frac{m_e}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2} = \frac{E_1}{n^2}, \qquad n = 1, 2, 3, \cdots}$$

Summary

- n: principal quantum number
- ℓ: azimuthal quantum number
- m: magnetic quantum number

Ground State

The polynomial $v(\rho)$

$$v(\rho) = L^{2\ell+1}_{n-\ell-1}(2\rho)$$

- Associated Laguerre polynomial
- qth Laguerre polynomial

$$\boxed{\psi_{n\ell m} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-\ell-1)!}{2n(n+\ell)!}} e^{-r/na} \left(\frac{2r}{na}\right)^{\ell} \left[L^{2\ell+1}_{n-\ell-1}(2r/na)\right] Y^m_\ell(\theta, \phi)}$$

4.2.2 The Spectrum of Hydrogen

$$E_\gamma = E_i - E_f = -13.6\text{eV}\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right)$$

$$\frac{1}{\lambda} = \mathcal{R}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

4.3 Angular Momentum

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}$$

$$L_x = yp_z - zp_y, \quad L_y = zp_x - xp_z, \quad L_z = xp_y - yp_x$$

4.3.1 Eigenvalues

Fundamental commutation relations for angular momentum

$$[L_x, L_y] = i\hbar L_z \qquad [L^2, L_x] = 0 \qquad [L^2, \mathbf{L}] = 0 \qquad \sigma_{L_x}\sigma_{L_y} \geqslant \frac{\hbar}{2}|\langle L_z\rangle|$$

Find simultaneous eigenstates

$$L^2 f = \lambda f \qquad \text{and} \qquad L_z f = \mu f$$

Let

$$L_\pm \equiv L_x \pm iL_y \qquad \rightarrow \qquad \begin{cases} [L_z, L_\pm] = \pm\hbar L_\pm \\ \left[L^2, L_\pm\right] = 0 \\ L^2 = L_\pm L_\mp + L_z^2 \mp \hbar L_z \end{cases} \qquad \Rightarrow$$

f is an eigenfuction of L^2 and L_z

$$\begin{aligned} L^2(L_\pm f) &= L_\pm(L^2 f) = L_\pm(\lambda f) \\ &= \lambda(L_\pm f) \end{aligned}$$

$$\begin{aligned} L_z(L_\pm f) &= (L_z L_\pm - L_\pm L_z)f + L_\pm L_z f = \pm\hbar L_\pm f + L_\pm(\mu f) \\ &= (\mu \pm \hbar)(L_\pm f) \end{aligned}$$

- top rung

  $$L_+ f_t = 0$$

  let $L_z = \hbar\ell f_t$

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

- bottom rung

  $$L_- f_b = 0$$

  let $L_z = \hbar\bar{\ell} f_b$

  $$\lambda = \hbar\bar{\ell}(\bar{\ell} - 1)$$

- compare them

  $$\bar{\ell} = \ell + 1; \qquad \bar{\ell} = -\ell; \qquad \ell = -\ell + N \qquad \Rightarrow$$

  $$\boxed{L^2 f_\ell^m = \hbar^2 \ell(\ell+1) f_\ell^m \qquad L_z f_\ell^m = \hbar m f_\ell^m}$$

  where

  $$\ell = 0, 1/2, 1, 3/2, \cdots; \quad m = -\ell, -\ell+1, \cdots, \ell-1, \ell$$

4.3.2 Eigenfunctions

$$\mathbf{L} = -i\hbar(\mathbf{r}\times\nabla) \quad \rightarrow \quad \nabla = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}$$

$$\mathbf{L} = -i\hbar\left(\hat{\phi}\frac{\partial}{\partial\theta} - \hat{\theta}\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\right)$$

$$\begin{cases}\hat{\theta} = (\cos\theta\cos\phi)\hat{\imath} + (\cos\theta\sin\phi)\hat{\jmath} + (-\sin\theta)\hat{k} \\ \hat{\phi} = -\sin\phi\hat{\imath} + \cos\phi\hat{\jmath}\end{cases} \quad \Rightarrow \quad \boxed{L_z = -i\hbar\frac{\partial}{\partial\phi}}$$

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

Conclusion: Spherical harmonics are the eigenfuctions of L^2 and L_z

4.4 Spin

$$[S_x, S_y] = i\hbar S_z \qquad S_\pm \pm iS_y$$

$$S^2\,|s\,m\rangle = \hbar^2 s(s+1)\,|s\,m\rangle$$

$$S_z\,|s\,m\rangle = \hbar m\,|s\,m\rangle$$

$$S_\pm\,|s\,m\rangle = \hbar\sqrt{s(s+1) - m(m\pm 1)}\,|s\,(m\pm 1)\rangle$$

where

$$s = 0, \frac{1}{2}, 2, \frac{3}{2}, \cdots \qquad m = -s, -s+1, \cdots, s-1, s$$

4.4.1 Spin 1/2

for $s = 1/2$, there are two eigenstates

- spin up ($\uparrow$): $\left|\frac{1}{2}\,\frac{1}{2}\right\rangle$
- spin down ($\downarrow$): $\left|\frac{1}{2}\left(-\frac{1}{2}\right)\right\rangle$

spinor

$$\chi = \begin{pmatrix} a \\ b \end{pmatrix} = a\chi_+ + b\chi_-$$

- spin up ($\uparrow$): $\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$
- spin down ($\downarrow$): $\chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

in Matrix

$$\begin{cases}\mathsf{S}^2\chi_+ = \frac{3}{4}\hbar^2\chi_+ \\ \mathsf{S}^2\chi_- = \frac{3}{4}\hbar^2\chi_-\end{cases} \qquad \Rightarrow \qquad \mathsf{S}^2 = \frac{3}{4}\hbar^2\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\begin{cases} \mathsf{S}_z\chi_+ = \dfrac{\hbar}{2}\chi_+ \\ \mathsf{S}_z\chi_- = -\dfrac{\hbar}{2}\chi_- \end{cases} \quad \Rightarrow \quad \mathsf{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\begin{cases} \mathsf{S}_+\chi_- = \hbar\chi_+ \\ \mathsf{S}_-\chi_+ = \hbar\chi_- \\ \mathsf{S}_+\chi_+ = \mathsf{S}_-\chi_- = 0 \end{cases} \quad \Rightarrow \quad \begin{matrix} \mathsf{S}_+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \\ \mathsf{S}_- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \end{matrix} \quad \Rightarrow \quad \begin{matrix} \mathsf{S}_x = \hbar/2\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \mathsf{S}_y = \hbar/2\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \end{matrix}$$

Pauli spin Matrix

$$\mathsf{S} = \frac{\hbar}{2}\boldsymbol{\sigma} \quad \Rightarrow \quad \boxed{\sigma_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}$$

The eigenspinors of S are:

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \left(\text{eigenvalue} \quad +\frac{\hbar}{2}\right); \quad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \left(\text{eigenvalue} \quad -\frac{\hbar}{2}\right)$$

The eigenspinors of S_x are: (normalized)

$$\chi_+^{(x)} = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}, \left(\text{eigenvalue} \quad +\frac{\hbar}{2}\right); \quad \chi_-^{(x)} = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}, \left(\text{eigenvalue} \quad -\frac{\hbar}{2}\right)$$

$$\Rightarrow \quad \chi = \left(\frac{a+b}{\sqrt{2}}\right)\chi_+^{(x)} + \left(\frac{a-b}{\sqrt{2}}\right)\chi_-^{(x)}$$

4.4.2 Electron in a Magnetic Field

Hamiltonian matrix for a spinning charged particle, at rest in $\mathbf{B}$

$$\begin{cases} \boldsymbol{\mu} = \gamma\mathbf{S} \\ H = -\boldsymbol{\mu}\cdot\mathbf{B} \end{cases} \quad \Rightarrow \quad \mathsf{H} = -\gamma\mathbf{B}\cdot\mathsf{S}$$

- $\boldsymbol{\mu}$: magnetic dipole momentum
- γ: gyromagnetic ratio

1. Larmor precession:

$$\mathbf{B} = B_0\hat{k} \quad \Rightarrow \quad \mathsf{H} = -\gamma B_0\mathsf{S}_z = -\frac{\gamma B_0\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\Rightarrow \quad \text{eigenstates}\begin{cases} \chi_+, \text{ with } E_+ = -(\gamma B_0\hbar)/2 \\ \chi_-, \text{ with } E_- = +(\gamma B_0\hbar)/2 \end{cases}$$

$$i\hbar\frac{\partial\chi}{\partial t} = \mathsf{H}\chi \qquad \Rightarrow$$

$$\chi(t) = a\chi_+e^{-iE_+t/\hbar} + b\chi_-e^{-iE_-t/\hbar} = \begin{pmatrix} ae^{i\gamma B_0t/2} \\ be^{-i\gamma B_0t/2} \end{pmatrix}$$

$$|a|^2 + |b|^2 = 1 \quad \Rightarrow \quad \chi(t) = \begin{pmatrix} \cos(\alpha/2)e^{i\gamma B_0 t/2} \\ \sin(\alpha/2)e^{-i\gamma B_0 t/2} \end{pmatrix}$$

$$\Downarrow$$

$$\begin{aligned} \langle S_x \rangle = \chi(t)^\dagger \mathsf{S}_x \chi(t) &= \frac{\hbar}{2} \sin\alpha \cos(\gamma B_0 t) \\ \langle S_y \rangle = \chi(t)^\dagger \mathsf{S}_y \chi(t) &= -\frac{\hbar}{2} \sin\alpha \sin(\gamma B_0 t) \\ \langle S_z \rangle = \chi(t)^\dagger \mathsf{S}_z \chi(t) &= \frac{\hbar}{2} \cos\alpha \end{aligned}$$

Larmor frequency:

$$\omega = \gamma B_0$$

2. The Stern-Gerlach experiment

4.4.3 Addition of Angular Momenta

Two Particles

$$\begin{aligned} S^{(1)^2} |s_1 s_2 m_1 m_2\rangle &= s_1(s_1+1)\hbar^2 |s_1 s_2 m_1 m_2\rangle \\ S^{(2)^2} |s_1 s_2 m_1 m_2\rangle &= s_2(s_2+1)\hbar^2 |s_1 s_2 m_1 m_2\rangle \\ S_z^{(1)} |s_1 s_2 m_1 m_2\rangle &= m_1\hbar |s_1 s_2 m_1 m_2\rangle \\ S_z^{(2)} |s_1 s_2 m_1 m_2\rangle &= m_2\hbar |s_1 s_2 m_1 m_2\rangle \end{aligned}$$

totol angular momentum

$$\mathbf{S} = \mathbf{S}^{(1)} + \mathbf{S}^{(2)}$$

z component

$$\left.\begin{aligned} S_z |s_1 s_2 m_1 m_2\rangle &= S_z^{(1)} |s_1 s_2 m_1 m_2\rangle + S_z^{(2)} |s_1 s_2 m_1 m_2\rangle \\ &= \hbar(m_1+m_2) |s_1 s_2 m_1 m_2\rangle = \hbar m |s_1 s_2 m_1 m_2\rangle \end{aligned}\right. \quad \Rightarrow \quad m = m_1 + m_2$$

Consider the spin-1/2 Particles

$$\boxed{\left\{\begin{array}{ccc} |1\,1\rangle & = & |\uparrow\uparrow\rangle \\ |1\,0\rangle & = & \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ |1\,-1\rangle & = & |\downarrow\downarrow\rangle \end{array}\right\} \quad s = 1\,(\text{triplet})}$$

- triplet states are eigenvectors of S^2 with eigenvalue $2\hbar^2$

$$\boxed{\left\{|0\,0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\right\} \quad s = 0\,(\text{singlet})}$$

- singlet state is an eigenvector of S^2 with eigenvalue 0

Clebsch-Gordan coefficients

$$|s\,m\rangle = \sum_{m_1+m_2=m} C^{s_1 s_2 s}_{m_1 m_2 m} |s_1\,s_2\,m_1\,m_2\rangle$$

4.5 Electromagnetic Interactions

4.5.1 Minimal Coupling

$$\boxed{i\hbar\frac{\partial\Psi}{\partial t} = \left[\frac{1}{2m}(-i\hbar\nabla - q\mathbf{A})^2 + q\varphi\right]\Psi}$$

- quantum implementation of the Lorentz force law
- minimal coupling rule

4.5.2 The Aharonov-Bohm Effect

Chapter 5

Identical Particles

5.1 Two-Particle System

- $\Psi(\mathbf{r}_1, \mathbf{r}_2, t)$
- $i\hbar \dfrac{\partial \Psi}{\partial t} = \hat{H}\Psi, \qquad \text{where} \quad \hat{H} = -\dfrac{\hbar^2}{2m_1}\nabla_1^2 - \dfrac{\hbar^2}{2m_2}\nabla_2^2 + V(\mathbf{r}_1, \mathbf{r}_2, t)$
- $\displaystyle\int |\Psi(\mathbf{r}_1, \mathbf{r}_2, t)|^2 \mathrm{d}^3\mathbf{r}_1 \mathrm{d}^3\mathbf{r}_2 = 1$
- $\Psi(\mathbf{r}_1, \mathbf{r}_2, t) = \psi(\mathbf{r}_1, \mathbf{r}_2)e^{-iEt/\hbar}$
- $-\dfrac{\hbar^2}{2m_1}\nabla_1^2\psi - \dfrac{\hbar^2}{2m_2}\nabla_2^2\psi + V\psi = E\psi$

1. Nointeracting Particles

$$V(\mathbf{r}_1, \mathbf{r}_2) = V(\mathbf{r}_1) + V(\mathbf{r}_2)$$

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, t) = \psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2)\mathrm{e}^{-i(E_a+E_b)t/\hbar} = \Psi_a(\mathbf{r}_1, t)\Psi_b(\mathbf{r}_2, t)$$

2. Central potential (helium atom)

$$V(|\mathbf{r}_1 - \mathbf{r}_2|) \qquad \leftarrow \qquad V(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{4\pi\epsilon_0}\left(-\frac{2e^2}{|\mathbf{r}_1|} - \frac{2e^2}{|\mathbf{r}_2|} + \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}\right)$$

5.1.1 Bosons and Fermions

1. Bosons state

$$\psi_+(\mathbf{r}_1, \mathbf{r}_2) = A[\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) + \psi_b(\mathbf{r}_1)\psi_a(\mathbf{r}_2)] \qquad A = \frac{1}{\sqrt{2}}$$

   - symmetric under interchange: $\psi_+(\mathbf{r}_1, \mathbf{r}_2) = \psi_+(\mathbf{r}_2, \mathbf{r}_1)$
   - all particles with integer spin are bosons

2. Fermions state

$$\psi_-(\mathbf{r}_1, \mathbf{r}_2) = A[\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) - \psi_b(\mathbf{r}_1)\psi_a(\mathbf{r}_2)] \qquad A = \frac{1}{\sqrt{2}}$$

- symmetric under interchange: $\psi_-(\mathbf{r}_1, \mathbf{r}_2) = -\psi_-(\mathbf{r}_2, \mathbf{r}_1)$
- all particles with half integer spin are fermions
- Pauli exclusion principle: two identical fermions cannot occupy the same state
$$\psi_-(\mathbf{r}_1, \mathbf{r}_2) = A[\psi_a(\mathbf{r}_1)\psi_a(\mathbf{r}_2) - \psi_a(\mathbf{r}_1)\psi_a(\mathbf{r}_2)] = 0$$

5.1.2 Exchange Forces

Suppose $\psi(x_1, x_2) = \psi_a(x_1)\psi_b(x_2)$
calculate $\left\langle (x_1 - x_2)^2 \right\rangle = \left\langle x_1^2 \right\rangle + \left\langle x_2^2 \right\rangle - 2\left\langle x_1 x_2 \right\rangle$

1. Distinguishable particles
$$\left\langle (x_1 - x_2)^2 \right\rangle_d = \left\langle x^2 \right\rangle_a + \left\langle x^2 \right\rangle_b + 2\left\langle x \right\rangle_a \left\langle x \right\rangle_b$$

2. Identical particles
$$\left\langle x_1^2 \right\rangle = \left\langle x_2^2 \right\rangle = \frac{1}{2}\left(\left\langle x^2 \right\rangle_a + \left\langle x^2 \right\rangle_b\right)$$
$$\left\langle x_1 x_2 \right\rangle = \left\langle x \right\rangle_a \left\langle x \right\rangle_b \pm |\left\langle x \right\rangle_{ab}|^2$$
where
$$\left\langle x \right\rangle_{ab} \equiv \int x\psi_a(x)^*\psi_b(x)\mathrm{d}x$$
thus
$$\left\langle (x_1 - x_2)^2 \right\rangle_\pm = \left\langle x^2 \right\rangle_a + \left\langle x^2 \right\rangle_b + 2\left\langle x \right\rangle_a \left\langle x \right\rangle_b \mp 2|\left\langle x \right\rangle_{ab}|^2$$
$$\Rightarrow \qquad \left\langle (\Delta x)^2 \right\rangle_\pm = \left\langle (\Delta x)^2 \right\rangle_d \mp 2|\left\langle x \right\rangle_{ab}|^2$$

Exchange force: (if $\left\langle x \right\rangle_{ab} \neq 0$)

- force of attraction between identical bosons
- force of repulsion between identical fermions

5.1.3 Spin

Pauli principle: two electrons in a given position state as long as their spins are in the singlet configuration
$$\psi(\mathbf{r}_1, \mathbf{r}_2)\chi(1, 2) = -\psi(\mathbf{r}_2, \mathbf{r}_1)\chi(2, 1)$$

5.1.4 Generlized Symmetrization Principle

general statement, if you have n identical particles
$$|(1, 2, \cdots, i, \cdots, j, \cdots, n)\rangle = \pm |(1, 2, \cdots, j, \cdots, i, \cdots, n)\rangle$$

5.2 Atoms

$$\hat{H} = \sum_{j=1}^{Z} \left\{ -\frac{\hbar^2}{2m}\nabla_j^2 - \left(\frac{1}{4\pi\epsilon_0}\right)\frac{Ze^2}{r_j} \right\} + \frac{1}{2}\left(\frac{1}{4\pi\epsilon_0}\right)\sum_{j\neq k}^{Z} \frac{e^2}{|\mathbf{r}_j - \mathbf{r}_j|}$$

- Z: atomic number
- Ze: electric charge
- in curly brackets: kinetic plus potential energy of the jth electron
- the second sum: the potential energy associated with the mutual repulsion of the electrons

5.2.1 Helium

$$\hat{H} = \left\{ -\frac{\hbar^2}{2m}\nabla_1^2 - \left(\frac{1}{4\pi\epsilon_0}\right)\frac{2e^2}{r_1} \right\} + \left\{ -\frac{\hbar^2}{2m}\nabla_2^2 - \left(\frac{1}{4\pi\epsilon_0}\right)\frac{2e^2}{r_2} \right\} + \frac{1}{4\pi\epsilon_0}\frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

ignore the last term

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \psi_{n\ell m}(\mathbf{r}_1)\psi_{n'\ell' m'}(\mathbf{r}_2) \qquad \text{with} \quad E = 4(E_n + E_{n'})$$

ground state

$$\psi_0(\mathbf{r}_1, \mathbf{r}_2) = \psi_{100}(\mathbf{r}_1)\psi_{100}(\mathbf{r}_2) = \frac{8}{\pi a^3}\mathrm{e}^{-2(r_1+r_2)/a} \qquad \text{with} \quad E = 8(-13.6\,\mathrm{eV}) = -109\,\mathrm{eV}$$

- symmetric function
- singlet

5.2.2 The Periodic Table

Hund's rules

$$^{2S+1}L_J$$

5.3 Solids

5.3.1 The Free Elctron Gas

Suppose

$$V(x,y,z) = \begin{cases} 0, & 0 < x < l_x, 0 < y < l_y, 0 < z < l_z \\ \infty & \textit{otherwise} \end{cases}$$

Wave functions are

$$\psi_{n_x,n_y,n_z} = \sqrt{\frac{8}{l_x l_y l_z}}\sin\left(\frac{n_x\pi}{l_x}x\right)\sin\left(\frac{n_y\pi}{l_y}y\right)\sin\left(\frac{n_z\pi}{l_z}z\right)$$

energies are

$$E_{n_x,n_y,n_z} = \frac{\hbar^2\pi^2}{2m}\left(\frac{n_x^2}{l_x^2} + \frac{n_y^2}{l_y^2} + \frac{n_z^2}{l_z^2}\right) = \frac{\hbar^2 k^2}{2m} \qquad \mathbf{k} \equiv (k_x, k_y, k_z)$$

5.3.2 Band Structure

Bloch's therem

$$V(x+a) = V(x) \qquad \rightarrow \qquad \psi(x+a) = \mathrm{e}^{iqa}\psi(x)$$

Dirac comb

$$V(x) = \alpha \sum_{j=0}^{N-1} \delta(x - ja)$$

Chapter 6

Symmeties and Conservation Laws

6.1 Introduction

what a symmetry is: that the Hamiltonian is unchanged by some transformation, such as a rotation or a translation

6.1.1 Transformations in Space

Translation Operator

$$\hat{T}(a)\psi(x) = \psi'(x) = \psi(x-a)$$

Parity Operator

$$\hat{\Pi}\psi(x) = \psi'(x) = \psi(-x)$$

$$\hat{\Pi}\psi(x,y,z) = \psi'(x,y,z) = \psi(-x,-y,-z)$$

$$\hat{\Pi}\psi(r,\theta,\varphi) = \psi'(x,y,z) = \psi(r,\pi-\theta,\phi+\pi)$$

Rotation Operator (about z axis through an φ)

$$\hat{R}_z(\varphi)\psi(r,\theta,\phi) = \psi'(r,\theta,\phi) = \psi(r,\theta,\phi-\varphi)$$

6.2 The Translation Operator

by Taylor series

$$\begin{aligned}\hat{T}(a)\psi(x) = \psi(x-a) &= \sum_{n=0}^{\infty}\frac{1}{n!}(-a)^n\frac{\mathrm{d}^n}{\mathrm{d}x^n}\psi(x) \\ &= \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{-ia}{\hbar}\hat{p}\right)^n\psi(x)\end{aligned} \qquad \Rightarrow$$

"generator" of translations

$$\boxed{\hat{T}(a) = \exp\left[-\frac{ia}{\hbar}\hat{p}\right]}$$

- $\hat{T}(a)$ is a unitary operator

$$\hat{T}(a)^{-1} = \hat{T}(-a) = \hat{T}(a)^{\dagger}$$

6.2.1 How Operators Transform

$$\begin{aligned}\langle\psi'|\hat{Q}|\psi'\rangle &= \langle\psi|\hat{Q}'|\psi\rangle \\ &= \langle\psi|\hat{T}^\dagger\hat{Q}\hat{T}|\psi\rangle\end{aligned} \quad \Rightarrow \quad \boxed{\hat{Q}' = \hat{T}^\dagger\hat{Q}\hat{T}}$$

6.2.2 Translational Symmetry

A system is translationally invariant if the Hamiltonian is unchanged by the transformation, then

$$\hat{H}' = \hat{T}^\dagger\hat{H}\hat{T} = \hat{H} \quad \Rightarrow \quad \left[\hat{H}, \hat{T}\right] = 0$$

1. Discrete translation symmetry and Bloch's Theorem
2. Continuous translational symmetry and MomentumConservation

6.3 Conservation Laws

- First Definition: $\langle Q\rangle$ is independent of time
- Second Definition: The probability of getting any particular value is independent o f time

6.4 Parity

6.4.1 Parity in One Dimension

- $\hat{\Pi}(a)$ is a unitary operator

$$\hat{\Pi}(a)^{-1} = \hat{\Pi}(-a) = \hat{\Pi}(a)^\dagger$$

- $\hat{\Pi}$ is Hermitian

Inversion symmetry

$$\left[\hat{H}, \hat{\Pi}\right] = 0$$

Parity Conservation

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\Pi\rangle = 0$$

6.4.2 Parity in Three Dimensions

6.4.3 Parity Selection Rules

6.5 Rotational Symmetry

6.5.1 Rotations About the z Axis

$$\hat{R}_z(\varphi) = \exp\left[-\frac{i\varphi}{\hbar}\hat{L}_z\right]$$

6.5.2 Rotations in Three Dimension

$$\boxed{\hat{R}_n(\varphi) = \exp\left[-\frac{i\varphi}{\hbar}\mathbf{n}\cdot\hat{\mathbf{L}}\right]}$$

6.6 Degeneracy

6.7 Rotational Selection Rules

6.7.1 Selection Rules for Scalar Operators

reduced matrix element

$$\boxed{\langle n'\ell'm'|\hat{f}|n\ell m\rangle = \delta_{\ell\ell'}\delta_{mm'}\langle n'\ell||f||n\ell\rangle}$$

6.7.2 Selection Rules for Vector Operators

6.8 Translation in Time

generator of translations in time

$$\boxed{\hat{U}(t) = \exp\left[-\frac{it}{\hbar}\hat{H}\right]}$$

6.8.1 The Heisenberg Picture

6.8.2 Time-Translation Invaraince

Energy Conservation is a consequence of time-translation invaraince

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\hat{H}\right\rangle = 0$$

Chapter 7

Time-Independent Perturbation Theory

7.1 Nondegenerate Perturbation Theory

7.1.1 General Formulation

Perturbation theory is a systematic procedure for obtaining approximation solutions to the perturbed problem, by building on the known exact solutions to the unperturbed theory

$$\begin{aligned} H &= H^0 + \lambda H' \\ \psi_n &= \psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \cdots \\ E_n &= E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \cdots \end{aligned}$$

- E_n^1: first-order correction to the nth eigenvalue
- ψ_n^1: first-order correction to the nth eigenfunction

Plugging into

$$H\psi_n = E_n \psi$$

we have

- to lowest order (λ^0)
$$H^0\psi_n^0 = E_n^0\psi_n^0$$
- to first order λ^1
$$H^0\psi_n^1 + H'\psi_n^0 = E_n^0\psi_n^1 + E_n^1\psi_n^0$$
- to second order λ^2
$$H^0\psi_n^2 + H'\psi_n^1 = E_n^0\psi_n^2 + E_n^1\psi_n^1 + E_n^2\psi_n^0$$

7.1.2 First-Order Theory

$$\left\langle \psi_n^0 \middle| H^0\psi_n^1 \right\rangle + \left\langle \psi_n^0 \middle| H'\psi_n^0 \right\rangle = E_n^0 \left\langle \psi_n^0 \middle| \psi_n^1 \right\rangle + E_n^1 \left\langle \psi_n^0 \middle| \psi_n^0 \right\rangle$$

$$\left\langle \psi_n^0 \middle| H^0\psi_n^1 \right\rangle = \left\langle H^0\psi_n^0 \middle| \psi_n^1 \right\rangle = E_n^0 \left\langle \psi_n^0 \middle| \psi_n^1 \right\rangle \qquad \Rightarrow \qquad \boxed{E_n^1 = \left\langle \psi_n^0 \middle| H' \middle| \psi_n^0 \right\rangle}$$

rewrite first-order wave function

$$(H^0 - E_n^0)\psi_n^1 = -(H' - E_n^1)\psi_n^0 \qquad \leftarrow \qquad \psi_n^1 = \sum_{m\neq n} c_m^{(n)}\psi_m^0$$

Taking the inner product with ψ_l^0

$$\sum_{m\neq n}(E_m^0 - E_n^0)c_m^{(n)}\left\langle\psi_l^0\middle|\psi_m^0\right\rangle = -\left\langle\psi_l^0\middle|H'\middle|\psi_n^0\right\rangle + E_n^1\left\langle\psi_l^0\middle|\psi_n^0\right\rangle$$

If $l \neq m$

$$\Rightarrow \qquad \boxed{\psi_n^1 = \sum_{m\neq n}\frac{\langle\psi_m^0|H'|\psi_n^0\rangle}{E_n^0 - E_m^0}\psi_m^0}$$

7.1.3 Second-Order Energies

$$\left\langle\psi_n^0\middle|H^0\psi_n^2\right\rangle + \left\langle\psi_n^0\middle|H'\psi_n^1\right\rangle = E_n^0\left\langle\psi_n^0\middle|\psi_n^2\right\rangle + E_n^1\left\langle\psi_n^0\middle|\psi_n^1\right\rangle + E_n^2\left\langle\psi_n^0\middle|\psi_n^0\right\rangle$$

$$\Rightarrow \qquad E_n^2 = \left\langle\psi_n^0\middle|H'\middle|\psi_n^1\right\rangle = \sum_{m\neq n}\frac{\langle\psi_m^0|H'|\psi_n^0\rangle\,\langle\psi_n^0|H'|\psi_m^0\rangle}{E_n^0 - E_m^0}$$

$$\Rightarrow \qquad \boxed{E_n^2 = \sum_{m\neq n}\frac{|\langle\psi_m^0|H'|\psi_n^0\rangle|^2}{E_n^0 - E_m^0}}$$

7.2 Degenerate Perturbation Theory

7.2.1 Two-Fold Degeneracy

Suppose that

$$H^0\psi_a^0 = E^0\psi_a^0, \qquad H^0\psi_b^0 = E^0\psi_b^0, \qquad \left\langle\psi_a^0\middle|\psi_b^0\right\rangle = 0$$

Note that

$$\psi_0 = \alpha\psi_a^0 + \beta\psi_b^0, \qquad H^0\psi^0 = E^0\psi^0$$

The fundamental result of degenerate perturbation theory

$$\boxed{E_\pm^1 = \frac{1}{2}\Big[W_{aa} + W_{bb} \pm \sqrt{(W_{aa} - W_{bb})^2 + 4|W_{ab|^2}}\Big]}$$

7.2.2 "Good" States

Theorem: Let A be a hermitian operator that commutes with H^0 and H'. If ψ_a^0 and ψ_b^0 (the degenerate eigenfunction of H^0) are also eigenfunctions of A, with distinct eigenvalues,

$$A\psi_a^0 = \mu\psi_a^0, \quad A\psi_a^0 = \mu\nu_a^0, \quad \text{and } \mu \neq \nu$$

then ψ_a^0 and ψ_b^0 are the "good" states to use in perturbation theory.
Proof:

7.2.3 Higher-Order Degeneracy

7.3 The Fine Structure of Hydrogen

7.3.1 The Relativistic Correction

$$\begin{aligned} T &= \frac{mc^2}{\sqrt{1-(v/c)^2}} - mc^2 \\ p &= \frac{mv}{\sqrt{1-(v/c)^1}} \end{aligned} \quad \Rightarrow$$

expanding in powers of small number (p/mc)

$$\begin{aligned} T =& \sqrt{p^2c^2 + m^2c^4} - mc^2 \\ =& mc^2\left[\sqrt{1+\left(\frac{p}{mc}\right)^2} - 1\right] = mc^2\left[1 + \frac{1}{2}\left(\frac{p}{mc}\right)^2 - \frac{1}{8}\left(\frac{p}{mc}\right)^4 \cdots - 1\right] \\ =& \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + \cdots \end{aligned}$$

$$E_r^1 = \langle H_r' \rangle = -$$

7.4 The Zeeman Effect

7.5 Hyperfine Splitting in Hydrogen

Chapter 8

The Variational Principle

8.1 Theory

Variational principle

$$\boxed{E_{gs} \leqslant \langle\psi|H|\psi\rangle \equiv \langle H\rangle}$$

- Pick any normalized function ψ whatsoever
- E_{gs}: ground state energy
- Proof:

$$\psi = \sum_n c_n\psi_n, \quad \text{with} \quad H\psi_n = E_n\psi_n$$

$$1 = \langle\psi|\psi\rangle = \sum_n |c_n|^2 \qquad \langle H\rangle = \sum_n E_n|c_n|^2$$

$$\because E_{gs} \leqslant E_n \qquad \therefore \langle H\rangle \geqslant E_{gs}\sum_n |c_n|^2 = E_{gs}$$

Examples:

- 1-d harmonic oscillator

$$\text{"trial wave function"}: \quad \psi(x) = Ae^{-bx^2} \qquad A = \left(\frac{2b}{\pi}\right)^{1/4}$$

$$\langle H\rangle = \langle T\rangle + \langle V\rangle = \frac{\hbar^2 b}{2m} - \frac{m\omega}{8b^2} = 0 \quad \Rightarrow \frac{\mathrm{d}\langle H\rangle}{\mathrm{d}b} = 0 \Rightarrow \quad b = \frac{m\omega}{2\hbar} \quad \Rightarrow \langle H\rangle_{\min} = \frac{1}{2}\hbar\omega$$

- delta function potential

$$\text{"trial wave function"}: \quad \psi(x) = Ae^{-bx^2} \qquad A = \left(\frac{2b}{\pi}\right)^{1/4}$$

$$\langle H\rangle = \frac{\hbar^2 b}{2m} - \frac{\alpha}{\sqrt{2\pi b}} \qquad \Rightarrow b = \frac{2m^2\alpha^2}{\pi\hbar^4} \qquad \Rightarrow \langle H\rangle_{\min} = -\frac{m\alpha^2}{\pi\hbar^2}$$

8.2 The Ground State of Helium

$$H = -\frac{\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2\right) - \frac{e^2}{4\pi\epsilon_0}\left(\frac{2}{r_1} + \frac{2}{r_2} - \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}\right)$$

The ground state energy measured in lab:

$$E_{gs} = -78.975\,\mathrm{eV} \qquad \text{experimental}$$

If ignore V_{ee}

$$\psi_0(\mathbf{r}_1, \mathbf{r}_2) \equiv \psi_{100}(\mathbf{r}_1)\psi_{100}(\mathbf{r}_2) = \frac{8}{\pi a^3}\mathrm{e}^{-2(r_1+r_2)/a} \qquad \text{with } 8E_1 = -109\,\mathrm{eV}$$

$$\Rightarrow \quad H\psi_0 = (8E_1 + V_{ee})\psi_0 \qquad \Rightarrow \quad \langle H\rangle = 8E_1 + \langle V_{ee}\rangle$$

trial function

$$\psi_1(\mathbf{r}_1, \mathbf{r}_2) \equiv \frac{Z^3}{\pi a^3}\mathrm{e}^{-Z(r_1+r_2)/a}$$

- Z: effective nuclear charge, variational parameter

rewrite H

$$\begin{aligned} H = &-\frac{\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2\right) - \frac{e^2}{4\pi\epsilon_0}\left(\frac{Z}{r_1} + \frac{Z}{r_2}\right) \\ &+ \frac{e^2}{4\pi\epsilon_0}\left(\frac{(Z-2)}{r_1} + \frac{(Z-2)}{r_2} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}\right) \end{aligned}$$

$$\langle H\rangle = 2Z^2E_1 + 2(Z-2)\left(\frac{e^2}{4\pi\epsilon_0}\right)\left\langle\frac{1}{r}\right\rangle + \langle V_{ee}\rangle$$

$$\left\langle\frac{1}{r}\right\rangle = \frac{Z}{a} \qquad \langle V_{ee}\rangle = \frac{5Z}{8a}\left(\frac{e^2}{4\pi\epsilon_0}\right) = -\frac{5Z}{4}E_1$$

$$\Rightarrow \quad \langle H\rangle = \left[-aZ^2 + (27/4)Z\right]E_1 \qquad \rightarrow \qquad \frac{\mathrm{d}}{\mathrm{d}Z}\langle H\rangle = 0$$

$$\Rightarrow \qquad Z = \frac{27}{16} \qquad \langle H\rangle = \frac{1}{2}\left(\frac{3}{2}\right)^6 E_1 = -77.5\,\mathrm{eV}$$

8.3 The Hydrogen Molecule Ion

Hamiltonian

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r} + \frac{1}{r'}\right)$$

Trial wave function

$$\psi_0(\mathbf{r}) = \frac{1}{\sqrt{\pi a^3}}\mathrm{e}^{-r/a}$$

8.4 The Hydrogen Molecule

Chapter 9

The WKB Approximation

Imagine a particle of energy E moving through a region where the potential $V(x)$ is constant.

- if $E > V$

$$\psi(x) = A\mathrm{e}^{\pm ikx}, \quad \text{with} \quad k \equiv \frac{2m\sqrt{E-V}}{\hbar}$$

- if $E < V$

$$\psi(x) = A\mathrm{e}^{\pm \kappa x}, \quad \text{with} \quad \kappa \equiv \frac{2m\sqrt{V-E}}{\hbar}$$

- if $E \approx V$

9.1 The "Classical" Region

Rewrite

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -\frac{p^2}{\hbar^2}\psi \qquad p(x) \equiv \sqrt{2m[E-V(x)]}$$

Assume $E > V(x)$, use prime and put ↓ into ↑ $\psi(x) = A(x)\mathrm{e}^{i\phi(x)}$

$$\Rightarrow \qquad A'' + 2iA'\phi' + iA\phi'' - A(\phi')^2 = -\frac{p^2}{\hbar^2}A$$

one for real part

$$\left(A^2\phi'\right)' = 0 \quad \Rightarrow \quad A = \frac{C}{\sqrt{|\phi'|}}$$

and one for imaginary part, Assume amplitude A varises slowly

$$(\phi')^2 = \frac{p^2}{\hbar^2} \quad \Rightarrow \quad \phi(x) = \pm\frac{1}{\hbar}\int p(x)\mathrm{d}x$$

$$\Rightarrow \qquad \boxed{\psi(x) \approx \frac{C}{\sqrt{p(x)}}\mathrm{e}^{\pm\frac{i}{\hbar}\int p(x)\mathrm{d}x}}$$

- $p(x)$ is real
- the two part are entirely equivalent to the original Schrodinger equation

- probability of finding the particle at point x is inverselu proportional to its (classical) momentum

$$|\psi(x)|^2 \approx \frac{|C|^2}{p(x)}$$

- the general approximate solution will be a linear combination

9.2 Tunneling

$$\boxed{\psi(x) \approx \frac{C}{\sqrt{|p(x)|}} \mathrm{e}^{\pm\frac{1}{\hbar}\int p(x)\mathrm{d}x}}$$

9.3 The Connection Formulas

Chapter 10

Scattering

10.1 Introduction

10.1.1 Classical Scattering Theory

10.1.2 Quantum Scattering Theory

10.2 Partial Wave Analysis

10.2.1 Formalism

10.2.2 Strategy

10.3 Phase Shifts

10.4 The Born Approximation

10.4.1 Integral Form of the Schrodinger Equation

10.4.2 The First Born Approximation

10.4.3 The Born Series

Chapter 11

Quantum Dynamics

11.1 Two-level System

Suppose two states of (unperturbed) System

$$\hat{H}^0\psi_b = E_a\psi_a \qquad \hat{H}^0\psi_b = E_b\psi_b$$

$$\langle\psi_i|\psi_j\rangle = \delta_{ij}, \qquad (i,j=a,b)$$

11.1.1 The Perturbed System

$$\Psi(t) = c_a(t)\psi_a \mathrm{e}^{-iE_at/\hbar} + c_b(t)\psi_b \mathrm{e}^{-iE_bt/\hbar}$$

$$|c_a|^2 + |c_b|^2 = 1$$

Solve for $c_a(t)$ and $c_b(t)$

$$\hat{H}\Psi = i\hbar\frac{\partial\Psi}{\partial t}, \quad \text{where} \quad \hat{H} = \hat{H}^0 + \hat{H}'(t)$$

We find

$$c_a\Big(\hat{H}'\psi_a\Big)\mathrm{e}^{-iE_at/\hbar} + c_b\Big(\hat{H}'\psi_b\Big)\mathrm{e}^{-iE_bt/\hbar} = i\hbar\big(\dot{c}_a\psi_a\mathrm{e}^{-iE_at/\hbar} + \dot{c}_b\psi_b\mathrm{e}^{-iE_bt/\hbar}\big)$$

We define

$$H'_{ij} \equiv \langle\psi_i|\hat{H}'|\psi_j\rangle \qquad \Rightarrow \qquad \hat{H}'_{ji} = \big(H'_{ij}\big)^*$$

Take the inner product with ψ_a and ψ_b

$$\begin{cases} \dot{c}_a = -\dfrac{i}{\hbar}\Big[c_a\hat{H}'_{aa} + c_b\hat{H}'_{ab}\mathrm{e}^{-i(E_b-E_a)t/\hbar}\Big] \\ \dot{c}_b = -\dfrac{i}{\hbar}\Big[c_a\hat{H}'_{bb} + c_b\hat{H}'_{ba}\mathrm{e}^{i(E_b-E_a)t/\hbar}\Big] \end{cases}$$

$$\hat{H}'_{aa} = \hat{H}'_{bb} = 0 \qquad \Rightarrow \boxed{\begin{aligned} \dot{c}_a &= -\frac{i}{\hbar}\hat{H}'_{ab}\mathrm{e}^{-i\omega_0 t}c_b \\ \dot{c}_b &= -\frac{i}{\hbar}\hat{H}'_{ba}\mathrm{e}^{-i\omega_0 t}c_a \end{aligned}} \text{with} \quad \omega_0 \equiv \frac{E_a - E_b}{\hbar}$$

11.1.2 Time-Dependent Perturbation Theory

Suppose the particles states out in the lower state:

$$c_a(0) = 1 \qquad c_b(0) = 0$$

Zeroth Order:

$$c_a^{(0)}(t) = 1 \qquad c_b^{(0)}(t) = 0$$

First Order:

$$\Rightarrow \quad \begin{aligned} \frac{\mathrm{d}c_a^{(1)}}{\mathrm{d}t} &= 0 && \Rightarrow && c_a^{(1)}(t) = 1 \\ \frac{\mathrm{d}c_b^{(1)}}{\mathrm{d}t} &= -\frac{i}{\hbar}\hat{H}'_{ba}\mathrm{e}^{-i\omega_0 t} && \Rightarrow && c_b^{(1)}(t) = -\frac{i}{\hbar}\int_0^t \hat{H}'_{ba}(t')\mathrm{e}^{i\omega_0 t'}\mathrm{d}t' \end{aligned}$$

11.1.3 Sinusoidal Perturbations

Suppose

$$\hat{H}'(\mathbf{r}, t) = V(\mathbf{r})\cos(\omega t) \quad \Rightarrow \quad \begin{aligned} H'_{ab} &= V_{ab}\cos(\omega t) \\ V_{ab} &\equiv \langle \psi_a | V | \psi_b \rangle \end{aligned}$$

Assume

$$\omega_0 + \omega \gg |\omega_0 - \omega|$$

we have

$$\begin{aligned} c_b(t) \approx c_b^{(1)}(t) &= -\frac{iV_{ba}}{2\hbar}\int_0^t \left[\mathrm{e}^{i(\omega_0+\omega)t'} + \mathrm{e}^{i(\omega_0-\omega)t'}\right]\mathrm{d}t' \\ &= -\frac{V_{ba}}{2\hbar}\left[\frac{\mathrm{e}^{i(\omega_0+\omega)t} - 1}{\omega_0+\omega} + \frac{\mathrm{e}^{i(\omega_0-\omega)t} - 1}{\omega_0-\omega}\right] \\ &\approx -\frac{V_{ba}}{2\hbar}\frac{\mathrm{e}^{i(\omega_0-\omega)t/2}}{\omega_0-\omega}\left[\mathrm{e}^{i(\omega_0-\omega)t/2} - \mathrm{e}^{-i(\omega_0-\omega)t/2}\right] \\ &= -i\frac{V_{ba}}{\hbar}\frac{\sin\left[(\omega_0-\omega)t/2\right]}{\omega_0-\omega}\mathrm{e}^{i(\omega_0-\omega)t/2} \end{aligned}$$

Transition probability

$$\boxed{P_{a\to b}(t) = |c_b(t)|^2 \approx \frac{|V_{ba}|^2}{\hbar^2}\frac{\sin^2\left[(\omega_0-\omega)t/2\right]}{(\omega_0-\omega)^2}}$$

11.2 Emission and Absortion of Radiationj

11.2.1 Electromagnetic Waves

The atom is exposed to a sinusoidally oscillating electric field

$$\mathbf{E} = E_0\cos(\omega t)\hat{k} \qquad H' = -qE_0 z\cos(\omega t)$$

$$\Rightarrow \quad H_{ba} = -\wp E_0\cos(\omega t), \quad \text{where } \wp \equiv q\langle \psi_b | z | \psi_a \rangle$$

in section 11.1.3, with

$$V_{ba} = -\wp E_0$$

11.2.2 Absorption, Stimulation Emission, and Spontaneous Emission

1. Absorption (start off in the lower state)

$$P_{a\to b}(t) = \left(\frac{|\wp|E_0}{\hbar}\right)^2 \frac{\sin^2[(\omega_0-\omega)t/2]}{(\omega_0-\omega)^2}$$

   - $c_a(0) = 1, c_b(0) = 0$
   - the atom absorts energy $E_b - E_a = \hbar\omega_0$ from the electromagnetic field

2. Stimulation Emission (start off in the upper state)

$$P_{b\to a}(t) = |c_a(t)|^2 = P_{a\to b}(t)$$

   - $c_a(0) = 0, c_b(0) = 1$
   - The electromagnetic field gains energy $\hbar\omega_0$ form the atom

3. Spontaneous Emission

   - An atom in the excited state makes a transition downward, with the release of a photon, but without any applied electromagnetic field to initate the process

11.2.3 Incoherent Perturbations

11.3 Spontaneous Emission

11.3.1 Einstein's A and B

11.3.2 The Life tiem of an Excites State

11.3.3 Selection Rules

$$\boxed{\Delta\ell \equiv \ell' - \ell = \pm 1, \qquad \Delta m \equiv m' - m = 0 \,\text{or}\, \pm 1}$$

- if $m' = m$, then

$$\langle n'\ell'm'|x|n\ell m\rangle = \langle n'\ell'm'|y|n\ell m\rangle = 0$$

- if $m' = m \pm 1$, then

$$\langle n'\ell'm'|x|n\ell m\rangle = \pm i\langle n'\ell'm'|y|n\ell m\rangle$$

$$\langle n'\ell'm'|z|n\ell m\rangle = 0$$

- otherwise

$$\langle n'\ell'm'|x|n\ell m\rangle = \langle n'\ell'm'|y|n\ell m\rangle = \langle n'\ell'm'|z|n\ell m\rangle = 0$$

11.4 Fermi's Golden Rule

11.5 The Adiabatic Approximation