Chap 6 Time-independent perturbation theory (定态)

6.1 Nondegenerate perturbation theory

6.1.1 General formulation

Suppose we have exactly solved

$$H^{(0)}\psi_n^{(0)} = E_n^{(0)}\psi_n^{(0)}$$ ← zeroth order

$H^{(0)}$: unperturbed Hamiltonian; $\psi_n^{(0)}$: eigen states; $E_n^{(0)}$: eigen energies

Orthonormal $\langle\psi_n^{(0)}|\psi_m^{(0)}\rangle = \delta_{n,m}$ (Delta Kronecker, dimensionless)

Delta function $\delta(ax) = \frac{1}{a}\delta(x)$

Full Hamiltonian $H = H^{(0)} + H'$ ← Perturbation ($H' \ll H^{(0)}$)

We cannot solve H

Perturbation theory:

To obtain approximate solutions, based on the known exact solution

To begin with, we write

$$H = H^{(0)} + \lambda H' \qquad \lambda = 1$$ to index different orders of perturbation equations

Assume

$$\psi_n = \psi_n^{(0)} + \lambda\psi^{(1)} + \lambda^2\psi_n^{(2)} + \cdots$$
$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots$$

Put them into $H\psi_n = E_n\psi_n$

$$(H^{(0)} + \lambda H')\left[\psi_n^{(0)} + \lambda\psi_n^{(1)} + \lambda^2\psi_n^{(2)} + \cdots\right]$$
$$= \left(E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots\right)\left[\psi_n^{(0)} + \lambda\psi_n^{(1)} + \lambda^2\psi_n^{(2)} + \cdots\right]$$

Or in powers of λ

The 1st order of λ

$$H^{(0)}\psi_n^{(1)} + H'\psi_n^{(0)} = E_n^{(0)}\psi_n^{(1)} + E_n^{(1)}\psi_n^{(0)} \quad [6.7]$$

The 2nd order of λ

$$H^{(0)}\psi_n^{(2)} + H'\psi_n^{(1)} = E_n^{(0)}\psi_n^{(2)} + E_n^{(1)}\psi_n^{(1)} + E_n^{(2)}\psi_n^{(0)} \quad [6.8]$$

6.1.2 1st-order theory

[Trick] Inner product $\langle\psi_n^{(0)}|[6.7]\rangle$

$$\langle\psi_n^{(0)}|H^{(0)}|\psi_n^{(1)}\rangle + \langle\psi_n^{(0)}|H'|\psi_n^{(0)}\rangle = \langle\psi_n^{(0)}|E_n^{(0)}|\psi_n^{(1)}\rangle + \langle\psi_n^{(0)}|E_n^{(1)}|\psi_n^{(0)}\rangle$$

$E_n^{(0)}\langle\psi_n^{(0)}|$: Hamiltonian is hermitian; ?; operator; number; number

$H = (n+\frac{1}{2})\hbar\omega$, $H|n\rangle = E_n|n\rangle$, $\langle x|n\rangle \equiv \psi(x)$

$$\Rightarrow E_n^{(0)}\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle + \langle\psi_n^{(0)}|H'|\psi_n^{(0)}\rangle = E_n^{(0)}\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle + E_n^{(1)}$$

$$\Rightarrow \boxed{E_n^{(1)} = \langle\psi_n^{(0)}|H'|\psi_n^{(0)}\rangle} \quad [6.9]$$

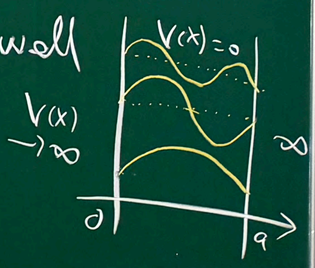
unperturbed; perturbation

First-order correction to the energy

Example 6.1 1D infinite square well

The unperturbed wave functions

$$\psi_n^{(0)}(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right) \qquad a = \text{width}$$
$$\equiv \langle x|\psi_n^{(0)}\rangle$$



↑ 投影背景墙面，注意保护，严禁书写！ ↑

Perturbation $H' = V_0$ Constant

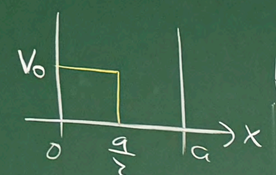
[Solution]: $E_n^{(1)} = \langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle = V_0 \langle \psi_n^{(0)} | \psi_n^{(0)} \rangle$
$= V_0$

$$E_n = E_n^{(0)} + E_n^{(1)} = \frac{\hbar^2}{2m}\left(\frac{\pi n}{a}\right)^2 + V_0 \qquad \frac{\hbar^2 k^2}{2m}$$

Energy up to the 1st order correction

$k \to \frac{\pi}{a} n$ wave vector

Perturbation



$$H'(x) = \begin{cases} V_0, & 0 \le x \le \frac{a}{2} \\ 0, & \text{otherwise} \end{cases}$$

$\Updownarrow$ $H(x, x')$, $\delta(x = x')$

$$\langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle \xrightarrow[\text{to the real space}]{\text{projection}} \int dx\, \psi_n^*(x) H'(x) \psi_n(x)$$

Completeness 完备性 $\int dx\, |x\rangle\langle x| = \hat{1}$ identity operator

$$E_n^{(1)} = \int dx \int dx' \underbrace{\langle \psi_n^{(0)} | x \rangle}_{\psi_n^{(0)*}(x)} \langle x | H' | x' \rangle \underbrace{\langle x' | \psi_n^{(0)} \rangle}_{\psi_n(x)}$$

$\psi_n(x)$ ← wave function

$$= \int dx \int dx'\, \psi_n^{(0)*}(x) \underbrace{\langle x | \hat{H}' | x' \rangle}_{H'(x)\delta(x-x')} \psi_n^{(0)}(x)$$

$H'(x)\delta(x-x')$ ← delta function

$$\int dx'\, f(x')\delta(x-x') = f(x)$$

$$\begin{bmatrix} H(x=1) & & 0 \\ & H(x=2) & \\ 0 & & \ddots \end{bmatrix}_{x, x'}$$

$$= \int dx\, \psi_n^{(0)*}(x) H'(x) \psi_n^{(0)}(x)$$

$$E_n^{(1)} = \int_0^{a/2} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) V_0 \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) dx + \int_{a/2}^{a} dx\, 0$$

$$= \frac{2V_0}{a} \int_0^{a/2} \sin^2\left(\frac{n\pi}{a}x\right) dx = \frac{V_0}{2}$$

$$E_n = E_n^{(0)} + E_n^{(1)}$$

First-order correction to wave function $\psi_n^{(1)}$

Rewrite Eq. [6.7]

$$[H^{(0)} - E_n^{(0)}]\psi_n^{(1)} = -[H' - E_n^{(0)}]\psi_n^{(0)}$$

to find

Assume $\boxed{\psi_n^{(1)} = \sum_{m \ne n} C_m^{(n)} \psi_m^{(0)}}$ ← Known eigen states as a basis to expand $\psi_n^{(1)}$

Why? $\psi_n = \psi_n^{(0)} + \psi_n^{(1)}$

superposition coefficients to be determined

$$[H^{(0)} - E_n^{(0)}] \sum_{m \ne n} C_m^{(n)} \psi_m^{(0)} = -[H' - E_n^{(1)}]\psi_n^{(0)}$$

$$\Rightarrow \sum_{m \ne n} C_m^{(n)} [H^{(0)} - E_n^{(0)}] \psi_m^{(0)} = -[H' - E_n^{(1)}]\psi_n^{(0)}$$

[Trick] $\langle \psi_l^{(0)} | \times$

$$\Rightarrow \langle \psi_l^{(0)} | \sum_{m \ne n} C_m^{(n)} [H^{(0)} - E_n^{(0)}] | \psi_m^{(0)} \rangle = -\langle \psi_l^{(0)} | [H' - E_n^{(0)}] | \psi_n^{(0)} \rangle$$

$$\Rightarrow \sum_{m \ne n} C_m^{(n)} \left[\langle \psi_l^{(0)} | H^{(0)} | \psi_m^{(0)} \rangle - \langle \psi_l^{(0)} | E_n^{(0)} | \psi_m^{(0)} \rangle \right]$$

$E_m^{(0)} | \psi_m^{(0)} \rangle$ number

$$= -\langle \psi_l^{(0)} | H' | \psi_n^{(0)} \rangle + \langle \psi_l^{(0)} | E_n^{(1)} | \psi_n^{(0)} \rangle$$

$$\Rightarrow \sum_{m \ne n} C_m^{(n)} (E_m^{(0)} - E_n^{(0)}) \langle \psi_l^{(0)} | \psi_m^{(0)} \rangle = -\langle \psi_l^{(0)} | H' | \psi_n^{(0)} \rangle + E_n^{(1)} \langle \psi_l^{(0)} | \psi_n^{(0)} \rangle$$

If $l = n \Rightarrow \langle \psi_l^{(0)} | \psi_m^{(0)} \rangle = \delta_{n,m}$, but $m \ne n$

$\Rightarrow$ Left $= 0$

If $l \ne n$

$$\sum_{m \ne n} C_m^{(n)} (E_m^{(0)} - E_n^{(0)}) \delta_{l,m} = -\langle \psi_l^{(0)} | H' | \psi_n^{(0)} \rangle + E_n^{(1)} \delta_{l,n}^{F^0}$$

$$\Rightarrow C_l^{(n)} [E_l^{(0)} - E_n^{(0)}] = -\langle \psi_l^{(0)} | H' | \psi_n^{(0)} \rangle$$

$$\Rightarrow C_{\underline{\underline{l}}\,m}^{(n)} = \frac{\langle \psi_l^{(0)} | H' | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_{\underline{\underline{l}}\,m}^{(0)}}$$

$$\psi_n^{(1)} = \sum_{m\neq n} \frac{\langle \psi_m^{(0)} | H' | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} \psi_m^{(0)} \quad [6.13]$$

6.1.3 2nd-order correction to energy $E_n^{(2)}$

[Trick] $\langle \psi_n^{(0)} |$ (6.8) $\Rightarrow$

$\langle \psi_n^{(0)} | H^{(0)} | \psi_n^{(2)} \rangle + \langle \psi_n^{(0)} | H' | \psi_n^{(1)} \rangle$

$= E_n^{(0)} \langle \psi_n^{(0)} | \psi_n^{(2)} \rangle + E_n^{(1)} \langle \psi_n^{(0)} | \psi_n^{(1)} \rangle + E_n^{(2)} \langle \psi_n^{(0)} | \psi_n^{(0)} \rangle$ (= 1)

$\Rightarrow E_n^{(2)} = \langle \psi_n^{(0)} | H' | \psi_n^{(1)} \rangle = \sum_{m\neq n} \langle \psi_n^{(0)} | H' | \sum_{m\neq n} C_m^{(n)} | \psi_m^{(0)} \rangle$ (because $\psi_n^{(1)} = \sum_{m\neq n} C_m^{(n)} \psi_m^{(0)}$, $\in 0$)

$= \sum_{m\neq n} \frac{\langle \psi_m^{(0)} | H' | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} \langle \psi_n^{(0)} | H' | \psi_m^{(0)} \rangle$

H' is hermitian, $H'_{nm} = (H'_{mn})^*$ (* complex conjugate, nm → mn transpose)

$$E_n^{(2)} = \sum_{m\neq n} \frac{|\langle \psi_m^{(0)} | H' | \psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_m^{(0)}} \quad [6.15]$$

What if degenerate? $E_n^{(0)} = E_m^{(0)}$

$\psi_n^{(1)} \sim \frac{1}{E_n^{(0)} - E_m^{(0)}}$, $E_n^{(2)} \sim \frac{1}{E_n^{(0)} - E_m^{(0)}}$ Divergence

We need to look for other way

6.2 Degenerate perturbation theory = Diagonalization 对角化

6.2.1 Two-fold degeneracy (only two states)

Suppose $H^{(0)}\psi_a^{(0)} = E^{(0)}\psi_a^{(0)}$, $H^{(0)}\psi_b^{(0)} = E^{(0)}\psi_b^{(0)}$

$\langle \psi_a^{(0)} | \psi_b^{(0)} \rangle = \delta_{a,b}$

Note that, any state can be written as

$\psi^{(0)} = \alpha\psi_a^{(0)} + \beta\psi_b^{(0)}$ is also an eigenstate of $H^{(0)}$

(α, β: superposition coefficients)

[Proof] $= \langle \psi^{(0)} | H^{(0)} | \psi^{(0)} \rangle$

$= [\alpha^* \langle \psi_a^{(0)}| + \beta^* \langle \psi_b^{(0)}|] H^{(0)} [\alpha|\psi_a^{(0)}\rangle + \beta|\psi_b^{(0)}\rangle]$

$= |\alpha|^2 \langle \psi_a^{(0)} | H^{(0)} | \psi_a^{(0)} \rangle + |\beta|^2 \langle \psi_b^{(0)} | H^{(0)} | \psi_b^{(0)} \rangle$

$+ \alpha^*\beta \langle \psi_b^{(0)} | H^{(0)} | \psi_a^{(0)} \rangle + \alpha\beta^* \langle \psi_b^{(0)} | H^{(0)} | \psi_a^{(0)} \rangle$

($E^{(0)}$; $\langle \psi_a^{(0)} | \psi_b^{(0)} \rangle = 0$; $\langle \psi_b^{(0)} | \psi_a^{(0)} \rangle = 0$)

$= (|\alpha|^2 + |\beta|^2) E^{(0)} = E^{(0)}$

because $|\alpha|^2 + |\beta|^2 = 1$ as required by the superposition coefficients

We want to solve

$H\psi = E\psi$ with $H = H^{(0)} + \lambda H'$, $\lambda = 1$

Assume $E = E^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + \cdots$

$\psi = \psi^{(0)} + \lambda\psi^{(1)} + \lambda^2\psi^{(2)} + \cdots$

$\psi^{(0)} = \alpha\psi_a^{(0)} + \beta\psi_b^{(0)}$ (to be determined) — Good state — under which the Hamiltonian is diagonalized

Put them together, we have

$H^{(0)}\psi^{(0)} + \lambda(H'\psi^{(0)} + H^{(0)}\psi^{(1)}) + \cdots = E^{(0)}\psi^{(0)} + \lambda(E^{(1)}\psi^{(0)} + E^{(0)}\psi^{(1)}) + \cdots$

At the order of λ, we have

$H^{(0)}\psi^{(1)} + H'\psi^{(0)} = E^{(0)}\psi^{(1)} + E^{(1)}\psi^{(0)}$ [Trick] $\langle \psi_a^{(0)}|$

$\Rightarrow \langle \psi_a^{(0)} | H^{(0)} | \psi^{(1)} \rangle + \langle \psi_a^{(0)} | H' | \psi^{(0)} \rangle = E^{(0)} \langle \psi_a^{(0)} | \psi^{(1)} \rangle + E^{(1)} \langle \psi_a^{(0)} |$

($E^{(0)} \langle \psi_a^{(0)} | \psi^{(1)} \rangle$; $\psi^{(0)} = \alpha\psi_a^{(0)} + \beta\psi_b^{(0)}$)

$\Rightarrow \langle \psi_a^{(0)} | H' | \alpha\psi_a^{(0)} + \beta\psi_b^{(0)} \rangle = E^{(1)} (\alpha \langle \psi_a^{(0)} | \psi_a^{(0)} \rangle + \beta \langle \psi_a^{(0)} | \psi_b^{(0)} \rangle)$ (= 1; $\in 0$)

$\Rightarrow \alpha \langle \psi_a^{(0)} | H' | \psi_a^{(0)} \rangle + \beta \langle \psi_a^{(0)} | H' | \psi_b^{(0)} \rangle = E^{(1)}\alpha$

$\Rightarrow \boxed{\alpha W_{aa} + \beta W_{ab} = E^{(1)}\alpha}$ We have defined $W_{ij} \equiv \langle \psi_i^{(0)} | H' | \psi_j^{(0)} \rangle$

Similarly, $\langle \psi_b^{(0)}|$ 1st order equation of λ $\Rightarrow$

$\boxed{\alpha W_{ba} + \beta W_{bb} = \beta E^{(0)}}$

$$\Rightarrow \begin{bmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = E^{(0)} \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

$\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \alpha \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ ($\psi_a^{(0)}$, $\psi_b^{(0)}$)

Next step : Diagonalization

⬆ 投影背景墙面，注意保护，严禁书写！⬆

SUSTech

Chap 6.2 Degenerate Perturbation Theory

6.2.1 Two-fold (only 2 states) case

$H = H^{(0)} + H'$
($H^{(0)}$: unperturbed, H': perturbation)

The matrix representation of H' in the Hilbert space spanned by $|\psi_a^{(0)}\rangle$ and $|\psi_b^{(0)}\rangle$ is

$$H' = W = \begin{bmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{bmatrix}$$

The degenerate perturbation theory is to diagonalize the matrix of H'

[Must know] Eigen energies $E_{\pm}^{(1)} = \frac{W_{aa}+W_{bb}}{2} \pm \sqrt{\left(\frac{W_{aa}-W_{bb}}{2}\right)^2 + W_{ab}W_{ba}}$

$H'\begin{pmatrix} a \\ b \end{pmatrix} = E\begin{pmatrix} a \\ b \end{pmatrix} \Rightarrow \begin{bmatrix} W_{aa}-E & W_{ab} \\ W_{ba} & W_{bb}-E \end{bmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = 0$

P178 Eq.[4.155]

$$\chi_+ = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix}, \quad \chi_- = \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2}e^{i\phi} \end{pmatrix}$$

$$\cos\theta \equiv \frac{\frac{W_{aa}-W_{bb}}{2}}{\sqrt{\left(\frac{W_{aa}-W_{bb}}{2}\right)^2 + W_{ab}W_{ba}}}, \quad W_{ab} \equiv |W_{ab}|e^{-i\phi}$$

Definition of ϕ

Equivalent to "Spin"

$$\begin{bmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{bmatrix} = \frac{W_{aa}+W_{bb}}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \sqrt{\left(\frac{W_{aa}-W_{bb}}{2}\right)^2 + W_{ab}W_{ba}}\begin{bmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{bmatrix}$$

$$= \frac{W_{aa}+W_{bb}}{2}\sigma_0 + (\cos\theta\,\sigma_z + \sin\theta\cos\phi\,\sigma_x + \sin\theta\sin\phi\,\sigma_y)$$

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

(check the orthonormal properties)

$\langle\psi_+^{(0)}|\psi_-^{(0)}\rangle = \langle\chi_+|\chi_-\rangle = \left(\cos\frac{\theta}{2}, \sin\frac{\theta}{2}e^{-i\phi}\right)\begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2}e^{i\phi} \end{pmatrix}$

Hermite conjugate $= \cos\frac{\theta}{2}\sin\frac{\theta}{2} - \sin\frac{\theta}{2}\cos\frac{\theta}{2} = 0$

$\langle\psi_+^{(0)}|H'|\psi_+^{(0)}\rangle = \left(\cos\frac{\theta}{2}, \sin\frac{\theta}{2}e^{-i\phi}\right)\frac{W_{aa}+W_{bb}}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix}$

$+ \left(\cos\frac{\theta}{2}, \sin\frac{\theta}{2}e^{-i\phi}\right)\sqrt{\left(\frac{W_{aa}-W_{bb}}{2}\right)^2 + W_{ab}W_{ba}}\begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix}\begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix}$

$= \frac{W_{aa}+W_{bb}}{2} + \sqrt{\left(\frac{W_{aa}-W_{bb}}{2}\right)^2 + W_{ab}W_{ba}}\left(\cos\frac{\theta}{2}, \sin\frac{\theta}{2}e^{-i\phi}\right)_{1\times 2}\begin{pmatrix} \cos\theta\cos\frac{\theta}{2} + \sin\theta\sin\frac{\theta}{2} \\ \sin\theta\cos\frac{\theta}{2}e^{i\phi} - \cos\theta\sin\frac{\theta}{2}e^{i\phi} \end{pmatrix}_{2\times 1}$

$= \frac{W_{aa}+W_{bb}}{2} + \sqrt{\dots}$

$\langle\psi_+^{(0)}|H'|\psi_-^{(0)}\rangle = 0$

Good states

In the basis formed by $|\psi_+^{(0)}\rangle$ and $|\psi_-^{(0)}\rangle$, the Matrix of $H' = \begin{bmatrix} E_+^{(1)} & 0 \\ 0 & E_-^{(1)} \end{bmatrix}$

$E = E^{(0)} + E_{\pm}^{(1)}$ ← Splitting

6.2.2 Higher-order degeneracy

N-fold degeneracy = N states with the same energies

Use the basis $\{\psi_1, \psi_2, \psi_3, \dots, \psi_N\}$ to express H'

$\Rightarrow$ N×N Matrix of H', the diagonalize H'

Example 6.2 3D Cubical well

$$V(x,y,z) = \begin{cases} 0, & x,y,z \in [0,a] \\ \infty, & \text{elsewhere} \end{cases}$$ Potential

Unperturbed eigen energies $E_{n_x n_y n_z}^{(0)} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2(n_x^2+n_y^2+n_z^2)$

eigen states $\psi_{n_x n_y n_z}^{(0)} = \left(\frac{2}{a}\right)^{\frac{3}{2}}\sin\left(\frac{n_x\pi x}{a}\right)\sin\left(\frac{n_y\pi y}{a}\right)\sin\left(\frac{n_z\pi z}{a}\right)$

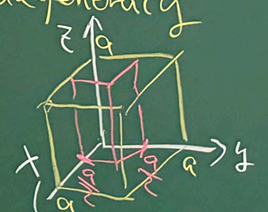
Wave vector $k \to \frac{\pi}{a}n$ Quantization

positive integers

Ground state $E_{111}^{(0)} = \frac{\pi^2\hbar^2}{2ma^2}(1+1+1)$ only one state

1st excited states $\psi_a = \psi_{112}^{(0)}, \psi_b = \psi_{121}^{(0)}, \psi_c = \psi_{211}^{(0)}$

$E_{a,b,c}^{(0)} = \frac{\pi^2\hbar^2}{2ma^2}(1+1+2^2) = 3\frac{\pi^2\hbar^2}{ma^2}$ Three-fold degeneracy



Perturbation $H' = \begin{cases} V_0, & x,y \in [0,\frac{a}{2}] \\ 0, & \text{elsewhere} \end{cases}$

Corrections to energies

Ground states $E_{111}^{(1)} = \langle\psi_{111}^{(0)}|H'|\psi_{111}^{(0)}\rangle$

$= \left(\frac{2}{a}\right)^3 V_0 \int_0^{a/2} dx \sin^2\frac{\pi}{a}x \int_0^{a/2} dy \sin^2\frac{\pi}{a}y \int_0^a dz \sin^2\frac{\pi}{a}z$

$= \frac{8}{a^3}V_0\left(\frac{a}{2}\cdot\frac{1}{2}\right)^2\frac{a}{2} = \frac{V_0}{4}$

↑ 投影背景墙面，注意保护，严禁书写！ ↑

1st excited states $H' = \begin{bmatrix} W_{aa} & W_{ab} & W_{ac} \\ W_{ba} & W_{bb} & W_{bc} \\ W_{ca} & W_{cb} & W_{cc} \end{bmatrix}$ basis $\{\psi_a, \psi_b, \psi_c\}$

$W_{aa} \equiv \langle \psi_a | H' | \psi_a \rangle = \langle \psi^{(0)}_{112} | H' | \psi^{(0)}_{112} \rangle$

$= \left(\frac{2}{a}\right)^3 V_0 \int_0^{a/2} dx \sin^2\frac{\pi}{a}x \int_0^{a/2} dy \sin^2\frac{\pi}{a}y \int_0^a dz \sin^2\frac{2\pi}{a}z$ ($\sin^2\frac{2\pi}{a}z$: $\downarrow \frac{2\pi}{a}$)

$= \left(\frac{2}{a}\right)^2 V_0 \frac{a}{4}\frac{a}{4}\frac{a}{2} = \frac{V_0}{4}$ Similarly $W_{bb} = W_{cc} = W_{aa}$

$W_{ab} \equiv \langle \psi_a | H' | \psi_b \rangle = \langle \psi^{(0)}_{112} | H' | \psi^{(0)}_{121} \rangle$

$= \left(\frac{2}{a}\right)^3 V_0 \int_0^{a/2} dx \sin^2\frac{\pi}{a}x \int_0^{a/2} dy \sin\frac{\pi}{a}y \sin\frac{2\pi}{a}y$

$\times \int_0^a dz \sin\frac{2\pi}{a}z \sin\frac{\pi}{a}z = 0$

$W_{ab} = 0$

H' does not couple ψ_a and ψ_b

Similarly $W_{ac} = 0$, H' does not couple ψ_a and ψ_c

$W_{bc} \equiv \langle \psi^{(0)}_{121} | H' | \psi^{(0)}_{211} \rangle = \left(\frac{2}{a}\right)^3 V_0 \int_0^{a/2} dx \sin\frac{\pi}{a}x \sin\frac{2\pi}{a}x$

$\times \int_0^{a/2} dy \sin\frac{2\pi}{a}y \sin\frac{\pi}{a}y \times \int_0^a dz \sin^2\frac{\pi}{a}z$

$= \frac{16}{9\pi^2} V_0 \neq 0$ H' couples ψ_b and ψ_c

$W_{cb} = W^*_{bc} = \frac{16}{9\pi^2} V_0 \equiv \frac{V_0}{4}\kappa$ ← kappa

$\Rightarrow H' = \begin{bmatrix} \frac{V_0}{4} & 0 & 0 \\ 0 & \frac{V_0}{4} & \frac{V_0}{4}\kappa \\ 0 & \frac{V_0}{4}\kappa & \frac{V_0}{4} \end{bmatrix} = \frac{V_0}{4}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \kappa \\ 0 & \kappa & 1 \end{bmatrix}$ basis ψ_a, ψ_b, ψ_c

$\Rightarrow E_1 = \frac{V_0}{4}$, Eigen state $\psi_a = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$

Eigen energy

$E_{2,3} = \frac{V_0}{4}\left[\frac{1+1}{2} \pm \sqrt{\left(\frac{1-1}{2}\right)^2 + \kappa^2}\right] = \frac{V_0}{4}(1 \pm \kappa)$

$E_2 = \frac{V_0}{4}(1+\kappa)$, $\psi_2 = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}\psi_b + \frac{1}{\sqrt{2}}\psi_c$

$E_3 = \frac{V_0}{4}(1-\kappa)$, $\psi_3 = \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2}e^{i\phi} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}}\psi_b - \frac{1}{\sqrt{2}}\psi_c$

$\cos\theta = \frac{\frac{1-1}{2}}{\sqrt{\left(\frac{1-1}{2}\right)^2 + \kappa^2}} = 0 \Rightarrow \cos\frac{\theta}{2} = \sqrt{\frac{1}{2}(1+\cos\theta)} = \sqrt{\frac{1}{2}}$

$\sin\frac{\theta}{2} = \sqrt{\frac{1}{2}(1-\cos\theta)} = \sqrt{\frac{1}{2}}$

$\kappa = |\kappa| e^{i\phi} \Rightarrow \phi = 0$

$E = E^{(0)}_{a,b,c} + \begin{cases} \frac{V_0}{4} \\ \frac{V_0}{4}(1+\kappa) \\ \frac{V_0}{4}(1-\kappa) \end{cases}$ $\frac{V_0}{4}(1+\kappa)$, $\frac{V_0}{4}$, $\frac{V_0}{4}(1-\kappa)$

H' lifts the degeneracy and split the energies

$\psi_a + \psi_b + \psi_c$

Problem 6.8 3D infinite cubic well

Perturbation $H' = a^3 V_0 \delta\left(x - \frac{a}{4}\right)\delta\left(y - \frac{a}{2}\right)\delta\left(z - \frac{3a}{4}\right)$

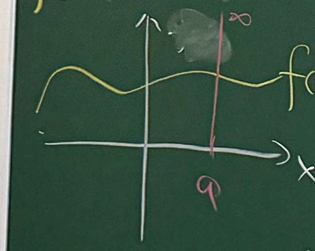
(a^3: length^3; V_0: dimension of energy; $\delta(ax) = \frac{1}{a}\delta(x)$: dimension of $\frac{1}{\text{length}}$)

Find the 1st-order corrections to the energies for the ground state and 1st excited states

$E^{(1)}_0 = \langle \psi_{111} | H' | \psi_{111} \rangle = \left(\frac{2}{a}\right)^3 a^3 V_0 \int_0^a dx \sin^2\frac{\pi}{a}x\, \delta\left(x - \frac{a}{4}\right)$

$\int f(x)\delta(x-a) = f(a)$

$\times \int_0^a dy \sin^2\frac{\pi}{a}y\, \delta\left(y - \frac{a}{2}\right) \times \int_0^a dz \sin^2\frac{\pi}{a}z\, \delta\left(z - \frac{3a}{4}\right)$



$= \left(\frac{2}{a}\right)^3 a^3 V_0 \sin^2\frac{\pi}{a}\frac{a}{4} \sin^2\frac{\pi}{a}\frac{a}{2} \sin^2\frac{\pi}{a}\frac{3a}{4}$

$= 8V_0 \cdot \frac{1}{2} \cdot 1 \cdot \frac{1}{2} = 2V_0$

Similarly,

$H' = \begin{bmatrix} W_{aa} & W_{ab} & W_{ac} \\ W_{ba} & W_{bb} & W_{bc} \\ W_{ca} & W_{cb} & W_{cc} \end{bmatrix}$ then diagonalize it

Chap 6.3 Fine structure energy of Hydrogen

(Spinless) Relativistic (6.3.1) + spin-orbit coupling (6.3.2)

(Also a relativistic effect)

- Low-energy limit of the Dirac equation in the Coulomb potential
- Dirac equation is a special relativistic quantum mechanics equation for spin-$\frac{1}{2}$ fermions

Recap Chap 4.2

Hydrogen atom

$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{1}{4\pi\epsilon_0}\frac{1}{r}$

Kinetic (Potential)

Bohr energies $= \frac{-13.6\,\text{eV}}{n^2}$

(Not the whole story)

$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} \approx \frac{1}{137}$

Fine-structure constant

Hierarchy

Bohr	$\alpha^2 mc^2$
Fine structure	$\alpha^4 mc^2$
Lamb shift	α^5
Hyperfine	α^8

Use the perturbation theory to figure out

Problem 6.11 Express Bohr energy in terms of α and mc^2

P149 Eq. [4.70]

$$E_n = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2} = -\frac{mc^2}{2}\left(\frac{e^2}{4\pi\epsilon_0\hbar c}\right)^2\frac{1}{n^2}$$

($\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c}$)

$$= -\frac{1}{2}mc^2\alpha^2\frac{1}{n^2} \quad [6.43]$$

6.3.1 (Spinless) Relativistic Correction

Kinetic energy $T = \frac{p^2}{2m} \longrightarrow -\frac{\hbar^2}{2m}\nabla^2$

$\hat{p} = -i\hbar\vec{\nabla}$

$[x, p] = i\hbar$ Uncertainty principle

No velocity

$v = \frac{1}{\hbar}\frac{\partial E}{\partial k}$ $\quad \hat{v} = \frac{1}{\hbar}\frac{\partial H}{\partial k}$

$\hat{p}\, e^{i\vec{p}\cdot\vec{x}/\hbar} = -i\hbar\vec{\nabla} e^{i\vec{p}\cdot\vec{x}/\hbar}$

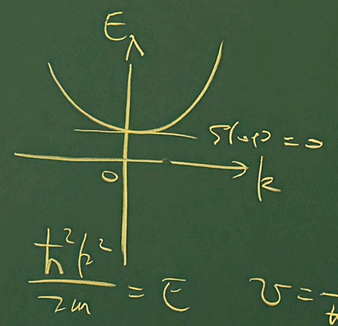
plane wave $= \vec{p}$

Relativistic kinetic energy $T = \frac{mc^2}{\sqrt{1-(\frac{v}{c})^2}} - mc^2$ ← from Lorentz transformation under the assumption that speed of light is the same constant in any reference systems

In QM, we express T in term of $\hat{p}$, not $\vec{v}$

$$p = \frac{mv}{\sqrt{1-(\frac{v}{c})^2}}$$

Note that $p^2c^2 + m^2c^4 = \frac{m^2v^2c^2}{1-(\frac{v}{c})^2} + m^2c^4$



$E = \hbar\omega$

$\frac{\hbar^2k^2}{2m} = E$ $\quad v = \frac{1}{\hbar}\frac{\partial E}{\partial k} = \frac{1}{\hbar}\frac{\hbar^2}{2m}2k = \frac{\hbar k}{m} = 0$ at $k=0$

↑ 投影背景墙面，注意保护，严禁书写！ ↑

6.3.1 (Spinless) Relativistic correction

Relativistic kinetic energy $T = \frac{mc^2}{\sqrt{1-(\frac{v}{c})^2}} - mc^2$

In QM, we express T in terms of p (momentum), not v (velocity)

$p = \frac{mv}{\sqrt{1-(\frac{v}{c})^2}}$ ← Lorentz transformation to make sure that speed of light is constant in any reference frames.

Note that $p^2c^2 + m^2c^4 = \frac{m^2v^2c^2}{1-(\frac{v}{c})^2} + m^2c^4$

$= \frac{m^2v^2c^2 + m^2c^4(1-(\frac{v}{c})^2)}{1-(\frac{v}{c})^2} = \frac{m^2c^4}{1-(\frac{v}{c})^2} = (T+mc^2)^2$

$\Rightarrow T = \sqrt{p^2c^2+m^2c^4} - mc^2$ kinetic energy in terms of p

Perturbation $T = mc^2\left[\sqrt{1+(\frac{p}{mc})^2} - 1\right]$ Taylor expansion $\sqrt{1+x} = 1 + \frac{1}{2}x - \frac{x^2}{8} + \cdots$

$= mc^2\left(1 + \frac{1}{2}(\frac{p}{mc})^2 - \frac{1}{8}(\frac{p}{mc})^4 + \cdots\right)$

$= \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + \cdots$

Classical — Perturbation from (spinless) relativistic correction

Perturbation $H_r' = -\frac{\hat{p}^4}{8m^3c^2} = -\frac{(\frac{p^2}{2m})^2}{2mc^2}$ $\sim 100\,eV$ $\sim MeV$ $\sim 10^6\,eV$

1st-order correction to energy

$E_r^{(1)} \equiv \langle \psi_{nlm} | H_r' | \psi_{nlm} \rangle$

Eq. [6.9] Non-degenerate

principal: $E_n = \frac{E_1}{n^2}$; $\hat{L}^2$; $\hat{L}_z$

$\hat{L}^2|\psi_{nlm}\rangle = \hbar^2 l(l+1)|\psi_{nlm}\rangle$

$\hat{L}_z|\psi_{nlm}\rangle = \hbar m|\psi_{nlm}\rangle$

$[\hat{L}^2, H^{(0)}] = 0$, $[L_z, H^{(0)}] = 0$

But, the eigenstates of Hydrogen (Bohr) are degenerate

$n=1, l=0, m=0$

$n=2, l=0,1, m=\pm1, 0$

To explain this confusion, Theorem on Page 259-260

[Conditions] unperturbed

① Hermitian operator $\hat{A}$ — perturbation

$[\hat{A}, H^{(0)}] = 0$, $[\hat{A}, H'] = 0$

② If $\psi_a^{(0)}$ and $\psi_b^{(0)}$ are also eigen states of $\hat{A}$ (eigen states of $H^{(0)}$)

but with distinct eigen values

$\hat{A}|\psi_a^{(0)}\rangle = \mu|\psi_a^{(0)}\rangle$, $\hat{A}|\psi_b^{(0)}\rangle = \nu|\psi_b^{(0)}\rangle$, $\mu \neq \nu$ (\mu, \nu)

[Conclusion]: Then, $W_{ab} \equiv \langle \psi_a^{(0)} | H' | \psi_b^{(0)} \rangle = 0$

No off-diagonal terms $\begin{bmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{bmatrix}$

[Proof]: $[\hat{A}, H'] = 0 \Rightarrow \langle \psi_a^{(0)} | [\hat{A}, H'] | \psi_b^{(0)} \rangle = 0$

$\Rightarrow \langle \psi_a^{(0)} | \hat{A}H' | \psi_b^{(0)} \rangle - \langle \psi_a^{(0)} | H'\hat{A} | \psi_b^{(0)} \rangle = 0$ ($AH' - H'A$)

$\Rightarrow \mu \langle \psi_a^{(0)} | H' | \psi_b^{(0)} \rangle - \nu \langle \psi_a^{(0)} | H' | \psi_b^{(0)} \rangle = 0$

$\Rightarrow (\mu - \nu)\langle \psi_a^{(0)} | H' | \psi_b^{(0)} \rangle = 0$

$\mu - \nu$: nonzero; $\langle \psi_a^{(0)} | H' | \psi_b^{(0)} \rangle$: This has to be zero ※QED

Application $\hat{A} \to \hat{L}^2, \hat{L}_z$, $H' \to H_r' \sim p^4$

$H^{(0)} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}$

We have known that $[L^2, H^{(0)}] = 0$, $[L_z, H^{(0)}] = 0$

But, How about $[L^2, H_r'] = ?$ $[L_z, H_r'] = ?$

Which is equivalent to show $[L^2, p^4] = 0$, $[L_z, p^4] = 0$

To show this, we need to use

$[AB, C] = A[B, C] + [A, C]B$

$[p^4, L_z] = p^2[p^2, L_z] + [p^2, L_z]p^2 = 0$ ($[p^2, L_z] = 0$)

Page 167 Problem 4.19 (c) $[L_z, p^2] = 0$

$p^2 = \vec{p}\cdot\vec{p}$, $\vec{L} = \vec{r} \times \vec{p}$

$[L_z, p^2] = [L_z, p_x^2] + [L_z, p_y^2] + [L_z, p_z^2]$

$= [L_z, p_x]p_x + p_x[L_z, p_x] + [L_z, p_y]p_y + p_y[L_z, p_y]$

$= i\hbar p_y p_x + p_x i\hbar p_y + (-i\hbar p_x)p_y + p_y(-i\hbar p_x) = 0$

$[x, p_x] = i\hbar$, $[y, p_y] = i\hbar$, $[x, p_y] = 0$, $[y, p_x] = 0$

$L_z = xp_y - yp_x$ independent of freedom

L_x, L_y, L_z are equivalent

$\Rightarrow [L_x, p^4] = [L_y, p^4] = 0$

↑ 投影背景墙面，注意保护，严禁书写！ ↑

$L^2 = L_x^2 + L_y^2 + L_z^2$, $[L^2, P^4] = L_x[P^4, L_x] + [P^4, L_x]L_x + \cdots + \cdots$ ($[P^4, L_x] = 0$, $[P^4, L_x] = 0$) $= 0$

$\Rightarrow \langle \psi_{n\ell m} | H_r' | \psi_{n\ell m} \rangle = 0$, $\langle \psi_{n\ell m} | H_r' | \psi_{n\ell' m'} \rangle = 0$ $\Rightarrow$ No off-diagonal terms

[Proof]: Because $[L^2, H_r'] = 0$, $[L_z, H_r'] = 0$

$0 = \langle \psi_{n\ell m} | [H_r', L^2] | \psi_{n\ell' m'} \rangle$

$= \langle \psi_{n\ell m} | H_r' L^2 - L^2 H_r' | \psi_{n\ell' m'} \rangle$

$= \hbar^2 \ell'(\ell'+1) \langle \psi_{n\ell m} | H_r' | \psi_{n\ell' m'} \rangle - \hbar^2 \ell(\ell+1) \langle \psi_{n\ell m} | H_r' | \psi_{n\ell' m'} \rangle$

$= \hbar^2 [\ell'(\ell'+1) - \ell(\ell+1)] \langle \psi_{n\ell m} | H_r' | \psi_{n\ell' m'} \rangle$

Nonzero; This part has to be zero.

Similarly, $\langle \psi_{n\ell m} | H_r' | \psi_{n\ell m'} \rangle = 0$

No need to do the diagonalization, so we can use Eq. (6.9)

Now, we evaluate $\langle \psi_{n\ell m} | H_r' | \psi_{n\ell m} \rangle$

[Trick]: $P^2 | \psi_{n\ell m} \rangle = 2m (E - V) | \psi_{n\ell m} \rangle$

(P: momentum; E: Eigen energy; V: potential energy)

$\Rightarrow \langle \psi | P^4 | \psi \rangle = \langle P^2 \psi | P^2 \psi \rangle = (2m)^2 \langle \psi_{n\ell m} | (E - V)^2 | \psi_{n\ell m} \rangle$

$\Rightarrow E_r^{(1)} = -\frac{1}{8m^3c^2}(2m)^2 \langle \psi_{n\ell m} | E_n^2 - 2E_n V + V^2 | \psi_{n\ell m} \rangle$ (E_n: Bohr energy)

$= -\frac{1}{8m^3c^2}(2m)^2 \left(E_n^2 - 2E_n \langle V \rangle + \langle V^2 \rangle \right)$

where $\langle V \rangle \equiv \langle \psi_{n\ell m} | -\frac{e^2}{4\pi\epsilon_0} \frac{1}{r} | \psi_{n\ell m} \rangle$

$\langle V^2 \rangle \equiv \langle \psi_{n\ell m} | \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \frac{1}{r^2} | \psi_{n\ell m} \rangle$

We evaluate $\langle V \rangle$ using Eq. [3.97] Stationary Virial theorem

1D $2\langle T \rangle = \langle x \frac{dV}{dx} \rangle$

3D $2\langle T \rangle = \langle \vec{r} \cdot \nabla V \rangle$ (T: Kinetic energy; ∇V: Gradient)

Because $V(\vec{r}) = V(r)$ has the spherical symmetry (has nothing to do with θ or φ)

We use the spherical coordinates

$\nabla V(\vec{r}) = -\frac{e^2}{4\pi\epsilon_0} \left[\frac{d}{dr}\left(\frac{1}{r}\right) \hat{r} + \cdots \hat{\theta} + \cdots \hat{\varphi} \right]$

$= \frac{e^2}{4\pi\epsilon_0} \frac{1}{r^2} \hat{r}$

$\Rightarrow 2\langle T \rangle = \langle \vec{r} \cdot \nabla V(\vec{r}) \rangle = \frac{e^2}{4\pi\epsilon_0} \left\langle \frac{1}{r^2} \vec{r} \cdot \hat{r} \right\rangle$ ($\vec{r} \parallel \hat{r}$; direction)

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

$\Rightarrow 2\langle T \rangle = -\langle V \rangle$ for $V(r) = -\frac{e^2}{4\pi\epsilon_0} \frac{1}{r}$

Along with $\langle T \rangle + \langle V \rangle = E_n$ $\Rightarrow \langle V \rangle = 2E_n$ ← Bohr

[Note]: $\langle T \rangle = \langle V \rangle$ for harmonic oscillator $H = \frac{1}{2}m\omega x^2 + \frac{1}{2m}\frac{\partial^2}{\partial x^2}$

The result by the Virial theorem is case by case

Problem 6.33 $\left\langle \frac{1}{r^2} \right\rangle = \frac{1}{(\ell + \frac{1}{2}) n^3 a^2}$ ← Bohr radius

($\ell^2(\psi_{n\ell m}) = \hbar^2 \ell(\ell+1)(\psi_{n\ell m})$; $E_n = \frac{E_1}{n^2}$)

$\langle V^2 \rangle = \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \left\langle \frac{1}{r^2} \right\rangle$

$E_r^{(1)} = -\frac{1}{2mc^2}\left[E_n^2 - 2E_n(2E_n) + \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \frac{1}{(\ell + \frac{1}{2}) n^3 a^2} \right]$ ($\langle V \rangle$; Bohr radius)

Express Bohr energy in terms of Bohr radius a

[6.55] $\left\langle \frac{1}{r} \right\rangle = \frac{1}{a}\frac{1}{n^2}$ $\Leftrightarrow \langle V \rangle = 2E_n = -\frac{e^2}{4\pi\epsilon_0}\left\langle \frac{1}{r} \right\rangle$

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

[4.77] Bohr radius $a \equiv \frac{4\pi\epsilon_0 \hbar^2}{me^2}$

$\Rightarrow E_n = -\frac{1}{2}\frac{e^2}{4\pi\epsilon_0}\frac{1}{a}\frac{1}{n^2} = -\frac{\hbar^2}{2m}\frac{1}{a^2}\frac{1}{n^2}$

Potential-like; Kinetic-like

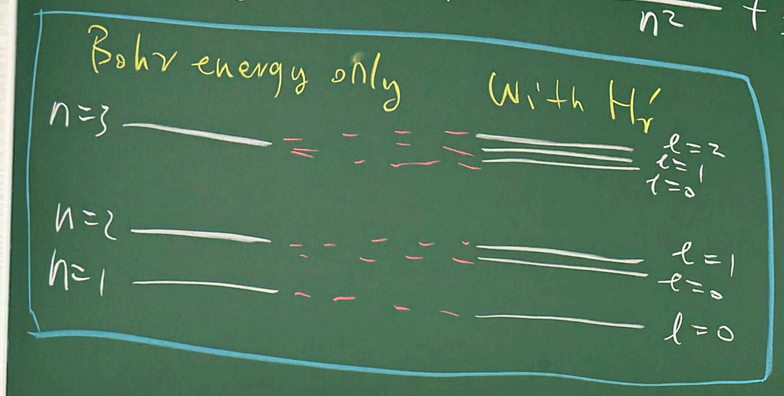
$$\Rightarrow E_r^{(1)} = -\frac{1}{2mc^2}\left[\cdots + \cdots + \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 \frac{4n}{4(l+\frac{1}{2})n^3a^2}\right]$$

$$= -\frac{1}{2mc^2}\left[E_n^2 - 4E_n^2 + E_n^2\frac{4n}{l+\frac{1}{2}}\right] \quad E_n^2\frac{4n}{l+\frac{1}{2}} \leftarrow \text{potential-like}$$

$$= \frac{E_n^2}{2mc^2}\left(3 - \frac{4n}{l+\frac{1}{2}}\right) \sim 10^{-5}E_n \sim \frac{E_n}{2mc^2}E_n \quad E_n \sim 10\,\text{eV},\ 2mc^2 \sim 10^6\,\text{eV}$$

Up to the (spinless) relativistic correction

$$E_{n,l} = E_n + E_r^{(1)} = -\frac{13.6\,\text{eV}}{n^2} + \frac{E_n^2}{2mc^2}\left(3 - \frac{4n}{l+\frac{1}{2}}\right)$$



Fine Structure

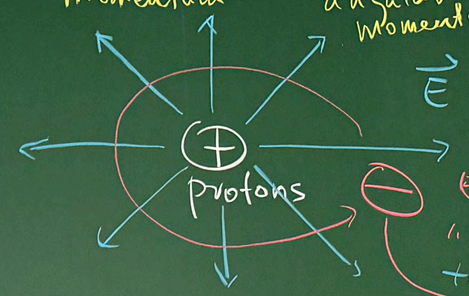
= (Spinless) relativistic

+ Spin-orbit Coupling

6.3.2 Spin-orbit coupling (Also a relativistic effect)

Spin angular momentum

Orbital angular momentum



$\vec{E}$ electric field of protons

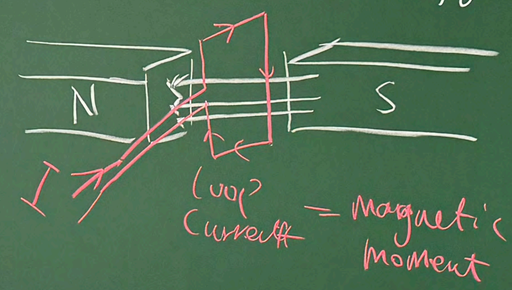
Electron feels an effective "magnetic" field, because the electric field is "moving"

$\Rightarrow$ Zeeman like energy $H = -\vec{\mu}\cdot\vec{B}$ [6.158]

Electron magnetic moment

proton electric field (orbital motion of electron)

Minus sign means anti-parallel has lower energy



Loop Current = Magnetic Moment

↑ 投影背景墙面，注意保护，严禁书写！ ↑

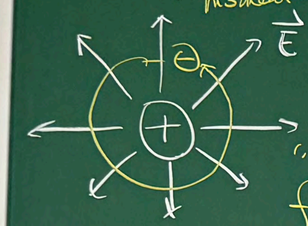
① "Magnetic" field of proton

② Magnetic moment of electron

SUSTech

6.3.2 Spin-orbit coupling (Also a relativistic effect)

Spin angular momentum — orbital angular momentum



Zeeman-like

$H = -\vec{\mu} \cdot \vec{B}$

$\vec{\mu}$: moment of electron spin; $\vec{B}$: "magnetic" field from orbital motion of electron

① Magnetic field of proton

Biot-Savart law $B = \frac{\mu_0 I}{2r}$

Current $I = \frac{e}{T}$ ← proton charge; ← period of the orbit of proton (electron)

Our task: to relate the "magnetic" field to the orbital angular momentum L

$$L = rMv = rM\frac{2\pi r}{T} = \frac{2\pi M r^2}{T} \Rightarrow \frac{1}{T} = \frac{L}{2\pi M r^2}$$

$$\Rightarrow B = \frac{\mu_0}{2r}\frac{e}{T} = \frac{\mu_0}{2r} e \frac{L}{2\pi M r^2} \Rightarrow \vec{B} = \frac{e\mu_0}{2r}\frac{\vec{L}}{2\pi M r^2} = \frac{e}{4\pi\epsilon_0 M c^2 r^3}\vec{L}$$

$\mu_0\epsilon_0 = \frac{1}{c^2}$, $\frac{e}{4\pi\epsilon_0 Mc^2 r^3}$

$\vec{L}$ and $\vec{B}$ are along the same direction

② Magnetic dipole moment of electron (to be related to spin angular momentum)

Angular momentum + charge = magnetic moment

Imagine electron as a rotating ring of { charge q, radius r, period T }

Angular momentum is an axial vector, which has to be treated as a loop current

Magnetic moment μ = current × area of ring $= \frac{q}{T}\cdot\pi r^2 = \frac{q\pi r^2}{T}$

Mass of the ring (electron) is m, its angular moment is moment of inertia × angular velocity

Inertia $= \int dm\, r = \int_0^{2\pi} r\, d\varphi \frac{m}{2\pi} r = mr^2$

Spin angular momentum $S = mr^2\frac{2\pi}{T} = \frac{2\pi m r^2}{T} \Rightarrow \vec{\mu} = \frac{q}{2m}\vec{S}$ ← spin angular momentum, an independent degree of freedom

$\vec{L}$ — $|n l m\rangle$ (Bohr) — $|m_s\rangle$ (Spin)

Consider the difference between classical and quantum

$$\vec{\mu}_e = -\frac{e}{m}\vec{S} \quad [6.60]$$

[6.58] $H = -\vec{\mu}\cdot\vec{B}$ Zeeman-like

[6.59] $\vec{B} = \frac{1}{4\pi\epsilon_0}\frac{e}{mc^2 r^3}\vec{L}$

[6.60] $\vec{\mu}_e = -\frac{e}{m}\vec{S}$

$$\Rightarrow H = \frac{e}{m}\vec{S}\frac{1}{4\pi\epsilon_0}\frac{e}{mc^2 r^3}\vec{L} = \frac{e^2}{4\pi\epsilon_0}\frac{1}{m^2c^2r^3}\vec{S}\cdot\vec{L}$$

Spin-orbit coupling

exchange of angular momenta

$$\vec{S}\cdot\vec{L} = S_x L_x + S_y L_y + S_z L_z = \frac{1}{2}(S_+ L_- + S_- L_+) + S_z L_z$$

$S_\pm = S_x \pm i S_y$, $L_\pm = L_x \pm i L_y$

$S_\pm |m_s\rangle \rightarrow |m_s \pm 1\rangle$, $L_\pm |m\rangle \rightarrow |m \pm 1\rangle$

$S_+ L_- |m, m_s\rangle \rightarrow |m-1, m_s+1\rangle$ ← exchge of angular momentum of $\hbar$

After considering the Thomas precession

Perturbation $H'_{SO} = \frac{e^2}{8\pi\epsilon_0}\frac{1}{M^2c^2 r^3}\vec{S}\cdot\vec{L}$

$\vec{S}\cdot\vec{L}$: Angular part; r^3: Radial part

Alternatively, this can be found from the Dirac equation

With SOC, $H = H^{(0)} + H'_{SO}$ no longer commute with $\vec{L}$ and $\vec{S}$

$H^{(0)}$: Bohr + (Spinless) relativistic

$[H'_{SO}, \vec{L}] \neq 0$, $[H'_{SO}, \vec{S}] \neq 0 \Rightarrow$ m and m_s are not conserved

$[\vec{L}\cdot\vec{S}, \vec{L}] \neq 0$ $\quad [\vec{L}\cdot\vec{S}, \vec{S}] \neq 0$

To show this

$$[\vec{S}\cdot\vec{L}, S] = [S_x L_x + S_y L_y + S_z L_z, (S_x, S_y, S_z)]$$

Scalar — Vector

$$= ([S_x L_x + S_y L_y + S_z L_z, S_x], [\cdots, S_y], [\cdots, S_z])$$

$$= ([S_y, S_x]L_y + [S_z, S_x]L_x, \cdots, \cdots) \neq 0$$

$[S_y, S_x] = -i\hbar S_z$, $[S_z, S_x] = i\hbar S_y$

Quantum Mechanics definition of an angular momentum

Pico Eq.(4.99) $[L_x, L_y] = i\hbar L_z$ ⇐ $\vec{L} \equiv \vec{r}\times\vec{p}$, $[x, p_x] = i\hbar$

(L_x: y, z; L_y: z, x; L_z: x, y)

In other words, $\hat{L}_z$ and $\hat{S}_z$ are not "good" to be used in the perturbation theory. Instead, we use the eigen states of (L^2, S^2, J^2, J_z) → only diagonal elements

(L^2, L_z, S^2, S_z) with off-diagonal elements

$\vec{J} = \vec{L} + \vec{S}$ Total angular momentum

$J^2 = (\vec{L}+\vec{S})\cdot(\vec{L}+\vec{S}) = L^2 + S^2 + 2\vec{L}\cdot\vec{S}$ ← $\vec{L}\cdot\vec{S} + \vec{S}\cdot\vec{L}$

$\Rightarrow \vec{L}\cdot\vec{S} = \frac{1}{2}(J^2 - L^2 - S^2)$

$[\vec{L}\cdot\vec{S}, J^2] = 0$, $[\vec{L}\cdot\vec{S}, L^2] = 0$, $[\vec{L}\cdot\vec{S}, S^2] = 0$

The eigenvalue of $\vec{L}\cdot\vec{S}$ is $\frac{1}{2}\hbar^2[j(j+1) - \ell(\ell+1) - s(s+1)]$

Our task is to evaluate the expectation value $\langle H'_{so}\rangle$ ($H'_{so} \propto \vec{L}\cdot\vec{S}$ always)

= Radial part + Angular part

Problem 6.35(c), 6.34

$\left\langle \frac{1}{r^3}\right\rangle = \frac{1}{\ell(\ell+\frac{1}{2})(\ell+1)n^3 a^3}$ ← Bohr radius

Example $|n=1, m_s=-\frac{1}{2}\rangle \xrightarrow{L_+ S_-} |n=0, m_s=\frac{1}{2}\rangle$

which means $\langle n=1, m_s=-\frac{1}{2}|\, H'_{so}\, |n=0, m_s=\frac{1}{2}\rangle \neq 0$

$m + m_s = m_j = \frac{1}{2}$ Conserved

off-diagonal elements of the matrix of $\langle H'_{so}\rangle$

Recall that Bohr energy $E_n = -\frac{e^2}{8\pi\epsilon_0 a}\frac{1}{n^2} = -\frac{\hbar^2}{2m}\frac{1}{a^2}\frac{1}{n^2}$

$\Rightarrow \frac{1}{a^3} = \frac{1}{a}\frac{1}{a^2} = \left(-E_n\frac{8\pi\epsilon_0}{e^2}n^2\right)\left(-E_n\frac{2m}{\hbar^2}n^2\right)$

$= E_n^2\frac{2m}{\hbar^2}\frac{8\pi\epsilon_0}{e^2}n^4$

Correction to energy from spin-orbit coupling

$E^{(1)}_{so} = \langle H'_{so}\rangle = \langle n\ell s j m_j|\hat{H}'_{so}|n\ell s j m_j\rangle$

(E_n, L^2, S^2, J^2, J_z)

$= \frac{e^2}{8\pi\epsilon_0 m^2c^2}\left\langle\frac{1}{r^3}\right\rangle\langle\vec{S}\cdot\vec{L}\rangle$

$= \frac{e^2}{8\pi\epsilon_0 m^2c^2}\frac{1}{\ell(\ell+\frac{1}{2})(\ell+1)n^3}E_n^2\frac{2m}{\hbar^2}\frac{8\pi\epsilon_0}{e^2}n^4$

$\times\frac{1}{2}\hbar^2[j(j+1) - \ell(\ell+1) - s(s+1)]$

$= \frac{E_n^2}{mc^2}n\,\frac{j(j+1) - \ell(\ell+1) - \frac{3}{4}}{\ell(\ell+\frac{1}{2})(\ell+1)}$ [6.65]

$\Rightarrow$ Fine Structure $E^{(1)}_{fs} = E^{(1)}_r + E^{(1)}_{so} =$ Eq.(6.57)+(6.65)

$= \frac{E_n^2}{2mc^2}\left(3 - \frac{4n}{j+\frac{1}{2}}\right)$ ← $j = \ell \pm \frac{1}{2}$

Using $E_n = -\frac{mc^2}{2}\alpha^2\frac{1}{n^2}$

$\Rightarrow E^{(1)}_{fs} = E_n\alpha^2\frac{1}{n^2}\left(\frac{n}{j+\frac{1}{2}} - 3\right)$

So far, the energy of Hydrogen atom

$E_{nj} = E_n + E^{(1)}_{fs} = -\frac{13.6\,eV}{n^2}\left[1 + \frac{\alpha^2}{n^2}\left(\frac{n}{j+\frac{1}{2}} - \frac{3}{4}\right)\right]$

Bohr

$j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$

6.4 Zeeman effect

An energy because of the angular momenta (orbital + spin) of electron

$H'_z = -(\vec{\mu}_\ell + \vec{\mu}_s)\cdot\vec{B}_{ext}$ ← A real external magnetic field

where $\vec{\mu}_s = -\frac{e}{m}\vec{S}$ magnetic dipole moment of spin

$\vec{\mu}_\ell = -\frac{e}{2m}\vec{L}$ orbital angular momentum

$\Rightarrow H'_z = \frac{e}{2m}(\vec{L}+2\vec{S})\cdot\vec{B}_{ext}$

B_{ext} External real magnetic field

B_{int} Internal "magnetic" field from spin-orbit coupling

Problem 6.20 Estimate $B_{int} \sim H'_{so}$

$H'_{so} = \cdots\vec{L}\cdot\vec{S} = \vec{B}_{int}\cdot\vec{\mu}_s$ ($\vec{\mu}_s = -\frac{e}{2m}\vec{S}$) $\Rightarrow B_{int} = \frac{1}{4\pi\epsilon_0}\frac{e}{mc^2r^3}\vec{L}$

Approximation $\vec{L} \to \hbar$, $r \to a$ Bohr radius

$$\Rightarrow B_{int} \sim \frac{(1.6\times10^{-19}\,\text{Coulomb})\times(1.05\times10^{-34}\,\text{Joul}\cdot\text{Sec})}{4\pi(8.9\times10^{-12}\,\text{Coulomb}^2/\text{N}\cdot\text{m}^2)(9.1\times10^{-31}\,\text{kg})(3\times10^{8}\,\text{m/s})\,(0.53\times10^{-10}\,\text{m})^3}$$

$$\approx 12\ \text{Tesla} = \frac{\text{Volt}\cdot\text{Sec}}{\text{Meter}^2}$$

Later, we will discuss 3 regimes

① $B_{ext} \ll B_{int}$ $|n l s j m_j\rangle$ → diagonal

② $B_{ext} \gg B_{int}$ $|n l s m m_s\rangle$ → diagonal

③ $B_{ext} \sim B_{int}$ Both with off-diagonal elements

6.4.1 Weak-field Zeeman effect ($B_{ext} \ll B_{int}$)

SOC

Total Hamiltonian of Hydrogen in a magnetic field

$$H = \underbrace{H_{Bohr} + H_{fs}}_{\text{Unperturbed}} + \underbrace{H_Z'}_{\text{Perturbation}}$$

Because of the spin-orbit coupling $\vec{L}\cdot\vec{S}$

m_l and m_s are not good quantum numbers

Now, good quantum numbers are n, l, j, m_j

$J^2|j\rangle = \hbar^2 j(j+1)|j\rangle$, $J_z|m_j\rangle = \hbar m_j|m_j\rangle$

6.4.1 Weak-field Zeeman effect

Total Hamiltonian of Hydrogen (So far)

$$H = \underbrace{H_{Bohr} + H_{fs}}_{\text{unperturbed}} + \underbrace{H'_z}_{\text{perturbation}}$$

Because of the spin-orbit coupling $\vec{L}\cdot\vec{S}$

$$\vec{L}\cdot\vec{S} = \frac{1}{2}(L_+S_- + L_-S_+) + L_zS_z$$

$L_\pm = L_x \pm iL_y$, $S_\pm = S_x \pm iS_y$

$$L_\pm|m_\ell\rangle = \hbar\sqrt{\ell(\ell+1) - m(m\pm1)}\,|m_\ell \pm 1\rangle$$ Problem 4.18

As a result, m_ℓ and m_s are no longer good quantum numbers

Now, the "good" quantum numbers are n, ℓ, j, m_j (H_{Bohr}: L^2, J^2, J_z)

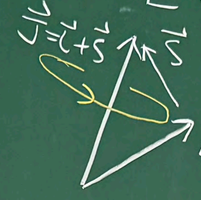
$\vec{J} = \vec{L} + \vec{S}$ total angular momentum

$J^2|j\rangle = \hbar^2 j(j+1)|j\rangle$, $J_z|m_j\rangle = \hbar m_j|m_j\rangle$

The Zeeman correction to energy

$$E_z^{(1)} = \langle n\ell j m_j | H'_z | n\ell j m_j\rangle$$
$$= \langle n\ell j m_j | \frac{e}{2m}\vec{B}_{ext}\cdot(\vec{L}+2\vec{S}) | n\ell j m_j\rangle$$
$$= \frac{e}{2m}\vec{B}_{ext}\cdot\langle n\ell j m_j | (\vec{L}+2\vec{S}) | n\ell j m_j\rangle$$

Where $\vec{L}+2\vec{S} = \vec{J}+\vec{S}$ → $\vec{J}+\vec{S}_{ave}$ (only the projection along $\vec{J}$ counts)



$\vec{L}$ and $\vec{S}$ process about $\vec{J}$

$$\vec{S}_{ave} = \left(\frac{\vec{S}\cdot\vec{J}}{J}\right)\left(\frac{\vec{J}}{J}\right) = \frac{\vec{S}\cdot\vec{J}}{J^2}\vec{J}$$

(average; magnitude, direction)

Also, $\vec{L} = \vec{J} - \vec{S}$

$$\Rightarrow L^2 = J^2 + S^2 - 2\vec{J}\cdot\vec{S}$$
$$\Rightarrow \langle\vec{S}\cdot\vec{J}\rangle = \left\langle\frac{1}{2}(J^2+S^2-L^2)\right\rangle$$
$$= \frac{\hbar^2}{2}\left[j(j+1) + \tfrac{1}{2}(\tfrac{1}{2}+1) - \ell(\ell+1)\right]$$

$$\Rightarrow \langle n\ell j m_j | \vec{L}+2\vec{S} | n\ell j m_j\rangle = \langle n\ell j m_j | \left(1 + \frac{\vec{S}\cdot\vec{J}}{J^2}\right)\vec{J} | n\ell j m_j\rangle$$
$$= \left[1 + \frac{\frac{\hbar^2}{2}[j(j+1) + \frac{3}{4} - \ell(\ell+1)]}{\hbar^2 j(j+1)}\right]\langle n\ell j m_j | \vec{J} | n\ell j m_j\rangle$$

Landé g-factor

$$\equiv g_J\langle\vec{J}\rangle$$ (vector)

[check] = Free electron $\ell=0$, $j=\frac{1}{2}$

$$g_J = 1 + \frac{\frac{3}{4}+\frac{3}{4}-0}{\frac{3}{4}} = 2$$

$$\Rightarrow E_z^{(1)} = \frac{e}{2m}\vec{B}_{ext}\cdot\langle\vec{L}+2\vec{S}\rangle = \frac{e}{2m}\vec{B}_{ext}\cdot g_J\langle\vec{J}\rangle$$
$$= \frac{e}{2m}g_J\vec{B}_{ext}\cdot\langle\vec{J}\rangle$$

We choose $\vec{B}_{ext} = B_{ext}\hat{z}$ The field direction defines the z axis

$$\Rightarrow E_z^{(1)} = \frac{e}{2m}g_J B_{ext}\hat{z}\cdot\langle J_x\hat{x} + J_y\hat{y} + J_z\hat{z}\rangle$$
$$= \frac{e}{2m}g_J B_{ext}\langle n\ell j m_j | J_z | n\ell j m_j\rangle \quad (E_0)$$
$$= \frac{e}{2m}g_J B_{ext}\hbar m_j \quad (\hbar m_j)$$

$$\Rightarrow E_z^{(1)} = \left(\frac{e\hbar}{2m}\right) g_J B_{ext} m_j$$

Bohr magneton; Tesla; dimensionless

$$\mu_B \equiv \frac{e\hbar}{2m} \approx 5.788\times10^{-5}\ eV/Tesla$$

$$\Rightarrow E_z^{(1)} = \mu_B g_J B_{ext} m_j$$

In other words, the Zeeman Hamiltonian can be written as

$$H'_z = \mu_B g_J B_{ext}\frac{\hat{J}_z}{\hbar}$$

Now, the total energy = Bohr + fine-structure + Zeeman

For example, the ground state $n=1$, $\ell=0$, $j=\frac{1}{2}$, $m_j=\pm\frac{1}{2}$

$$\Rightarrow E_{total} = -\underbrace{13.6eV}_{\hbar^2}\left[1 + \underbrace{\frac{\alpha^2}{n^2}}_{1}\left(\frac{n}{\underbrace{j+\frac{1}{2}}_{1}} - \frac{3}{4}\right)\right] \pm \mu_B g_J B_{ext}\frac{1}{2}$$

(2)

⬆ 投影背景墙面，注意保护，严禁书写！ ⬆

6.4.3. Zeeman effect – Intermediate regime

($B_{ext} \sim B_{int}$)

$H_z' \sim H_{so}'$

$$H = \underbrace{H_{Bohr}}_{\text{unperturbed}} + \underbrace{H_r' + H_{so}' + H_z'}_{\text{perturbation}}$$

$n\ell j m_j$ — L^2, J^2, J_z

$n\ell m_\ell m_s$ — L^2, L_z, S_z

We have to treat H_{so}' and H_z' on an equal footing

Steps ① Basis ② Find Matrices of H_{fs}' and H_z'
③ Diagonalization ⇒ Eigen energies

Example The $n=2$ states of hydrogen

How many states? 8 states ← the basis

$n=2 \Rightarrow \ell = 0, 1$, $s = \frac{1}{2}$ always $\Rightarrow j = \ell \pm s = \ell \pm \frac{1}{2}$

$\ell = 0 \Rightarrow j = \frac{1}{2} \Rightarrow m_j = \pm\frac{1}{2}$ (2 States)

$\ell = 1 \Rightarrow \begin{cases} j = \frac{1}{2} \Rightarrow m_j = \pm\frac{1}{2} & \text{(2 States)} \\ j = \frac{3}{2} \Rightarrow m_j = -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2} & \text{(4 States)} \end{cases}$

Representation 表象	Total angular momentum $\lvert j m_j \rangle$	$\lvert m_\ell m_s \rangle$
$\ell=0$ (2 States)	$\psi_1 = \lvert j=\frac{1}{2}, m_j=\frac{1}{2} \rangle$	$= \lvert m_\ell=0 \rangle \lvert m_s=\frac{1}{2} \rangle$
	$\psi_2 = \lvert j=\frac{1}{2}, m_j=-\frac{1}{2} \rangle$	$= \lvert m_\ell=0 \rangle \lvert m_s=-\frac{1}{2} \rangle$
C-G $\langle j, m_j \rvert m_\ell, m_s \rangle$	$\psi_3 = \lvert j=\frac{3}{2}, m_j=\frac{3}{2} \rangle$	$= \lvert \ell=1, m_\ell=1 \rangle \lvert s=\frac{1}{2}, m_s=\frac{1}{2} \rangle$
	$\psi_4 = \lvert j=\frac{3}{2}, m_j=-\frac{3}{2} \rangle$	$= \lvert m_\ell=-1 \rangle \lvert m_s=-\frac{1}{2} \rangle$
$\ell=1$ (6 States)	$\psi_5 = \lvert j=\frac{3}{2}, m_j=\frac{1}{2} \rangle$	$= \sqrt{\frac{2}{3}} \lvert m_\ell=0 \rangle \lvert m_s=\frac{1}{2} \rangle + \sqrt{\frac{1}{3}} \lvert m_\ell=1 \rangle \lvert m_s=-\frac{1}{2} \rangle$
	$\psi_6 = \lvert j=\frac{1}{2}, m_j=\frac{1}{2} \rangle$	$= \sqrt{\frac{1}{3}} \lvert m_\ell=0 \rangle \lvert m_s=\frac{1}{2} \rangle - \sqrt{\frac{2}{3}} \lvert m_\ell=1 \rangle \lvert m_s=-\frac{1}{2} \rangle$
	$\psi_7 = \lvert j=\frac{3}{2}, m_j=-\frac{1}{2} \rangle$	$= \sqrt{\frac{2}{3}} \lvert m_\ell=0 \rangle \lvert m_s=-\frac{1}{2} \rangle + \sqrt{\frac{1}{3}} \lvert m_\ell=-1 \rangle \lvert m_s=\frac{1}{2} \rangle$
	$\psi_8 = \lvert j=\frac{1}{2}, m_j=-\frac{1}{2} \rangle$	$= \sqrt{\frac{1}{3}} \lvert m_\ell=0 \rangle \lvert m_s=-\frac{1}{2} \rangle - \sqrt{\frac{2}{3}} \lvert m_\ell=-1 \rangle \lvert m_s=\frac{1}{2} \rangle$

6.4.2 Strong-field Zeeman effect ($B_{ext} \gg B_{int}$)

H_z H_{so}

Total Hamiltonian $H = \underbrace{H_{Bohr} + H_r + H_z}_{\text{Unperturbed } H^{(0)}} + \underbrace{H_{so}'}_{\text{Perturbation}}$

$$H_z = \frac{e}{2m}\vec{B}_{ext} \cdot (\vec{L} + 2\vec{S}) = \frac{e}{2m} B_{ext} (\hat{L}_z + 2\hat{S}_z)$$

Where $\vec{B}_{ext} = B_{ext}\hat{z}$ direction of field defines $\hat{z}$

Because $H_z \in H^{(0)}$, we can use m_ℓ and m_s as good quantum numbers

Unperturbed energy $E_{n m_\ell m_s} = -\frac{13.6\,eV}{n^2} + \mu_B B_{ext}(m_\ell + 2m_s)$

Perturbation Fine-structure correction to energy

$H_{fs}' = H_r' + H_{so}'$

$$H_{fs}' = \langle n\ell m_\ell m_s \rvert H_r' + H_{so}' \rvert n\ell m_\ell m_s \rangle = E_r^{(1)} + E_{so}^{(1)}$$

Eq. [6.57] $\Rightarrow E_r^{(1)} = -\frac{E_n^2}{2mc^2}\left(\frac{4n}{\ell+\frac{1}{2}} - 3\right) \Leftarrow H_r' = -\frac{p^4}{8m^3c^2}$

For spin-orbit coupling $H_{so}' \propto \vec{L}\cdot\vec{S}$, so we need to evaluate

$$\langle \vec{S}\cdot\vec{L} \rangle = \langle m_\ell m_s \rvert \frac{1}{2}(S_+L_- + S_-L_+) + S_zL_z \rvert m_\ell m_s \rangle$$

S_+L_- 不在 $H^{(0)}$

$$\langle m_s \rvert S_+ \rvert m_s \rangle \langle m_\ell \rvert L_- \rvert m_\ell \rangle \propto \langle m_s \rvert m_s+1 \rangle \langle m_\ell \rvert m_\ell - 1 \rangle = 0$$

$$\langle m_s \rvert S_z \rvert m_s \rangle \langle m_\ell \rvert L_z \rvert m_\ell \rangle = \hbar m_s \hbar m_\ell$$

$\Rightarrow \langle \vec{S}\cdot\vec{L} \rangle = \hbar^2 m_s m_\ell$

$\Rightarrow E_{fs}^{(1)} = E_r^{(1)} + E_{so}^{(1)}$ "Hack QM II" ⟶ [6.82]

$$\Rightarrow E_{fs}^{(1)} = -\frac{E_n^2}{2mc^2}\left(\frac{4n}{\ell+\frac{1}{2}} - 3\right) + \frac{e^2}{8\pi\epsilon_0}\frac{1}{m^2c^2}\left\langle\frac{1}{r^3}\right\rangle\langle\vec{S}\cdot\vec{L}\rangle$$

[6.54] [6.64] [6.81]

Clebsch-Gordan coefficients (P188 Table 4.8)

$\begin{pmatrix} j, & m_j \\ m_\ell, & m_s \end{pmatrix}$ Input output

$\ell = 1 \times \frac{1}{2} = s$

		$\frac{3}{2}$ $+\frac{3}{2}$						
$+1$	$+\frac{1}{2}$	1	$\frac{3}{2}$ $+\frac{1}{2}$	$\frac{1}{2}$ $+\frac{1}{2}$				
$+1$	$-\frac{1}{2}$		$\frac{1}{3}$	$\frac{2}{3}$	$\frac{3}{2}$	$\frac{1}{2}$		
0	$+\frac{1}{2}$		$\frac{2}{3}$	$-\frac{1}{3}$	$-\frac{1}{2}$	$-\frac{1}{2}$		
			0	$-\frac{1}{2}$	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{3}{2}$	
			-1	$+\frac{1}{2}$	$\frac{1}{3}$	$-\frac{2}{3}$	$-\frac{3}{2}$	
					-1	$-\frac{1}{2}$	1	

$\leftarrow j$

$\leftarrow m_j$

$\uparrow m_\ell$ $\uparrow m_s$

A $\sqrt{\ }$ is understood, minus sign goes outside

Why both representations?

Eq. [6.67] $\Rightarrow$ We need j to evaluate $E_{fs}^{(1)}$

Eq. [6.71] $\Rightarrow$ We need m_ℓ and m_s for $E_z^{(1)}$

Problem 6.25

Find the Matrix of $H'_{fs} + H'_z$ in the basis of $\{\psi_1, \psi_2, \dots, \psi_8\}$

[Solution]:

(1) Fine-Structure

[6.67] $E_{fs}^{(1)} = \frac{E_1}{n^2}\frac{\alpha^2}{n^2}\left(\frac{n}{j+\frac{1}{2}} - \frac{3}{4}\right)$

For $|\psi_1\rangle = |j=\frac{1}{2}, m_j=\frac{1}{2}\rangle$

$\langle\psi_1|H'_{fs}|\psi_1\rangle = \frac{E_1}{2^2}\frac{\alpha^2}{2^2}\left(\frac{2}{\frac{1}{2}+\frac{1}{2}} - \frac{3}{4}\right) = \frac{E_1\alpha^2}{4^3}5$

$\equiv -5\gamma$, where $\gamma \equiv -E_1\left(\frac{\alpha}{8}\right)^2$

Similarly, for $\psi_{2,6,8}$, $j=\frac{1}{2}$, the same as $\langle\psi_1|H'_{fs}|\psi_1\rangle$

$\langle\psi_3|H'_{fs}|\psi_3\rangle \equiv -\gamma$

4 4

5 5

7 7

投影背景墙面，注意保护，严禁书写！

$$H'_{fs} + H'_z = \begin{bmatrix} -5\gamma+\beta & & & & & & & \\ & -5\gamma-\beta & & & & & & \\ & & -\gamma+2\beta & & & & & \\ & & & -\gamma-2\beta & & & & \\ & & & & -\gamma+\frac{2}{3}\beta & -\frac{\sqrt{2}}{3}\beta & & \\ & & & & -\frac{\sqrt{2}}{3}\beta & -5\gamma+\frac{1}{3}\beta & & \\ & & & & & & -\gamma-\frac{2}{3}\beta & -\frac{\sqrt{2}}{3}\beta \\ & & & & & & -\frac{\sqrt{2}}{3}\beta & -5\gamma-\frac{1}{3}\beta \end{bmatrix}_{8\times 8}$$

Next time

(2) Matrix of H'_z

Problem 6.25 Find the matrix of $H'_{fs}+H'_z$ in the basis of $\{\psi_1, \psi_2, \dots, \psi_8\}$ Hydrogen $n=2$

[Solution]: (1) Last time H'_{fs} SOC (J, m_J)

(2) Matrix of Zeeman H'_z (M_ℓ, M_S)

[6.71] $\Rightarrow$ $\boxed{H'_z = \mu_B B_{ext}(\hat{M}_\ell + 2\hat{M}_S)}$ (μ_B: Bohr magneton)

$\hat{L}_z \equiv \hbar \hat{M}_\ell$, $\hat{S}_z \equiv \hbar \hat{M}_S$

For $|\psi_1\rangle = |J=\frac{1}{2}, m_J=\frac{1}{2}\rangle = |\ell=0, M_\ell=0\rangle|S=\frac{1}{2}, M_S=\frac{1}{2}\rangle$ (For convenience of SOC)

$\langle\psi_1|H'_z|\psi_1\rangle = \langle\frac{1}{2},\frac{1}{2}|\langle 0,0|\,\mu_B B_{ext}(\hat{M}_\ell + 2\hat{M}_S)\,|0,0\rangle|\frac{1}{2},\frac{1}{2}\rangle$ (For Zeeman)

$= \langle\frac{1}{2},\frac{1}{2}|\langle 0,0|\,\mu_B B_{ext}(0 + 2\cdot\frac{1}{2})\,|\frac{1}{2},\frac{1}{2}\rangle|0,0\rangle$

$= \mu_B B_{ext} \equiv \beta$

$\hat{J} = \frac{3}{2}$, $m_j = \frac{3}{2}$ ($|\psi_3\rangle$) or $-\frac{3}{2}$ ($|\psi_4\rangle$) $\Rightarrow$ $m_\ell = 1$, $m_S = \frac{1}{2}$ / $m_\ell = -1$, $m_S = -\frac{1}{2}$

$\hat{J} = \frac{1}{2}$, $m_j = -\frac{1}{2}$ ($|\psi_2\rangle$) $\Rightarrow$ $m_\ell = 0$, $m_S = -\frac{1}{2}$

$\langle\psi_2|H'_z|\psi_2\rangle = \mu_B B_{ext}(0 + 2\cdot(-\frac{1}{2})) = -\beta$

$\langle\psi_3|H'_z|\psi_3\rangle = \mu_B B_{ext}(1 + 2\cdot\frac{1}{2}) = 2\beta$

$\langle\psi_4|H'_z|\psi_4\rangle = \mu_B B_{ext}(-1 + 2(-\frac{1}{2})) = -2\beta$

$|\psi_5\rangle = \sqrt{\frac{2}{3}}\,|1,0\rangle|\frac{1}{2},\frac{1}{2}\rangle + \sqrt{\frac{1}{3}}\,|1,1\rangle|\frac{1}{2},-\frac{1}{2}\rangle$

$|\psi_6\rangle = -\sqrt{\frac{1}{3}}\,|1,0\rangle|\frac{1}{2},\frac{1}{2}\rangle + \sqrt{\frac{2}{3}}\,|1,1\rangle|\frac{1}{2},-\frac{1}{2}\rangle$

$\hat{H}'_z(\psi_5) = \mu_B B_{ext}(\hat{M}_\ell + 2\hat{M}_S)\left[\sqrt{\frac{2}{3}}\,|10\rangle|\frac{1}{2}\frac{1}{2}\rangle + \sqrt{\frac{1}{3}}\,|11\rangle|\frac{1}{2},-\frac{1}{2}\rangle\right]$

$= \mu_B B_{ext}\left[\sqrt{\frac{2}{3}}(0+2\cdot\frac{1}{2})|10\rangle|\frac{1}{2}\frac{1}{2}\rangle + \sqrt{\frac{1}{3}}\underbrace{\left[1+2\cdot(-\frac{1}{2})\right]}_{=0}|11\rangle|\frac{1}{2},-\frac{1}{2}\rangle\right]$

$= \mu_B B_{ext}\sqrt{\frac{2}{3}}\,|10\rangle|\frac{1}{2}\frac{1}{2}\rangle$

$\langle\psi_5|H'_z|\psi_5\rangle = \left[\sqrt{\frac{2}{3}}\langle\frac{1}{2}\frac{1}{2}|\langle 10| + \sqrt{\frac{1}{3}}\langle\frac{1}{2},-\frac{1}{2}|\langle 11|\right]\mu_B B_{ext}\sqrt{\frac{2}{3}}\,|10\rangle|\frac{1}{2}\frac{1}{2}\rangle$

Where $\langle 10|\langle\frac{1}{2}\frac{1}{2}|\frac{1}{2}\frac{1}{2}\rangle|10\rangle = 1$, $\langle\frac{1}{2},-\frac{1}{2}|\langle 11|10\rangle|\frac{1}{2},\frac{1}{2}\rangle = 0$ (orthogonal)

$\Rightarrow \langle\psi_5|H'_z|\psi_5\rangle = \sqrt{\frac{2}{3}}\,\mu_B B_{ext}\sqrt{\frac{2}{3}} = \frac{2}{3}\beta$

$\langle\psi_6|H'_z|\psi_5\rangle = \left(-\sqrt{\frac{1}{3}}\langle\frac{1}{2},\frac{1}{2}|\langle 1,0| + \sqrt{\frac{2}{3}}\langle\frac{1}{2},-\frac{1}{2}|\langle 1,1|\right]\mu_B B_{ext}$

$\times\sqrt{\frac{2}{3}}\,|10\rangle|\frac{1}{2},\frac{1}{2}\rangle$ ($\langle 11|10\rangle = 0$, $\langle 10|10\rangle = 1$)

$= -\sqrt{\frac{1}{3}}\,\mu_B B_{ext}\sqrt{\frac{2}{3}} = -\frac{\sqrt{2}}{3}\beta$

$|\psi_5\rangle$ and $|\psi_6\rangle$ share the same basis $|10\rangle|\frac{1}{2}\frac{1}{2}\rangle$, $|11\rangle|\frac{1}{2},-\frac{1}{2}\rangle$

So H'_z can couple $|\psi_5\rangle$ and $|\psi_6\rangle$

$\langle\psi_5|H'_z|\psi_6\rangle = \langle\psi_6|H'_z|\psi_5\rangle^*$ ← Complex Conjugate

$\langle\psi_{5,6}|H'_z|\psi_{7,8}\rangle = 0$ because they have different basis

$\langle\psi_7|H'_z|\psi_8\rangle = -\frac{\sqrt{2}}{3}\beta$

Share the same basis

Similarly, we can have all the matrix elements

$-W \equiv -\{\psi_1, \dots, \psi_8\}(H'_{fs}+H'_z)\begin{pmatrix}\psi_1\\ \vdots\\ \psi_8\end{pmatrix}$

$= \begin{bmatrix} 5\gamma-\beta & & & & & & & \\ & 5\gamma+\beta & & & & & & \\ & & \gamma-2\beta & & & & & \\ & & & \gamma+2\beta & & & & \\ & & & & \gamma-\frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta & & \\ & & & & \frac{\sqrt{2}}{3}\beta & 5\gamma-\frac{\beta}{3} & & \\ & & & & & & \gamma+\frac{2}{3}\beta & \frac{\sqrt{2}}{3}\beta \\ & & & & & & \frac{\sqrt{2}}{3}\beta & 5\gamma+\frac{\beta}{3} \end{bmatrix}$ (give the corrections to energy directly)

$-h = \begin{bmatrix} -\gamma+\frac{2}{3}\beta & -\frac{\sqrt{2}}{3}\beta \\ -\frac{\sqrt{2}}{3}\beta & -5\gamma+\frac{1}{3}\beta \end{bmatrix}$

$= (-3\gamma+\frac{1}{2}\beta)\begin{pmatrix}1&0\\0&1\end{pmatrix} + \begin{bmatrix} 2\gamma+\frac{\beta}{6} & -\frac{\sqrt{2}}{3}\beta \\ -\frac{\sqrt{2}}{3}\beta & -2\gamma-\frac{\beta}{6} \end{bmatrix}$

$\frac{1}{2}(h_{11}+h_{22})$ $\qquad$ $\frac{1}{2}(h_{11}-h_{22})$ $\qquad$ $-\frac{1}{2}(h_{11}-h_{22})$

↑ 投影背景墙面，注意保护，严禁书写！ ↑

$\Rightarrow h = h_0\sigma_0 + h_x\sigma_x + h_y\sigma_y + h_z\sigma_z$

$\sigma_0 = \begin{pmatrix}1&0\\0&1\end{pmatrix}$, $\sigma_x = \begin{pmatrix}0&1\\1&0\end{pmatrix}$, $\sigma_y = \begin{pmatrix}0&-i\\i&0\end{pmatrix}$, $\sigma_z = \begin{pmatrix}1&0\\0&-1\end{pmatrix}$

$h_0 = -3\gamma + \frac{1}{2}\beta$, $h_x = -\frac{\sqrt{2}}{3}\beta$, $h_y = 0$

$h_z = 2\gamma + \frac{1}{6}\beta$ $\Rightarrow E_\pm = h_0 \pm \sqrt{h_x^2 + h_y^2 + h_z^2}$

$\Rightarrow \chi_+ = \begin{pmatrix}\cos\frac{\theta}{2}\\ \sin\frac{\theta}{2}e^{i\phi}\end{pmatrix}$ $\chi_- = \begin{pmatrix}\sin\frac{\theta}{2}\\ -\cos\frac{\theta}{2}e^{i\phi}\end{pmatrix}$

$= \cos\frac{\theta}{2}|\uparrow_S\rangle + \sin\frac{\theta}{2}e^{i\phi}|\uparrow_0\rangle$

$\cos\theta \equiv \frac{h_z}{\sqrt{h_x^2+h_y^2+h_z^2}}$, $\tan\phi \equiv \frac{h_y}{h_x}$

6.5. Hyperfine Splitting

Physics: Interaction between electron spin $\vec{S}_e$ and proton (nuclear) spin $\vec{S}_p$

Read [6.85]–[6.88] by yourselves

$\Rightarrow E_{hf}^{(1)} = \frac{\mu_0 g_p e^2}{3\pi m_p m_e a^3}\langle \vec{S}_p \cdot \vec{S}_e \rangle$

So the Hamiltonian can be written as

$\hat{H}'_{hf} = \text{Constant}\ \vec{S}_p \cdot \vec{S}_e$ (Conserved)

Because of $\vec{S}_p\cdot\vec{S}_e$, $\vec{S}_p$ and $\vec{S}_e$ are no longer

$[\vec{S}_e, \vec{S}_p\cdot\vec{S}_e] \neq 0$, $[\vec{S}_p, \vec{S}_p\cdot\vec{S}_e] \neq 0$

Recall $[\vec{S}\cdot\vec{L}, \vec{S}] \neq 0$, $[\vec{S}\cdot\vec{L}, \vec{L}] \neq 0$

But, $\vec{S} = \vec{S}_e + \vec{S}_p \Rightarrow S = \begin{cases} S_e + S_p = \frac{1}{2}+\frac{1}{2} = 1 \\ S_e - S_p = 0 \end{cases}$

$\Rightarrow S^2 = S_e^2 + S_p^2 + 2\vec{S}_e\cdot\vec{S}_p$

$\Rightarrow \vec{S}_e\cdot\vec{S}_p = \frac{1}{2}(S^2 - S_e^2 - S_p^2)$

$[S_e^2, \vec{S}_e\cdot\vec{S}_p] = 0$, $[S_p^2, \vec{S}_e\cdot\vec{S}_p] = 0$

(S_e^2: magnitudes of S_e and S_p do not change)

$S = \begin{cases} S_e + S_p = 1 \Rightarrow m = 0, \pm 1 & \text{triplets 三重态} \\ S_e - S_p = 0 \Rightarrow m = 0 & \text{Singlet 单态} \end{cases}$

Projection of $\vec{S}$ along the $\hat{z}$ direction: $\hat{S}_z|m\rangle = \hbar m|m\rangle$

$E_{hf}^{(1)} = \text{Const.}\langle S^2 - S_e^2 - S_p^2\rangle$

$= \text{Const.}\ \hbar^2 \begin{cases} 1(1+1) - \frac{1}{2}(1+\frac{1}{2}) - \frac{1}{2}(1+\frac{1}{2}) = \frac{1}{2} & \text{Triplets} \\ 0(0+1) - \frac{1}{2}(1+\frac{1}{2}) - \frac{1}{2}(1+\frac{1}{2}) = -\frac{3}{2} \end{cases}$

Energy splitting $= E_{hf,\text{triplet}}^{(1)} - E_{hf,\text{singlet}}^{(1)} = \text{Const.}\ \hbar^2$

7.1 Theory of Variational Principle 变分原理

The variational principle gives the upper bound of the ground-state energy (E_{gs})

Pick any normalized function ψ, we can claim (does not have to be the eigen state, but has to be normalized)

$E_{gs} \leq \langle\psi|\hat{H}|\psi\rangle \equiv \langle H\rangle$

[Proof]: The eigen states (unknown) of $\hat{H}$ form a complete set, ψ_n

So ψ can be expressed as a linear combination

$\psi = \sum_n C_n\psi_n$, with $\begin{cases}\hat{H}\psi_n = E_n\psi_n \\ \langle\psi_n|\psi_m\rangle = \delta_{n,m}\end{cases}$

Since ψ is normalized

$1 = \langle\psi|\psi\rangle = \langle\sum_n C_n\psi_n|\sum_m C_m\psi_m\rangle$, n, m dumb index

$= \sum_n\sum_m C_n^* C_m\langle\psi_n|\psi_m\rangle^{=\delta_{n,m}} = \sum_n\sum_m C_n^* C_m\delta_{n,m} = \sum_n |C_n|^2$

$\Rightarrow \sum_n |c_n|^2 = 1$

Meanwhile, $\langle H\rangle = \langle \sum_m c_m \psi_m | \hat{H} | \sum_n c_n \psi_n \rangle$

$= \sum_n \sum_m c_m^* c_n \langle \psi_m | \underbrace{\hat{H}|\psi_n\rangle}_{E_n|\psi_n\rangle}$

$= \sum_n \sum_m c_m^* c_n E_n \underbrace{\langle \psi_m | \psi_n \rangle}_{\delta_{n,m}}$

$= \sum_n |c_n|^2 E_n$

By definition, $E_{gs} \le E_n$

So, $\langle H\rangle = \sum_n E_n |c_n|^2 \ge \sum_n E_{gs} |c_n|^2 = E_{gs} \underbrace{\sum_n |c_n|^2}_{=1}$ (Const.)

$\Rightarrow \langle \psi | \hat{H} | \psi \rangle \ge E_{gs}$

to be determined using the Variational Principle

Example 7.1 1D harmonic oscillator

$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$, $[x, p_x] = i\hbar$ $\hat{p} = -i\frac{\partial}{\partial x}\hbar$

Find its E_{gs}

[Solution]:

Step 1 Pick a $\boxed{\text{normalized}}$ trial function

$\psi(x) = A e^{-bx^2}$ Gaussian

Coefficient 系数

normalization factor (因子)

Variational parameter (参数) to be determined

$\boxed{1} = \int |\psi(x)|^2 dx = |A|^2 \int_{-\infty}^{\infty} e^{-2bx^2} dx$ Gaussian integral

$= |A|^2 \sqrt{\int_{-\infty}^{\infty} dx\, e^{-2bx^2} \int_{-\infty}^{\infty} dy\, e^{-2by^2}}$ $\rho^2 = x^2 + y^2$

$= |A|^2 \sqrt{\int_0^{2\pi}\int_0^{\infty} \rho\, d\rho\, e^{-2b\rho^2}}$ Polar coordinates

$= |A|^2 \sqrt{2\pi \int_0^{\infty} d(\frac{1}{2}\rho^2) e^{-2b\rho^2}} = |A|^2 \sqrt{\frac{2\pi}{2b}} \sqrt{-e^{-2b\rho^2}\Big|_0^{\infty}}$

$= |A|^2 \sqrt{\frac{\pi}{2b}} \Rightarrow A = \left(\frac{2b}{\pi}\right)^{1/4}$

↑ 投影背景墙面，注意保护，严禁书写！↑

$\Rightarrow \psi = \left(\frac{2b}{\pi}\right)^{1/4} e^{-bx^2}$

Step 2 Calculate $\langle H\rangle = \langle \psi | H | \psi \rangle = \langle T\rangle + \langle V\rangle$ Kinetic Potential

$\langle T\rangle = \int \psi^* \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\psi\, dx$ $\psi \left|\frac{d^2}{dx^2}\right| \psi$

$= -\frac{\hbar^2}{2m}|A|^2 \int_{-\infty}^{\infty} e^{-bx^2} \frac{d^2}{dx^2} e^{-bx^2} dx$

$= -\frac{\hbar^2}{2m}|A|^2 \int_{-\infty}^{\infty} dx\, e^{-bx^2} \left[e^{-bx^2}(-2bx)^2 + e^{-bx^2}(-2b)\right]$

$= -\frac{\hbar^2}{2m}|A|^2 \int_{-\infty}^{\infty} dx\, e^{-2bx^2}(4bx^2 - 2b)$

$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$, $\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{\sqrt{\pi}}{2a^{3/2}}$

$= -\frac{\hbar^2}{2m}|A|^2 \left[(2b)^2 \frac{\sqrt{\pi}}{2(2b)^{3/2}} - 2b\sqrt{\frac{\pi}{2b}}\right]$

$= \frac{\hbar^2 b}{2m}$ as a function of b

$\langle V\rangle = \int_{-\infty}^{\infty} \psi^* \frac{1}{2}m\omega^2 x^2 \psi\, dx$

$= \int_{-\infty}^{\infty} A e^{-bx^2} \frac{1}{2}m\omega^2 x^2 e^{-bx^2} dx$

$= \frac{1}{2}m\omega^2 |A|^2 \int_{-\infty}^{\infty} e^{-2bx^2} dx = \frac{1}{2}m\omega^2 \sqrt{\frac{2b}{\pi}} \frac{\sqrt{\pi}}{2(2b)^{3/2}}$

$= \frac{m\omega^2}{8b}$

$\langle H\rangle = \langle T\rangle + \langle V\rangle = \frac{\hbar^2 b}{2m} + \frac{m\omega^2}{8b}$ A function of b

Step 3 Minimize $\langle H\rangle$ as a function of b

$\frac{d}{db}\langle H\rangle = \frac{\hbar^2}{2m} - \frac{m\omega^2}{8b^2} = 0 \Rightarrow b = \frac{m\omega}{2\hbar}$ (positive)

$\frac{d}{db^2}\langle H\rangle \propto \frac{1}{b^3}$ (positive)

> 0



minimal $\frac{df}{dx} = 0$ $\frac{d^2f}{dx^2} > 0$

At $b = \frac{m\omega}{2\hbar}$, $\langle H\rangle = \frac{1}{2}\hbar\omega$ happen to be the exact result

7.1 Variational principle

Example 7.2 Delta potential

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \alpha\delta(x)$$ (kinetic, potential), Find Egs

[Solution]:

Step 1 Trial wavefunction Gaussian $\psi(x) = \left(\frac{2b}{\pi}\right)^{1/4} e^{-bx^2}$ (normalized)

Step 2 $\langle H\rangle = \langle T\rangle + \langle V\rangle$

See Example 7.1 $\Rightarrow \langle T\rangle = \frac{\hbar^2 b}{2m}$ kinetic

$\langle V\rangle = \int_{-\infty}^{\infty} dx\, A e^{-bx^2}\,[-\alpha\delta(x)]\, A e^{-bx^2}$ (potential)

$= -\alpha|A|^2 e^{-2b0^2} = -\alpha\sqrt{\frac{2b}{\pi}}$ ($\pm\delta(x-0)$)

$\langle H\rangle = \langle T\rangle + \langle V\rangle = \frac{\hbar^2 b}{2m} - \alpha\sqrt{\frac{2b}{\pi}}$ (Variational parameter)

Step 3 Minimize $\langle H\rangle$ as a function of b

$$\frac{d}{db}\langle H\rangle = 0 \Rightarrow \frac{\hbar^2}{2m} - \alpha\sqrt{\frac{1}{2\pi b}} = 0 \Rightarrow b = \frac{2m^2\alpha}{\pi\hbar^4} > 0$$

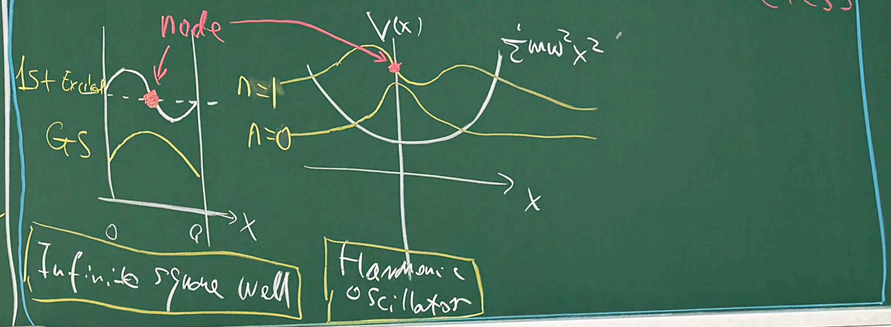
$$\frac{d^2}{db^2}\langle H\rangle \sim +\frac{1}{b^{3/2}} > 0$$ minimum

Step 4 $\langle H\rangle$ at $b_{min} = \frac{2m^2\alpha}{\pi\hbar^4}$

$$= \frac{\hbar^2}{2m}\frac{2m^2\alpha^2}{\pi\hbar^4} - \alpha\sqrt{\frac{2}{\pi}\frac{2m^2\alpha^2}{\pi\hbar^4}} = -\frac{m\alpha^2}{\pi\hbar^2}$$

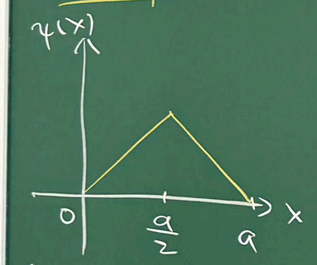
Eq. (2.129) $\Rightarrow$ Exact answer $= -\frac{m\alpha^2}{2\hbar^2}$ <

Ground-state wave function is nodeless



↑ 投影背景墙面，注意保护，严禁书写！ ↑

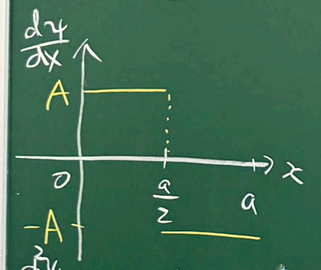
Example 7.3 1D infinite square well + "triangular" trial function



$$\psi(x) = \begin{cases} Ax, & x\in[0,\frac{a}{2}] \\ A(a-x), & x\in[\frac{a}{2},a] \\ 0, & \text{elsewhere}\end{cases}$$

[Solution] =

Step 1 Normalized trial wavefunction



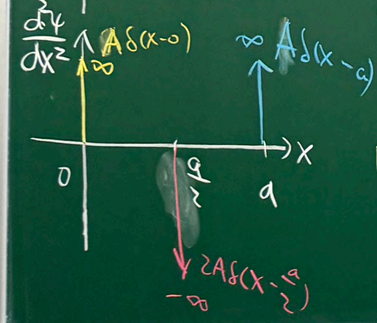
$$1 = |A|^2\left[\int_0^{a/2} dx\, x^2 + \int_{a/2}^{a}(a-x)^2 dx\right]$$

$$1 = |A|^2\left[\frac{1}{3}x^3\Big|_0^{a/2} + \frac{1}{3}(x-a)^3\Big|_{a/2}^{a}\right]$$

$$= \frac{1}{3}\frac{a^3}{4}|A|^2 \Rightarrow A = \frac{2}{a}\sqrt{\frac{3}{a}}$$

Step 2

$$\langle T\rangle = \int_0^a \psi^*\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right]\psi\, dx$$



where

$$\frac{d\psi}{dx} = \begin{cases} A, & x\in[0,\frac{a}{2}] \\ -A, & x\in[\frac{a}{2},a] \\ 0, & \text{elsewhere}\end{cases}$$

Considering $\frac{d\psi}{dx}(\text{upper bound}) = \int_{-\infty}^{\text{upper bound}} dx\, \frac{d^2\psi}{dx^2}$

$$\frac{d^2\psi}{dx^2} = A\,\delta(x-0) - 2A\delta(x-\tfrac{a}{2}) + A\delta(x-a)$$

$$\Rightarrow \langle T\rangle = \int_0^a \psi^*\left[-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}\right]\psi\, dx$$

$$= -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} dx\, \psi^*(x)\,A\left[\delta(x) - 2\delta(x-\tfrac{a}{2}) + A\delta(x-a)\right]$$

$$= -\frac{\hbar^2}{2m}A\left[\psi(0) - 2\psi(\tfrac{a}{2}) + \psi(a)\right]$$

$$= -\frac{\hbar^2}{2m}A\left(0 - 2A\frac{a}{2} + 0\right]$$

$$= \frac{12\hbar^2}{2ma^2} > \frac{\pi^2\hbar^2}{2ma^2}$$

[Summary]: Steps 1–4

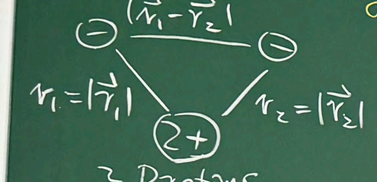
7.2 Ground state of Helium (Many-body wavefunction)

[Quiz] - How many Nobel Prize about Helium?

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

Electron 1 · Electron 2 · Two protons · electron-proton Coulomb interactions · electron-electron interaction

A real "3-body" problem (No exact solution)



[Our Goal]: To calculate E_{gs} using the variational principle

Experimentally measured as the energy to strip off both electrons $\approx -78.975\,eV$

[The trouble] = Coulomb interaction

$$V_{ee} = \frac{e^2}{4\pi\epsilon_0}\frac{1}{|\vec{r}_1 - \vec{r}_2|}$$

In the absence of V_{ee}

H reduces to $H_{e_1} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\frac{2}{r_1}$ (Bohr-like)

$H_{e_2} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\frac{2}{r_2}$

Each is a "Hydrogen", but $+e \to +2e$ two protons

[4.72] $\Rightarrow$ Bohr radius of Hydrogen $a \equiv \frac{4\pi\epsilon_0\hbar^2}{me^2}$ ($+e \to +2e$: $\to \frac{a}{2}$; electron, proton)

[4.80] $\Rightarrow$ The ground-state wave function of Hydrogen

$$\psi_{100} = \frac{1}{\sqrt{\pi a^3}} e^{-\frac{r}{a}}$$

($n=1$, ℓ, m) $\quad +e \to 2e,\ a \to \frac{a}{2}$

$$\to \sqrt{\frac{8}{\pi a^3}}\, e^{-\frac{2r}{a}}$$

one of the 2 electrons

With V_{ee}, the wave function is a product of two $\psi_{100}(a \to \frac{a}{2})$

$$\psi_0(\vec{r}_1, \vec{r}_2) = \psi_{100}(\vec{r}_1)\,\psi_{100}(\vec{r}_2)$$

($\vec{r}_2$: coordinates of electron 2; $\vec{r}_1$: coordinates of electron 1)

$$\psi_0(\vec{r}_1, \vec{r}_2) = \left(\sqrt{\frac{8}{\pi a^3}}\right)^2 e^{-\frac{2r_1}{a}} e^{-\frac{2r_2}{a}} = \frac{8}{\pi a^3} e^{-2(r_1+r_2)/a}$$

$r_1 = |\vec{r}_1|$, $r_2 = |\vec{r}_2|$ (Many-body wave function)

Eqs. [4.72] and [4.77] $\Rightarrow -13.6\,eV \approx E_1 = -\frac{\hbar^2}{2m}\frac{1}{a^2}$

$$E_1^{+2e} = -\frac{\hbar^2}{2m}\frac{4}{a^2}$$

($+e \to +2e$, $a \to \frac{a}{2}$)

The 2 "+2e-Hydrogen" $\Rightarrow 2E_1^{+2e} = -\frac{\hbar^2}{2m}\frac{4}{a^2}\cdot 2 = 8E_1 \approx 8\cdot(-13.6\,eV) \approx -109\,eV$

(far from experiment)

Now, we include V_{ee} and evaluate $\langle\psi_0(\vec{r}_1,\vec{r}_2)|V_{ee}|\psi_0(\vec{r}_1,\vec{r}_2)\rangle$

First, $H\psi_0 = (8E_1 + V_{ee})\psi_0$

(2 "+2e-Hydrogen"; V_{ee})

$$\langle\psi_0|H|\psi_0\rangle = 8E_1 + \langle\psi_0|V_{ee}|\psi_0\rangle$$

$$\langle\psi_0(\vec{r}_1,\vec{r}_2)|V_{ee}|\psi_0(\vec{r}_1,\vec{r}_2)\rangle = \int d^3\vec{r}_1 \int d^3\vec{r}_2\, \psi_0^*(\vec{r}_1,\vec{r}_2)\, V_{ee}\, \psi_0(\vec{r}_1,\vec{r}_2)$$

Six-fold integral

$$= \frac{e^2}{4\pi\epsilon_0}\left(\frac{8}{\pi a^3}\right)^2 \int \frac{e^{-4(r_1+r_2)/a}}{|\vec{r}_1 - \vec{r}_2|}\, d^3\vec{r}_1\, d^3\vec{r}_2$$

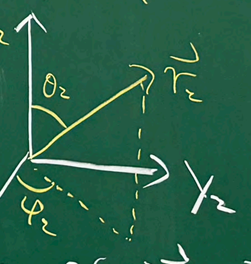
Cartesian coordinates: $\int dx_1 \int dy_1 \int dz_1 \int dx_2 \int dy_2 \int dz_2$

or $\int r_1^2 \sin\theta_1 d\theta_1 d\varphi_1 dr_1 \int r_2^2 \ldots$ Spherical coordinates

We do the $\vec{r}_2$ integral first

[Trick]: $z_2 \parallel \vec{r}_1$ ($\vec{r}_1 \parallel z_2$)

$$|\vec{r}_1 - \vec{r}_2| = \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta_2}$$



$$\Rightarrow \langle\psi_0|V_{ee}|\psi_0\rangle = \frac{e^2}{4\pi\epsilon_0}\left(\frac{8}{\pi a^3}\right)^2 \int d^3\vec{r}_1\, e^{-4r_1/a} \times \int d\vec{r}_2\, \frac{e^{-4r_2/a}}{|\vec{r}_1 - \vec{r}_2|} \equiv I_2$$

$$I_2 \equiv \int_0^{2\pi} d\phi_2 \int_0^{\pi} \sin\theta_2 d\theta_2 \int_0^{\infty} r_2^2 dr_2 \frac{e^{-4r_2/a}}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_2}}$$

(r_1 looks like a parameter)

2π

$$= 2\pi \int_0^{\infty} r_2^2 e^{-\frac{4r_2}{a}} dr_2 \int_0^{\pi} d\theta_2 \sin\theta_2 \frac{1}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_2}}$$

The θ_2 integral

$$= -\int_0^{\pi} d(\cos\theta_2) \frac{1}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_2}}$$

($x = \cos\theta_2$)

$$= -\int_1^{-1} dx \frac{1}{\sqrt{2r_1r_2}} \frac{1}{\sqrt{\frac{r_1^2+r_2^2}{2r_1r_2}-x}}$$

use $\int \frac{dx}{\sqrt{a-x}} = -2\sqrt{a-x}$

$$= \frac{1}{\sqrt{2r_1r_2}} (-2)\sqrt{\frac{r_1^2+r_2^2}{2r_1r_2}-x}\Big|_{x=1}^{a}$$

$$= \frac{1}{r_1r_2}\left[(r_1+r_2)-|r_1-r_2|\right] = \begin{cases} \frac{2}{r_1}, & r_2 < r_1 \\ \frac{2}{r_2}, & r_2 > r_1 \end{cases}$$

$$\Rightarrow I_2 = 2\pi \int_0^{\infty} r_2^2 dr_2 e^{-\frac{4r_2}{a}} \text{ (The } \theta_2 \text{ integral)}$$

$$= 2\pi \int_0^{r_1} dr_2 r_2^2 e^{-\frac{4r_2}{a}} \left(\frac{2}{r_1}\right) + 2\pi \int_{r_1}^{\infty} dr_2 r_2^2 e^{-\frac{4r_2}{a}} \left(\frac{2}{r_2}\right)$$

$$= 4\pi \left[\frac{1}{r_1}\int_0^{r_1} dr_2 r_2^2 e^{-\frac{4r_2}{a}} + \int_{r_1}^{\infty} dr_2 r_2 e^{-\frac{4r_2}{a}} \right]$$

Using Gaussian integrals $\int dx\, xe^x = e^x(x-1)$, $\int dx\, x^2e^x = e^x(x^2-2x+2)$

$$\Rightarrow I_2 = \frac{\pi a^3}{8r_1}\left[1-\left(1+\frac{2r_1}{a}\right)e^{-\frac{4r_1}{a}}\right]$$

$$\Rightarrow \langle V_{ee}\rangle = \frac{e^2}{4\pi\epsilon_0}\left(\frac{8}{\pi a^3}\right)^2 \int_0^{2\pi} d\phi_1 \int_0^{\pi} \sin\theta_1 d\theta_1 \int_0^{\infty} r_1^2 dr_1 \, I_2$$

($\int_0^{2\pi} d\phi_1 \int_0^{\pi} \sin\theta_1 d\theta_1 = 4\pi$)

$$= \frac{e^2}{4\pi\epsilon_0}\frac{8}{\pi a^3} 4\pi \int_0^{\infty} dr_1 \left(\underbrace{r_1 e^{-\frac{4r_1}{a}}}_{I_a} - \underbrace{r_1 e^{-\frac{8r_1}{a}}}_{I_b} - \underbrace{\frac{2r_1^2}{a} e^{-\frac{8r_1}{a}}}_{I_c} \right)$$

See "Hack QM II" in QQ

$$I_a = \left(\frac{a}{4}\right)^2, \quad I_b = -\left(\frac{a}{8}\right)^2, \quad I_c = -\frac{a^2}{128}$$

$$I_a + I_b + I_c = \frac{5}{128}a^2$$

$$\Rightarrow \langle V_{ee}\rangle = \frac{e^2}{4\pi\epsilon_0}\frac{8}{\pi a^3} 4\pi \frac{5}{128}a^2 = \frac{5}{4a}\frac{e^2}{4\pi\epsilon_0}$$

$$= -\frac{5}{2}E_1 \text{ where } E_1 = -\frac{e^2}{8\pi\epsilon_0 a} \approx -13.6\,\text{eV}$$

$$\approx 34\,\text{eV}$$

$$\Rightarrow \langle \psi_0(\vec{r}_1,\vec{r}_2)| \underbrace{2}_{\text{"+2e-Hydrogen"}} + V_{ee} |\psi_0(\vec{r}_1,\vec{r}_2)\rangle$$

$$= \underbrace{8E_1}_{} + \underbrace{\left(-\frac{5}{2}E_1\right)}_{} = -109\,\text{eV} + 34\,\text{eV} = -75\,\text{eV}$$

Close to the experiment, but we did not use the variational principle so far

Z^2E_1

Screening effect

Due to the other electron, one electron "sees" an attractive nuclear charge $Z < 2$



Z is the variational parameter

$1 < Z < 2$

Step 1 Trial wave function $\psi_0 \xrightarrow{Z \to Z} \psi_1$

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

Step 2 Evaluate $\langle \psi_1|H|\psi_1\rangle$ as a function of Z

$$H = \left[-\frac{\hbar^2}{2m}\nabla_1 - \frac{1}{4\pi\epsilon_0}\frac{Z}{r_1}\right] + \left[-\frac{\hbar^2}{2m}\nabla_2 - \frac{1}{4\pi\epsilon_0}\frac{Z}{r_2}\right] \Rightarrow Z^2E_1$$

$$+ \frac{e^2}{4\pi\epsilon_0}\left(\frac{Z-2}{r_1}+\frac{Z-2}{r_2}\right) + \frac{e^2}{4\pi\epsilon_0}\frac{1}{|\vec{r}_1-\vec{r}_2|}$$

⬆ 投影背景墙面，注意保护，严禁书写！⬆

SUSTech

7.2 Helium (Variational principle)

Step 1 Trial wave function

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

a: Bohr radius; Z: Variational parameter

Step 2 $\langle H\rangle(Z)$

$$H = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{1}{4\pi\epsilon_0}\frac{Z}{r_1} - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{1}{4\pi\epsilon_0}\frac{Z}{r_2}$$

$E_1 = -13.6\,eV$; Z^2E_1; Z^2E_1

$$+\frac{e^2}{4\pi\epsilon_0}\left(\frac{Z-Z}{r_1}+\frac{Z-Z}{r_2}\right) + \frac{e^2}{4\pi\epsilon_0}\frac{1}{|\vec{r}_1-\vec{r}_2|}$$

$$\Rightarrow \langle H\rangle \equiv \langle\psi_1(\vec{r}_1,\vec{r}_2)|H|\psi_1(\vec{r}_1,\vec{r}_2)\rangle$$

$$= 2Z^2E_1 + 2(Z-2)\frac{e^2}{4\pi\epsilon_0}\left\langle\frac{1}{r_1}\right\rangle + \langle V_{ee}\rangle$$

where $\left\langle\frac{1}{r_1}\right\rangle \equiv \left\langle\psi_1(\vec{r}_1,\vec{r}_2)\left|\frac{1}{r_1}\right|\psi_1(\vec{r}_1,\vec{r}_2)\right\rangle$

$$= \int d^3\vec{r}_1 \int d^3\vec{r}_2 \left(\frac{Z^3}{\pi a^3}\right)^2 e^{-2Z(r_1+r_2)/a}\,\frac{1}{r_1}$$

Use Eq. [6.55] $\Rightarrow \left\langle\frac{1}{r}\right\rangle = \frac{1}{a}$ ← Bohr radius (Hydrogen)

$$\Rightarrow \left\langle\frac{1}{r_1}\right\rangle \overset{+e\to Ze}{=} \frac{1}{a/Z}$$

For $Z=2$, $\langle\psi_0(\vec{r}_1,\vec{r}_2)|V_{ee}|\psi_0(\vec{r}_1,\vec{r}_2)\rangle = \frac{5}{8(\frac{2}{2})}\frac{e^2}{4\pi\epsilon_0}$

For $Z=Z$, $\langle\psi_1(\vec{r}_1,\vec{r}_2)|V_{ee}|\psi_1(\vec{r}_1,\vec{r}_2)\rangle = \frac{5}{8(\frac{2}{Z})}\frac{e^2}{4\pi\epsilon_0}$

$$= -\frac{5Z}{4}E_1$$

Put them together

$$\langle\psi_1|H|\psi_1\rangle = 2Z^2E_1 + 2(Z-2)\frac{e^2}{4\pi\epsilon_0}\frac{Z}{a} - \frac{5Z}{4}E_1$$

$E_1 = -\frac{e^2}{8\pi\epsilon_0 a}$

$$= E_1\left[2Z^2 - 4Z(Z-2) - \frac{5}{4}Z\right]$$

$$= E_1\left(-2Z^2 + \frac{27}{4}Z\right)$$

Step 3

$$\frac{d\langle H\rangle}{dZ} = 0 \Rightarrow E_1\left[-4Z+\frac{27}{4}\right] = 0 \Rightarrow Z = \frac{27}{16} \approx 1.69$$

Step 4 $\langle H\rangle = \left[-2\left(\frac{27}{16}\right)^2 + \frac{27}{4}\frac{27}{16}\right] \approx -77.5\,eV$

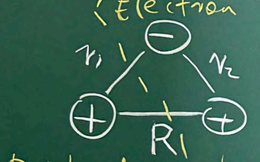
Experiment $-79\,eV$

[Note]: Many-body wavefunction $\psi_1(\vec{r}_1,\vec{r}_2)$

7.3 Hydrogen molecule ion (one-particle wavefunction) 单电子

H_2^+ < Hydrogen + proton

Energy



one electron shared by two protons

= Covalent bond (共价键)

= bound State (束缚态)

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r_1}+\frac{1}{r_2}\right) + \frac{e^2}{4\pi\epsilon_0}\frac{1}{R}$$

proton

Step 1 Trial wave function

For one proton $\psi_0(\vec{r}) = \frac{1}{\sqrt{\pi a^3}}e^{-r/a} \equiv \psi_{100}$

For two protons on equal footing

$$\psi = A\left[\psi_0(r_1) + \psi_0(r_2)\right]$$

A: normalization factor; r_1: distance between e and P_1; r_2: distance between e and P_2

LCAO = Linear Combination of Atomic Orbitals

Normalization

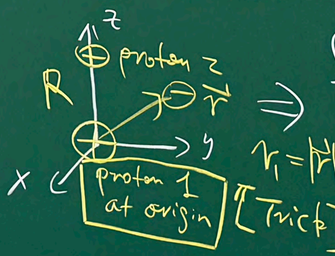
$$1 = \int|\psi|^2 d^3\vec{r} = |A|^2\left[\int|\psi_0(r_1)|^2 d^3\vec{r} + \int|\psi_0(r_2)|^2 d^3\vec{r} + 2\int\psi_0(r_1)\psi_0(r_2)\,d^3\vec{r}\right] \quad [7.38]$$

F1 F1

$\psi_0^*(r_1)\psi_0(r_2) + \psi_0(r_1)\psi_0^*(r_2)$

Integral over only one electron

The 1st and 2nd integral



[Trick]

$$\Rightarrow r_1 = |\vec{r}|$$

$$\int|\psi_0(r_1)|^2 d^3\vec{r} = \int|\psi_{100}(\vec{r})|^2 d^3\vec{r} = 1$$

r_1: distance between e and P_1

Similarly, Put P_2 at the origin

$$\Rightarrow \int|\psi_0(r_2)|^2 d^3\vec{r} = 1$$

Coordinates of electron

↑ 投影背景墙面，注意保护，严禁书写！↑

The 3rd integral

$$I \equiv \int \psi_0(r_1)\,\psi_0(r_2)\,d^3\vec{r} = \frac{1}{\pi a^3}\int e^{-\frac{r_1+r_2}{a}}\,d^3\vec{r}$$

where $r_1 = |\vec{r}| = r$, $r_2 = \sqrt{r^2+R^2-2rR\cos\theta}$

(put P_1 at the origin, put P_2 along the z direction)

$$\Rightarrow I = \frac{1}{\pi a^3}\int_0^{2\pi}d\varphi\int_0^{\pi}\sin\theta\,d\theta\int_0^{\infty}r^2 dr\, e^{-\frac{r}{a}}e^{-\frac{1}{a}\sqrt{r^2+R^2-2rR\cos\theta}}$$

"Hack QM II": Let $t = \sqrt{r^2+R^2-2rR\cos\theta} \Rightarrow dt^2 = d(r^2+R^2-2rR\cos\theta)$

$\Rightarrow 2t\,dt = 2rR\sin\theta\,d\theta \Rightarrow \sin\theta\,d\theta = \frac{t\,dt}{rR}$

Do the θ integral first, then the r integral

$$= e^{-\frac{R}{a}}\left[\frac{1}{3}\left(\frac{R}{a}\right)^2 + \frac{R}{a} + 1\right] \quad [7.42]$$

$[7.38] \Rightarrow |A|^2(2+2I) = 1 \Rightarrow |A|^2 = \frac{1}{2(1+I)}$

Step 2 Evaluate $\langle H\rangle$ as a function of $\frac{R}{a}$ ← variational parameter

Note that (4 terms):

$$\left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{1}{4\pi\epsilon_0}\frac{1}{r_1}\right)\psi_0(r_1) = E_1\psi_0(r_1) \quad \text{---} ①$$

$$\left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{1}{4\pi\epsilon_0}\frac{1}{r_2}\right)\psi_0(r_2) = E_1\psi_0(r_2) \quad \text{---} ②$$

$$H\psi = \left[-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r_1}+\frac{1}{r_2}\right)\right]A\left[\psi_0(r_1)+\psi_0(r_2)\right]$$

where 4 out of 6 terms $= A[① + ②]$

$$\Rightarrow H\psi = E_1\psi - A\frac{e^2}{4\pi\epsilon_0}\left[\frac{1}{r_2}|\psi_0(r_1)\rangle + \frac{1}{r_1}|\psi_0(r_2)\rangle\right]$$

($A[① + ②]$; rest 2 terms)

$$\Rightarrow \langle\psi|H|\psi\rangle = \langle\psi|E_1|\psi\rangle - A\left[\langle\psi_0(r_1)| + \langle\psi_0(r_2)|\right]$$

$$= E_1 - |A|^2\frac{e^2}{4\pi\epsilon_0}\left[\langle\psi_0(r_1)|\frac{1}{r_2}|\psi_0(r_1)\rangle + \langle\psi_0(r_2)|\frac{1}{r_1}|\psi_0(r_2)\rangle + \langle\psi_0(r_1)|\frac{1}{r_1}|\psi_0(r_2)\rangle + \langle\psi_0(r_2)|\frac{1}{r_2}|\psi_0(r_1)\rangle\right]$$

($\langle\psi|\psi\rangle = 1$; equivalent $r_1 \leftrightarrow r_2$)

$$= E_1 - 2|A|^2\frac{e^2}{4\pi\epsilon_0}\left[\langle\psi_0(r_1)|\frac{1}{r_2}|\psi_0(r_1)\rangle + \langle\psi_0(r_1)|\frac{1}{r_1}|\psi_0(r_2)\rangle\right]$$

Define $D \equiv a\langle\psi_0(r_1)|\frac{1}{r_2}|\psi_0(r_1)\rangle$ Direct

$X \equiv a\langle\psi_0(r_1)|\frac{1}{r_1}|\psi_0(r_2)\rangle$ eXchange

Problem 7.8 $\Rightarrow$

$$D = \frac{a}{R} - \left(1+\frac{a}{R}\right)e^{-\frac{2R}{a}}$$

$$X = \left(1+\frac{R}{a}\right)e^{-\frac{R}{a}}$$

Also, note that $\boxed{E_1 = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{2a}}$

$$\Rightarrow \langle\psi|H|\psi\rangle = E_1 + 2|A|^2\frac{e^2}{4\pi\epsilon_0}\frac{1}{a}(D+X)$$

($|A|^2 = \frac{1}{2(1+I)}$)

$$= E_1 + 4\frac{1}{2(1+I)}E_1(D+X) = E_1\left[1+\frac{2(D+X)}{1+I}\right]$$

(Electron only)

Also, the proton–proton repulsion

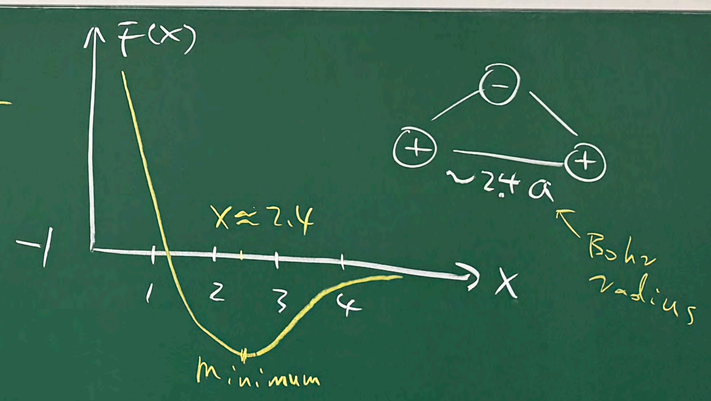
$$V_{pp} = \frac{e^2}{4\pi\epsilon_0}\frac{1}{R} = -\frac{2a}{R}\underbrace{\left(-\frac{e^2}{4\pi\epsilon_0}\frac{1}{2a}\right)}_{E_1} = -\frac{2a}{R}E_1$$

Define $x = \frac{R}{a}$ dimensionless variational parameter

The total energy in units of E_1

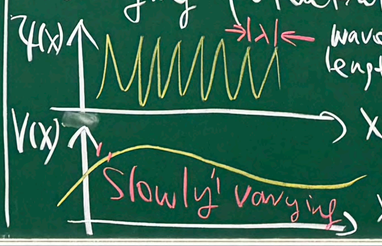
$$\frac{V_{pp}+\langle H\rangle}{E_1} \equiv F(x) = -1 + \frac{2}{x}\left[\frac{(1-\frac{2}{3}x^2)e^{-x} + (1+x)e^{-2x}}{1+(1+x+\frac{1}{3}x^2)e^{-x}}\right]$$

Fig 7.7.



Chap 8 WKB approximation (a semiclassical approximation)

The WKB method is to find approximate solutions to the 1D time-independent Schrödinger equation for "slowly" varying potential $V(x)$

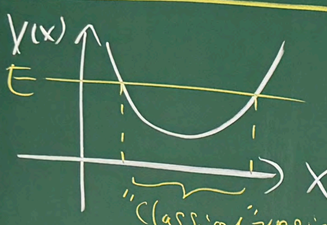


$\lambda = \frac{2\pi}{k}$ wave vector

$k \equiv \sqrt{2m(E-V)/\hbar}$

Three regions { ① Total energy E > Potential energy V "classical" → Bound state ; ② $E < V$ "Tunneling" ; ③ $E \sim V$ "Turning point" }

8.1 Classical region (Bound state) $E > V(x)$



The Schrödinger eqn.

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

$$\Rightarrow \frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}[E - V(x)]\psi$$

Refine $p(x) \equiv \sqrt{2m[E - V(x)]}$ (not momentum)

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

"Semiclassical", because { $[x, p] = i\hbar$, Cannot determine x and p simultaneously ; But, p is a function of x }

$E > V(x) \Rightarrow p(x)$ is real (实的)

In general, $\psi(x)$ is complex, we can express

$$\psi(x) = A(x)\, e^{i\phi(x)}$$

[Approximation 1] Both the amplitude $A(x)$ and the phase $\phi(x)$ are functions of x

$$\frac{d\psi}{dx} = A' e^{i\phi} + A e^{i\phi} i\phi' \qquad A' \equiv \frac{dA}{dx},\ \phi' \equiv \frac{d\phi}{dx}$$

$$\frac{d^2\psi}{dx^2} = (A'' + iA'\phi' + iA\phi'')e^{i\phi} + (A' + iA\phi')e^{i\phi} i\phi'$$
$$= [A'' + i2A'\phi' + iA\phi'' - A(\phi')^2]e^{i\phi}$$

$$\Rightarrow [A'' + i2A'\phi' + iA\phi'' - A(\phi')^2]e^{i\phi} = -\frac{p^2}{\hbar^2}A e^{i\phi}$$

The real part $A'' - A(\phi')^2 = -\frac{p^2}{\hbar^2}A$

or $A'' = A\left[(\phi')^2 - \frac{p^2}{\hbar^2}\right] = 0$ ← Approximation 2

The imaginary part $2A'\phi' + A\phi'' = 0 \Rightarrow (A^2\phi')' = 0$

$$\Rightarrow A^2\phi' = \text{constant} \Rightarrow A = \frac{C}{\sqrt{\phi'}} \text{ or } -\frac{C}{\sqrt{\phi'}}$$

[Approximation 2] Assume A varies slowly, so that $A'' \to 0$

$$\Rightarrow 0 = A\left[(\phi')^2 - \frac{p^2}{\hbar^2}\right] \Rightarrow \frac{d\phi}{dx} = \pm\frac{p}{\hbar}$$

$$\Rightarrow d\phi = \pm\frac{1}{\hbar}p(x)dx$$

Integrate on both sides $\phi(x) = \pm\frac{1}{\hbar}\int_0^x p(x')dx'$ ← For convenience

General solution

$$\psi(x) = C_+ \frac{1}{\sqrt{p(x)}} e^{\frac{i}{\hbar}\int p(x)dx} + C_- \frac{1}{\sqrt{p(x)}} e^{-\frac{i}{\hbar}\int p(x)dx}$$

[Note] = [8.1.2] mean this ↗

⬆ 投影背景墙面，注意保护，严禁书写！⬆

Chap 8 WKB approximation

8.1 Classical Region (Bound state, $E \geq V$)

General solution (一维定态薛定谔方程)

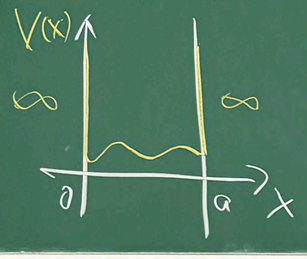
$$\psi(x) = \frac{C_+}{\sqrt{p(x)}} e^{\frac{i}{\hbar}\int p(x)dx} + \frac{C_-}{\sqrt{p(x)}} e^{-\frac{i}{\hbar}\int p(x)dx} \quad [8.10]$$

Total energy E, potential V

where $p(x) \equiv \sqrt{2m[E-V(x)]}$

An observation $|\psi(x)|^2 \sim \frac{1}{p(x)}$ — The probability to find the particle is inversely proportional to its "momentum"

Example 8.1 Potential well with 2 vertical walls



$$V(x) = \begin{cases} \text{some function}, & 0 < x < a \\ \infty, & \text{otherwise} \end{cases}$$

Inside well, if $E > V(x)$, we have

$$\psi(x) \cong \frac{1}{\sqrt{p(x)}}\left[C_+ e^{i\phi(x)} + C_- e^{-i\phi(x)}\right]$$

where $\phi(x) \equiv \frac{1}{\hbar}\int_{\text{A convenient lower bound}}^{x} p(x')dx'$

We can check $\frac{d}{dx}\phi(x) = \frac{1}{\hbar}p(x)$

Boundary conditions $\begin{cases} \psi(x=0) = 0 \\ \psi(x=a) = 0 \end{cases}$

The first one means: $\phi(x=0) = \frac{1}{\hbar}\int_0^{x=0} \cdots = 0$

The general solution can also be written as

$$\psi(x) \cong \frac{1}{\sqrt{p(x)}}\left[C_1 \sin\phi(x) + C_2 \cos\phi(x)\right] \Leftarrow e^{ix} = \cos x + i\sin x$$

Apply the boundary conditions

① $\phi(x=0)=0 \Rightarrow \cos\phi(x=0)=1,\ \sin\phi(x=0)=0$

Steps to solve a differential equation

① Trial solution $e^{\lambda x}$, e^{ikx} — Turn the differential eqn. to algebraic eqn.

② General solution

③ Boundary conditions / Initial conditions

Boundary condition $\psi(x=0)=0 \Rightarrow C_2 = 0$

② $\psi(x=a)=0 \Rightarrow$

$$\psi(x=a) \cong \frac{1}{\sqrt{p(x=a)}}\left[C_1 \sin\phi(x=a)\right] = 0$$

$\Rightarrow \sin\phi(x=a)=0 \Rightarrow \phi(x=a) = n\pi$, n integers

$\Rightarrow \phi(x=a) \equiv \frac{1}{\hbar}\int_0^{x=a} p(x')dx' = n\pi$

$\Rightarrow$ **$\int_0^a p(x)dx = n\pi\hbar$**, where $p(x) \equiv \sqrt{2m(E-V(x))}$

Quantization conditions (The first one) for two vertical walls

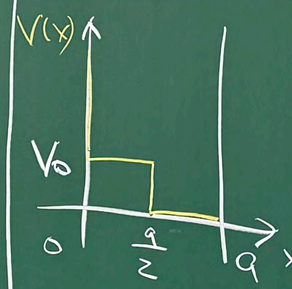
to be found, to be given

For example $V(x)=0$

$p(x) = \sqrt{2mE} \Rightarrow \int_0^a p(x)dx = \int_0^a \sqrt{2mE}\,dx = n\pi\hbar$

$\Rightarrow a\sqrt{2mE} = n\pi\hbar \Rightarrow E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$

Example 8.1 A well with 2 vertical walls and a "shelf"



$$V(x) = \begin{cases} V_0, & x \in [0, \frac{a}{2}] \\ 0, & x \in [\frac{a}{2}, a] \\ \infty, & \text{otherwise} \end{cases}$$

[Solution]: Use the quantization condition

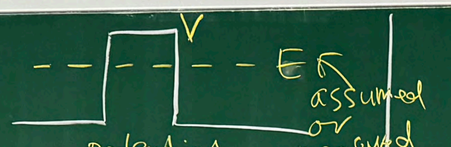
$\int_0^a p(x)dx = n\pi\hbar$, n integers, $p(x) \equiv \sqrt{2m[E-V(x)]}$

$\Rightarrow \int_0^{a/2}\sqrt{2m(E-V_0)}\,dx + \int_{a/2}^{a}\sqrt{2mE}\,dx = n\pi\hbar$

$\Rightarrow$ One hour later $E = E_n^{(0)} + \frac{1}{2}V_0 + \frac{V_0^2}{16E_n^{(0)}}$

$E_n^{(0)} = \frac{n^2\pi^2\hbar^2}{2ma^2}$

8.2 Tunneling ($E < V$)

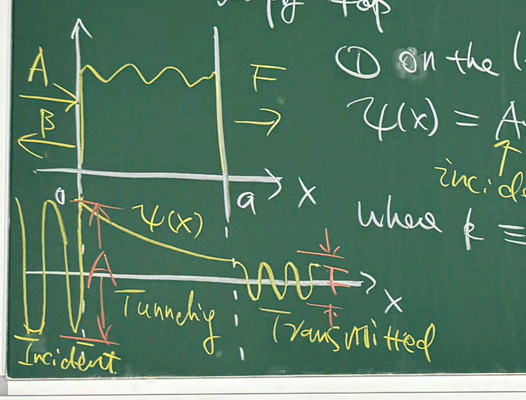


For $E < V(x)$, $p(x)$ is imaginary

$\Rightarrow$ General solution $\psi(x) \simeq \frac{C_+}{\sqrt{|p(x)|}} e^{\frac{1}{\hbar}\int |p(x)|dx} + \frac{C_-}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar}\int |p(x)|dx}$ (diverse / decay)

A physical consideration

Problem Scattering from a rectangular barrier with a bumpy top



① On the left side of the barrier ($x < 0$)

$\psi(x) = Ae^{ikx} + Be^{-ikx}$ (plane wave)

A: incident amplitude, B: reflected amplitude

where $k \equiv \sqrt{2mE}/\hbar$ wave vector

② On the right side ($x > a$)

$\psi(x) = Fe^{ikx}$ ← Transmitted amplitude

③ In the tunneling region ($0 \le x \le a$)

The WKB approximation gives

$\psi(x) = \frac{D}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar}\int_0^x |p(x')|dx'}$ only decay term

Matching the boundary conditions $\Rightarrow$

$\left|\frac{F}{A}\right| \sim e^{-\frac{1}{\hbar}\int_0^a |p(x)|dx}$, where $p(x) \equiv \sqrt{2m[E - V(x)]}$

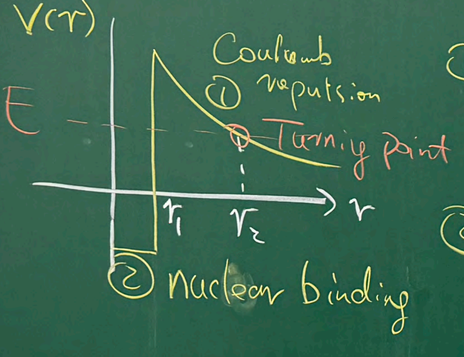
Define the transmission probability

$T \equiv \left|\frac{F}{A}\right|^2 \simeq e^{-2\gamma}$, where $\gamma \equiv \frac{1}{\hbar}\int_0^a |p(x)|dx$ (Gamma) (8.22)

We can check $\begin{cases} a \to \infty, \gamma \to \infty, T \to 0 \\ a \to 0, \gamma \to 0, T \to 1 \end{cases}$

Example 8.2 Gamow's theory of the α decay

α particle = 2 protons + 2 neutrons



① The α particle ($+2e$) is repelled by the leftover nucleus charge Ze ($+ze$) $V(r) = \frac{2e}{4\pi\epsilon_0}\frac{Ze}{r}$

② A barrier more than twice the energy of the emitted particle E

At the turning point $E = V(r_2)$

$\left.\begin{aligned} \frac{1}{4\pi\epsilon_0}\frac{2e\,Ze}{r_2} &= E \\ V(r) &= \frac{1}{4\pi\epsilon_0}\frac{2e\,Ze}{r} \end{aligned}\right\} \Rightarrow V(r) = E\frac{r_2}{r}$ (E given)

The decay exponent γ

$\gamma \equiv \frac{1}{\hbar}\int_{r_1}^{r_2} \sqrt{2m[V(r) - E]}\,dr = \frac{1}{\hbar}\int_{r_1}^{r_2} \sqrt{2m\left(E\frac{r_2}{r} - E\right)}dr$

(r_2 ← right boundary; r_1 ← left boundary of the barrier)

$= \frac{\sqrt{2mE}}{\hbar}\int_{r_1}^{r_2}\sqrt{\frac{r_2}{r} - 1}\,dr$

[Trick]: let $r \equiv r_2 \sin^2\theta$ "Hack QM II"

$\Rightarrow \gamma = \frac{\sqrt{2mE}}{\hbar}\left[r_2\frac{\pi}{2} - 2\sqrt{r_1 r_2}\right]$

where $E = \frac{1}{4\pi\epsilon_0}\frac{2e\,Ze}{r_2} \Rightarrow r_2 = \frac{2Ze^2}{4\pi\epsilon_0}\frac{1}{E}$

$\gamma = \frac{\sqrt{2mE}}{\hbar}\frac{\pi}{2}\frac{1}{4\pi\epsilon_0}\frac{2Ze^2}{E} - \frac{\sqrt{2mE}}{\hbar}2\sqrt{r_1\frac{1}{4\pi\epsilon_0}\frac{2Ze^2}{E}}$

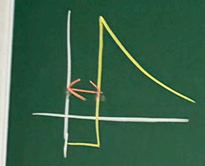
$\equiv k_1\frac{Z}{\sqrt{E}} - k_2\sqrt{Zr_1}$

where $k_1 \equiv \frac{e^2}{4\pi\epsilon_0}\frac{\pi\sqrt{2m}}{\hbar} \approx 1.980\,(\mathrm{MeV})^{1/2}$ (10^6), $k_2 \equiv \sqrt{\frac{e^2}{4\pi\epsilon_0}}\frac{4\sqrt{m}}{\hbar} \approx 1.485\,(\mathrm{fm})^{-1/2}$ (10^{-15} m)

Transmission probability $T \equiv e^{-2\gamma}$

[Experiement] ① The α particle have an average velocity v, So the frequency of collisions with the wall is $\frac{v}{2r_1}$

② The probability of escape at each collision is $e^{-2\gamma} = T$



$\Rightarrow$ The probability of emission per unit time $\frac{v}{2r_1} e^{-2\gamma}$

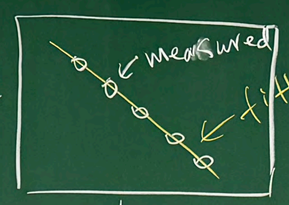
Inverse $\Rightarrow$ The lifetime $\tau = \frac{2r_1}{v} e^{2\gamma}$

Experimentally measurable $\Rightarrow$

$$\ln \tau = \ln \frac{2r_1}{v} + 2\gamma = \ln \frac{2r_1}{v} + 2\left[k_1 \frac{z}{\sqrt{E}} - k_2\sqrt{2r_1}\right]$$

$\ln\tau$ = y $= C_1 + C_2 \frac{1}{\sqrt{E}}$ = x

$y = \ln\tau$



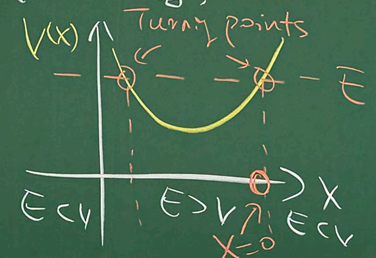
$\frac{1}{\sqrt{E}} \equiv x$

$\ln\tau$ is a linear function of $\frac{1}{\sqrt{E}}$

8.3 Connection formulas

To connect the WKB solutions on both sides of the turning point (C, B, D)

Previously, we have studied two regions



The problem At the turning points

$E = V \Rightarrow p(x) \equiv \sqrt{2m(E-V)} = 0$

$\psi \propto \frac{1}{\sqrt{p(x)}}$ WKB breaks down

⬆ 投影背景墙面，注意保护，严禁书写！ ⬆

For convenience, we set $x = 0$ at the turning point

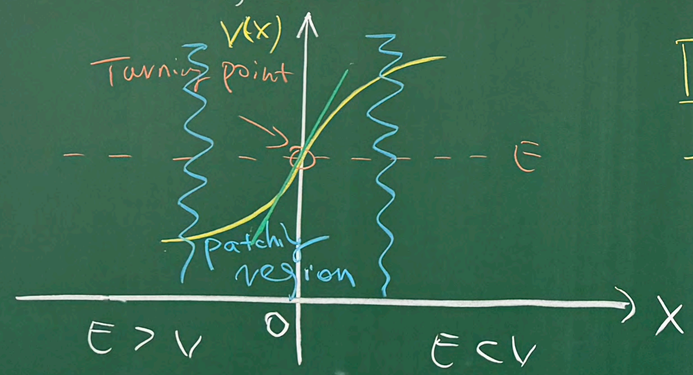


Fig. 8.7 One of the turning points

In the WKB approximation

$$\psi(x) \cong \begin{cases} \frac{1}{\sqrt{p(x)}}\left(B e^{\frac{i}{\hbar}\int_x^0 p(x')dx'} + C e^{-\frac{i}{\hbar}\int_x^0 p(x')dx'}\right), & x<0 \\ \frac{D}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar}\int_0^x |p(x')|dx'}, & x>0 \end{cases} \quad [8.31]$$

Our task is to connect the two solutions at the turning point, by using a "patching" wave function

[Trick]: Linearization $V(x) \approx V(x=0) + \left.\frac{dV}{dx}\right|_{x=0} x = E + V'(0)x$

Solve the Schrödinger eqn. of the linearized potential

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_p}{dx^2} + [E + V'(0)x]\psi_p = E\psi_p$$

linearized $V(x)$ — for patching

$$\Rightarrow \frac{\hbar^2}{2m}\frac{d^2\psi_p}{dx^2} = V'(0)x\psi_p \Rightarrow \frac{d^2\psi_p}{dx^2} = \frac{2mV'(0)}{\hbar^2}x\psi_p$$

$$\Rightarrow \frac{d^2\psi_p}{dx^2} = \alpha^3 x \psi_p \quad \text{where } \alpha \equiv \left(\frac{2m}{\hbar^2}V'(0)\right)^{1/3}$$

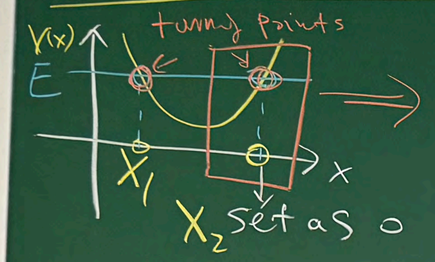
Define $z \equiv \alpha x$, so $x = \frac{z}{\alpha}$

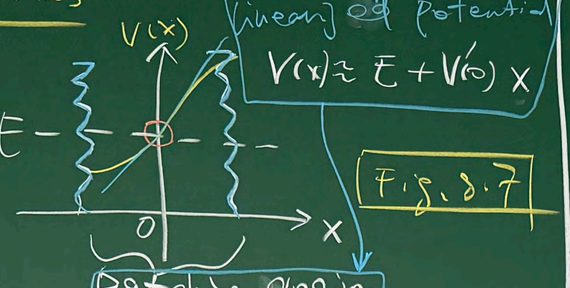
$$\Rightarrow \frac{d^2\psi_p}{d\left(\frac{z}{\alpha}\right)^2} = \alpha^3 \frac{z}{\alpha}\psi_p \Rightarrow \frac{d^2\psi_p}{dz^2} = z\psi_p$$ Airy's equation

Its solutions are called Airy functions $A_i(z)$, $B_i(z)$

SUSTech

8.3. Connection formulas



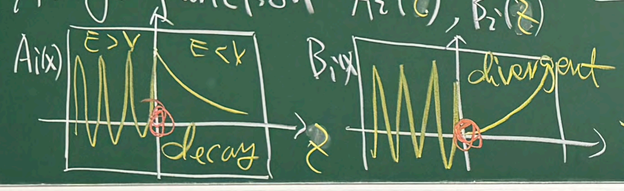


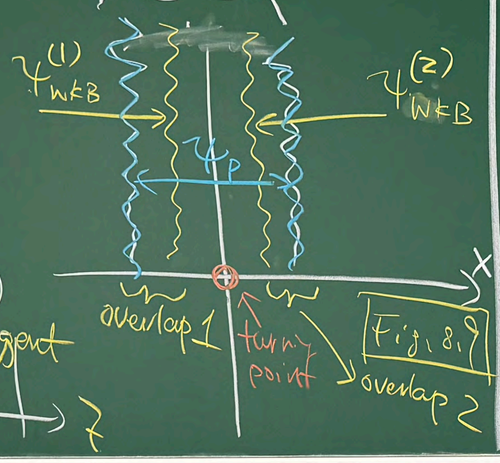
Put the linearized potential into the Schrödinger equation

$$\Rightarrow \frac{d^2\psi_p}{dz^2} = z\,\psi_p \quad \text{(Airy equation)}$$

Its solutions

Airy function $A_i(z)$, $B_i(z)$





The general solution of the patching region

$$\psi_p(x) = a\,Ai(\alpha x) + b\,Bi(\alpha x) \qquad \alpha \equiv \left[\frac{2m}{\hbar^2}V'(0)\right]^{1/3} \quad [8.37]$$

$z \equiv \alpha x$

a and b to be determined and to be used to connect B, C, and D in ψ_{WKB}

For the WKB solutions in the overlap zones, we also consider the linearized potential

$$p(x) \simeq \sqrt{2m[E-(E+V'(0)x)]} = \hbar\alpha^{3/2}\sqrt{-x}$$

[Tricky point]:

① The overlap zones are close to the turning point, so that the linearization is reasonable ($|x| \to 0$)

② The overlap zones are far enough away from the turning point, so that WKB solution is reliable ($|z| \gg 0$)

Overlap zone 2 ($E < V$)

$$p(x) \equiv \sqrt{2m[E-V(x)]} \quad \text{(linearized)}$$

Eq. [8.31] $\Rightarrow$

$$\psi^{(2)}_{WKB} = \frac{D}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar}\int_0^x |p(x')|dx'}$$

where $\int_0^x |p(x')|dx' \simeq \hbar\alpha^{3/2}\int_0^x \sqrt{x'}\,dx' = \frac{2}{3}\hbar(\alpha x)^{\frac{3}{2}}$ with linearized potential [8.38]

$$\Rightarrow \psi^{(2)}_{WKB}(x) = \frac{D}{\sqrt{\hbar\alpha^{3/2}\sqrt{x}}} e^{-\frac{2}{3}(\alpha x)^{3/2}} \quad [8.39]$$

Non-classical WKB solution with the linearized potential

Meanwhile, use the asymptotic form in Tab. 8.1 for $z \gg 0$, Eq. [8.34] reduces to

$$\psi_p(z) = a\,Ai(z) + b\,Bi(z)$$

$$\overset{z\gg 0}{\simeq} \frac{a}{2\sqrt{\pi}\,z^{1/4}} e^{-\frac{2}{3}z^{\frac{3}{2}}} + \frac{b}{\sqrt{\pi}\,z^{1/4}} e^{\frac{2}{3}z^{\frac{3}{2}}} \qquad (z \gg 0)$$

$z = \alpha x$ $\downarrow$

$$\psi_p(x) = \frac{a}{2\sqrt{\pi}(\alpha x)^{1/4}} e^{-\frac{2}{3}(\alpha x)^{\frac{3}{2}}} + \frac{b}{\sqrt{\pi}(\alpha x)^{1/4}} e^{\frac{2}{3}(\alpha x)^{3/2}}$$

Compare $\psi^{(2)}_{WKB}$ and ψ_p in the overlap zone 2

$$\Rightarrow \boxed{b = 0}, \quad \frac{a}{2\sqrt{\pi}(\alpha x)^{1/4}} = \frac{D}{\sqrt{\hbar\alpha^{3/2}\sqrt{x}}}$$

$$\Rightarrow \boxed{a = D}\,\frac{2\sqrt{\pi}\,\alpha^{1/4}}{\sqrt{\hbar}\,\alpha^{3/4}} = D\sqrt{\frac{4\pi}{\alpha\hbar}}$$

$$\Rightarrow \psi_p(x) = aAi(x) \quad \text{In the patching region}$$

$$\int_x^0 p(x')dx' = \frac{2}{3}\hbar(-\alpha x)^{\frac{3}{2}}$$

Overlap zone 1 (turning point)

[8.31] $\Rightarrow$

$$\int_x^0 p(x')dx' = \int_x^0 \hbar\alpha^{\frac{3}{2}}\sqrt{-x'}\,dx' \quad [8.38] \text{ Linearized Potential}$$

$$\psi^{(1)}_{WKB} = \frac{1}{\sqrt{p(x)}}\left(Be^{\frac{i}{\hbar}\int_x^0 p(x')dx'} + Ce^{-\frac{i}{\hbar}\int_x^0 p(x')dx'}\right)$$

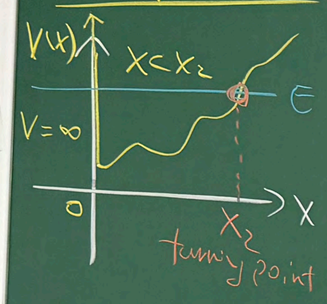
$$= \frac{1}{\sqrt{\hbar\alpha^{3/2}\sqrt{-x}}}\left[Be^{\frac{i}{\hbar}\frac{2}{3}\hbar(-\alpha x)^{\frac{3}{2}}} + Ce^{-\frac{i}{\hbar}\frac{2}{3}\hbar(-\alpha x)^{\frac{3}{2}}}\right]$$

Classical WKB solution with the linearized potential

$$\Rightarrow \psi(x) = \begin{cases} \frac{D}{\sqrt{p(x)}} \sin\left[\frac{\pi}{4} + \frac{1}{\hbar}\int_x^{x_2} p(x')dx'\right], & x < x_2 \\ \frac{D}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar}\int_{x_2}^{x} |p(x')|dx'}, & x > x_2 \end{cases} \quad [8.46]$$

For given $V(x)$ and boundary conditions, we can use Eq. [8.46] to determine E

Example 8.3 Potential well with one vertical wall



Boundary Condition $\psi(0) = 0$

$$[8.46] \Rightarrow 0 = \psi(0) \cong \frac{2D}{\sqrt{p(0)}} \sin\left[\frac{1}{\hbar}\int_0^{x_2} p(x')dx' + \frac{\pi}{4}\right]$$

$\sqrt{p(0)}$: finite; $\int_0^{x_2}$: $\neq 0$

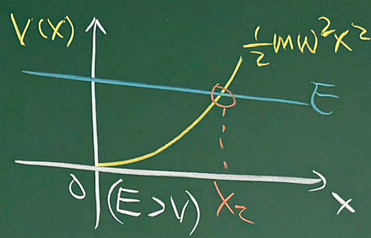
$$\Rightarrow \frac{1}{\hbar}\int_0^{x_2} p(x')dx' + \frac{\pi}{4} = n\pi, \quad n \text{ integers}$$

$$\Rightarrow \boxed{\int_0^{x_2} p(x)dx = (n - \tfrac{1}{4})\pi\hbar} \quad [8.47]$$

infinite wall; turning point

The 2nd quantization condition of WKB

"Half-harmonic" oscillator



$$V(x) = \begin{cases} \frac{1}{2}m\omega^2 x^2, & x > 0 \\ \infty, & \text{elsewhere} \end{cases}$$

To find the bound state energies E

Step 1 Find the turning point x_2

$$E = \frac{1}{2}m\omega^2 x_2^2 \Rightarrow x_2 = \frac{1}{\omega}\sqrt{\frac{2E}{m}}$$

Step 2 Find $p(x)$

$$p(x) = \sqrt{2m\left(E - \tfrac{1}{2}m\omega^2 x^2\right)} = \sqrt{2m\tfrac{1}{2}m\omega^2(x_2^2 - x^2)}$$

Use the asymptotic form of the Airy function for $z \ll 0$

$$\psi_p(x) = \frac{a}{\sqrt{\pi}(-\alpha x)^{1/4}} \sin\left[\frac{2}{3}(-\alpha x)^{\frac{3}{2}} + \frac{\pi}{4}\right]$$

$\sin x = \frac{e^{ix} - e^{-ix}}{2i}$

$$= \frac{a}{\sqrt{\pi}(-\alpha x)^{1/4} 2i}\left[e^{i\frac{\pi}{4}} e^{i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}} - e^{-i\frac{\pi}{4}} e^{-i\frac{2}{3}(-\alpha x)^{\frac{3}{2}}}\right] \quad [8.44]$$

Compare $\psi^{(1)}_{WKB}$ and ψ_p in the overlap zone 1

$$\frac{a e^{i\frac{\pi}{4}}}{\sqrt{\pi}(-\alpha x)^{1/4} 2i} = \frac{B}{\sqrt{\hbar}\,\alpha^{\frac{3}{4}}(-x)^{1/4}} \Rightarrow B = \frac{\sqrt{\hbar\alpha}}{2i\sqrt{\pi}} e^{i\frac{\pi}{4}} a$$

$$\frac{-a e^{-i\frac{\pi}{4}}}{\sqrt{\pi}(-\alpha x)^{1/4} 2i} = \frac{C}{\sqrt{\hbar}\,\alpha^{\frac{1}{4}}(-x)^{1/4}} \Rightarrow C = -\frac{\sqrt{\hbar\alpha}}{2i\sqrt{\pi}} e^{-i\frac{\pi}{4}} a$$

where $a = D\sqrt{\frac{4\pi}{\alpha\hbar}}$

$$\Rightarrow B = \frac{\sqrt{\hbar\alpha}}{2i\sqrt{\pi}} e^{i\frac{\pi}{4}} D\sqrt{\frac{4\pi}{\alpha\hbar}} = -i e^{i\frac{\pi}{4}} D$$

$$C = -\frac{\sqrt{\hbar\alpha}}{2i\sqrt{\pi}} e^{-i\frac{\pi}{4}} D\sqrt{\frac{4\pi}{\alpha\hbar}} = i e^{-i\frac{\pi}{4}} D$$

Put them into Eq. [8.31]

$$\psi(x) \cong \begin{cases} \frac{1}{\sqrt{p(x)}}\left[B e^{\frac{i}{\hbar}\int_x^0 p(x')dx'} + C e^{-\frac{i}{\hbar}\int_x^0 p(x')dx'}\right], & x < 0 \\ \frac{D}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar}\int_0^x |p(x')|dx'}, & x > 0 \end{cases} \quad [8.51]$$

$$\Rightarrow \psi(x) \cong \begin{cases} \frac{-iD}{\sqrt{p(x)}}\left(e^{i\frac{\pi}{4}} e^{\frac{i}{\hbar}\int_x^0 p(x')dx'} - e^{-i\frac{\pi}{4}} e^{-\frac{i}{\hbar}\int_x^0 p(x')dx'}\right), & x < 0 \\ \frac{D}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar}\int_0^x |p(x')|dx'}, & x > 0 \end{cases}$$

$\sin x = \frac{e^{ix} - e^{-ix}}{2i}$

↑ turning point, $0 \to x_2$

$p(x) = m\omega\sqrt{x_2^2 - x^2}$ $\quad E_n$

Step 3 Use the quantization condition to find

$$\int_0^{x_2} p(x)dx = m\omega \int_0^{x_2} \sqrt{x_2^2 - x^2}\, dx = m\omega \frac{\pi}{4} x_2^2$$

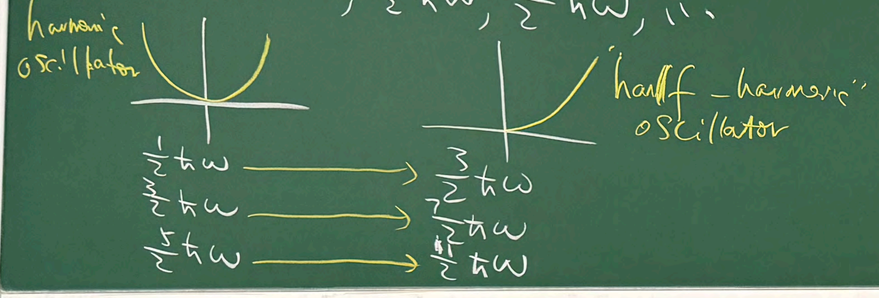
$$= m\omega \frac{\pi}{4} \frac{2E}{\omega^2 m}$$

$$\boxed{\int_0^a \sqrt{a^2 - x^2}\, dx = \frac{\pi}{4} a^2}$$

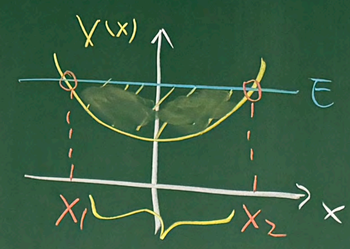
$$\Rightarrow \int_0^{x_2} p(x)dx = \frac{\pi E}{2\omega} = (n - \tfrac{1}{4})\pi\hbar$$

$$\Rightarrow E_n = (2n - \tfrac{1}{2})\hbar\omega, \; n \text{ integers}$$

$$= \tfrac{3}{2}\hbar\omega, \tfrac{7}{2}\hbar\omega, \tfrac{11}{2}\hbar\omega, \ldots$$



Example 8.4 Potential well with no vertical wall



We have found the WKB solutions near x_2

Problem 8.9 $\Rightarrow$ WKB solutions near x_1 [8.50]

[8.50] $\Rightarrow \psi(x) \cong \begin{cases} \frac{D'}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar}\int_x^{x_1} |p(x')|dx'}, & x < x_1 \\ \frac{2D'}{\sqrt{p(x)}} \sin\left[\frac{1}{\hbar}\int_{x_1}^{x} p(x')dx' + \frac{\pi}{4}\right], & x > x_1 \end{cases}$

This part should be equivalent to [8.46] for $x < x_2$

For $x_1 < x < x_2$, the solution can be written as

[8.46] $\Rightarrow \psi(x) \cong \frac{2D}{\sqrt{p(x)}} \sin\theta_2(x)$, $\theta_2(x) \equiv \frac{1}{\hbar}\int_x^{x_2} p(x')dx' + \frac{\pi}{4}$

↑ 投影背景墙面，注意保护，严禁书写！ ↑

[8.50] $\Rightarrow \psi(x) \cong \frac{-2D'}{\sqrt{p(x)}} \sin\theta_1(x)$, $\theta_1(x) \equiv -\frac{1}{\hbar}\int_{x_1}^{x} p(x')dx' + \frac{\pi}{4}$

The argument of the sin functions must be equal up to $n\pi$

$$\Rightarrow \theta_2 = \theta_1 + n\pi$$

$$\Rightarrow \frac{1}{\hbar}\int_x^{x_2} p(x')dx' + \frac{\pi}{4} = -\frac{1}{\hbar}\int_{x_1}^{x} p(x')dx' - \frac{\pi}{4} + n\pi$$

$$\Rightarrow \frac{1}{\hbar}\int_{x_1}^{x_2} p(x')dx' = (n - \tfrac{1}{2})\pi$$

$$\Rightarrow \boxed{\int_{x_1}^{x_2} p(x')dx' = (n - \tfrac{1}{2})\pi\hbar, \; n \text{ integers}}$$

The 3rd quantization condition

Example "Harmonic oscillator"

$$E = \tfrac{1}{2}m\omega^2 x_1^2 = \tfrac{1}{2}m\omega^2 x_2^2 \Rightarrow -x_1 = x_2 = \frac{1}{\omega}\sqrt{\frac{2E}{m}}$$

Use the quantization condition

$$\int_{-x_2}^{x_2} p(x)dx = 2\int_0^{x_2} \sqrt{x_2^2 - x^2}\, dx = \frac{2\pi E}{2\omega}$$

$$= (n - \tfrac{1}{2})\pi\hbar$$

$$\Rightarrow E_n = (n - \tfrac{1}{2})\hbar\omega, \quad n = 1, 2, 3, \ldots \; (E > V)$$

$$= (n + \tfrac{1}{2})\hbar\omega, \quad n = 0, 1, 2, \ldots$$

SUSTech

↑ 投影背景墙面，注意保护，严禁书写！↑

Recap of chap 6 - 8

Preliminary

1. Infinite square well

$E_n = \frac{n^2\pi^2(\hbar^2)}{(2m)a^2}$ [2.27] $\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$ [2.28]

$n = 1, 2, 3, \ldots$

2. Harmonic oscillator

$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2$

$a_\pm \equiv \frac{1}{\sqrt{2\hbar m\omega}}(\mp ip + m\omega x)$ [2.47]

$\Rightarrow \langle n|x'|n'\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n'}\,\delta_{n,n'-1} + \sqrt{n}\,\delta_{n',n-1}\right)$ [Problem 3.33]

$[x,p] = i\hbar$ [2.51] $\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$ [2.59]

$E_n = (n+\frac{1}{2})\hbar\omega$, $n = 0, 1, 2, \ldots$

$a_+|n\rangle = \sqrt{n+1}\,|n+1\rangle$, $a_-|n\rangle = \sqrt{n}\,|n-1\rangle$ [2.66]

$|n\rangle = \frac{1}{\sqrt{n!}}(a_+)^n|0\rangle$ [2.67]

3. Hydrogen

Bohr energy $E_n = -\left[\frac{m}{2\hbar}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2} = \frac{E_1}{n^2}$ [4.70] $n = 1, 2, 3, \ldots$

Bohr radius $a \equiv \frac{4\pi\epsilon_0\hbar^2}{me^2} \approx 0.529\times10^{-10}\,m$ [4.72]

Ground-state wave function [4.80] $\psi_{100}(r,\theta,\phi) = \frac{1}{\sqrt{\pi a^3}}e^{-r/a}$ (s wave)

$n \quad l \quad m$

$L^2|l\rangle = \hbar^2 l(l+1)|l\rangle$, $L_z|m\rangle = \hbar m|m\rangle \leftarrow |n,l,m\rangle$

4. Angular momentum

$[L_x, L_y] = i\hbar L_z$ [4.99]

$L_\pm = L_x \pm iL_y$, $L_\pm|lm\rangle = \hbar\sqrt{l(l+1) - m(m\pm1)}\,|l, m\pm1\rangle$

$S_\pm|S, M_S\rangle = \quad S \quad M_S$

5. delta function

$\delta(ax) = \frac{1}{a}\delta(x)$, $\int\delta(x)dx = 1$, $\int f(x)\delta(x-a)dx = f(a)$

6. Varial theorem

$2\langle T\rangle = \langle x\frac{dV}{dx}\rangle$ 1D, $2\langle T\rangle = \langle\vec{r}\cdot\nabla V\rangle$ 3D

Recap of chap 6 Perturbation

1. How [6.7] and [6.8] are derived?

[6.7] $H^{(0)}\psi_n^{(1)} + H'\psi_n^{(0)} = E_n^{(0)}\psi_n^{(1)} + E_n^{(1)}\psi_n^{(0)}$

[6.8] $H^{(0)}\psi_n^{(2)} + H'\psi_n^{(1)} = E_n^{(0)}\psi_n^{(2)} + E_n^{(1)}\psi_n^{(1)} + E_n^{(2)}\psi_n^{(0)}$

① $\lambda = 1$ is a tracer ② Assumption $E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + \ldots$

$\psi_n = \psi_n^{(0)} + \psi_n^{(1)} + \ldots$

2. Three formulas

1st-order correction to energy $E_n^{(1)} = \langle\psi_n^{(0)}|H'|\psi_n^{(0)}\rangle$ [6.9]

1st-order correction to wave function $\psi_n^{(1)} = \sum_{m\neq n}\frac{\langle\psi_m^{(0)}|H'|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}}$ [6.13]

2nd-order correction to energy $E_n^{(2)} = \sum_{m\neq n}\frac{|\langle\psi_m^{(0)}|H'|\psi_n^{(0)}\rangle|^2}{E_n^{(0)} - E_m^{(0)}}$ [6.15]

3. Degenerate perturbation = diagonalization

4. 2×2 Matrix (complex) $= C_0\sigma_0 + C_x\sigma_x + C_y\sigma_y + C_z\sigma_z$

$\sigma_x = \begin{pmatrix}0&1\\1&0\end{pmatrix}$, $\sigma_y = \begin{pmatrix}0&-i\\i&0\end{pmatrix}$, $\sigma_z = \begin{pmatrix}1&0\\0&-1\end{pmatrix}$, $\sigma_0 = \begin{pmatrix}1&0\\0&1\end{pmatrix}$

5. $H = \begin{pmatrix}W_{aa}&W_{ab}\\W_{ba}&W_{bb}\end{pmatrix}$ $W_{ab} = W_{ba}^*$ Hermitian

Eigen energies $E_\pm = \frac{W_{aa}+W_{bb}}{2} \pm \sqrt{\left(\frac{W_{aa}-W_{bb}}{2}\right)^2 + W_{ab}W_{ba}}$

Eigen states [4.155] $\chi_+ = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} e^{i\phi} \end{pmatrix}$ $\chi_- = \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} e^{i\phi} \end{pmatrix} = \begin{pmatrix} \sin\frac{\theta}{2} e^{-i\phi} \\ -\cos\frac{\theta}{2} \end{pmatrix}$

$\cos\theta \equiv \frac{(W_{aa}-W_{bb})/2}{\sqrt{(\frac{W_{aa}-W_{bb}}{2})^2 + W_{ab}W_{ba}}} \rightarrow \cos\frac{\theta}{2} = \sqrt{\frac{1}{2}(1+\omega_{10})}$, $\sin\frac{\theta}{2} = \sqrt{\frac{1}{2}(1-\omega_{10})}$

$W_{ab} \equiv |W_{ab}|e^{-i\phi}$, $W_{ba} \equiv |W_{ba}|e^{-i\phi}$

6. Hierarchy of Hydrogen energies

① Bohr ② Fine structure ③ Lamb shift ④ Hyperfine

7. Fine structure constant $\alpha \equiv \frac{e^2}{4\pi\epsilon_0 \hbar c} \sim \frac{1}{137}$ [6.43]

8. Fine structure = Spinless relativistic $\sim p^4$
+ Spin-orbit coupling $\sim \vec{L}\cdot\vec{S}$
(also relativistic effect)

9. Dirac equation (Spin-½ Special relativistic Quantum Mechanical equation)

low energy Limit; $\vec{B}$; Coulomb potential $\sim \frac{1}{r}$

Schrödinger equation + Zeeman + SOC + Spin

10. How [6.50] $H_r' = -\frac{p^4}{8m^3c^2}$ is derived?

① classical $\vec{v}$ → Quantum $\vec{p}$

② $T = \sqrt{p^2c^2+m^2c^4} - mc^2$

Taylor expansion $= mc^2\left[1 + \frac{1}{2}\left(\frac{p}{mc}\right)^2 - \frac{1}{8}\left(\frac{p}{mc}\right)^4 + \cdots - 1\right]$

$f(x) = f(x_0) + \left.\frac{df}{dx}\right|_{x=x_0}(x-x_0) + \frac{1}{2}\left.\frac{d^2f}{dx^2}\right|_{x=x_0}(x-x_0)^2 + \cdots$

11. How Eq. [6.61] $H_{so}' = \frac{e^2}{8\pi\epsilon_0}\frac{1}{m^2c^2r^3}\vec{S}\cdot\vec{L}$ is derived?

$[\vec{S}\cdot\vec{L}, \vec{S}] \neq 0$, $[\vec{S}\cdot\vec{L}, \vec{L}] \neq 0$, $[\vec{S}\cdot\vec{L}, \vec{L}+\vec{S}] = 0$

($\vec{S} = (S_x, S_y, S_z)$, $\vec{L}+\vec{S} = \vec{J}$)

$[\vec{S}\cdot\vec{L}, L^2] = 0$, $[\vec{S}\cdot\vec{L}, S^2] = 0$, $[\vec{S}\cdot\vec{L}, J^2] = 0$

$\vec{S}\cdot\vec{L} = \frac{1}{2}(S_+L_- + S_-L_+) + S_zL_z$

12. Zeeman effect

$H_z' = \frac{e}{2m}(\vec{L}+2\vec{S})\cdot\vec{B}_{ext} \Rightarrow \mu_B g_J \vec{B}_{ext}\cdot\vec{J}$

Bohr magneton $\mu_B \equiv \frac{e\hbar}{2M}$, g-factor

$g_J = 1 + \frac{j(j+1) - l(l+1) + s(s+1)}{2j(j+1)}$

13. Estimate $B_{int} \sim \frac{e^2}{8\pi\epsilon_0}\frac{1}{m^2c^2a^3}\hbar \sim 12$ Tesla

So ↑ c

14. Good quantum number in

{ Weak Zeeman $n\ l\ j\ m_j$ ← $\vec{L}\cdot\vec{S}$
Strong Zeeman $n\ l\ m_l\ m_s$

15. Chap 6.4.3 Intermediate Zeeman regime $n=2$

$l=0 \xrightarrow{s=\frac{1}{2}} j=\frac{1}{2} \rightarrow m_j = -\frac{1}{2}, \frac{1}{2}$

$l=1$: $j=l-s \rightarrow j=\frac{1}{2} \rightarrow m_j = -\frac{1}{2}, \frac{1}{2}$; $j=l+s \rightarrow j=\frac{3}{2} \rightarrow m_j = -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$

$n=3 \Rightarrow l=0,1,2$

16. Hyperfine $\vec{S}_e \cdot \vec{S}_p$ ← proton spin

[4.177], [4.178]

Singlet $\frac{1}{\sqrt{2}}(|\uparrow\rangle_e|\downarrow\rangle_p - |\downarrow\rangle|\uparrow\rangle_p) = |0,0\rangle$

triplets $\begin{cases} |\uparrow\rangle_e|\uparrow\rangle_p = |1,1\rangle \\ \frac{1}{\sqrt{2}}(|\uparrow\rangle_e|\downarrow\rangle_p + |\downarrow\rangle_e|\uparrow\rangle_p) = |1,0\rangle \\ |\downarrow\rangle_e|\downarrow\rangle_p = |1,-1\rangle \end{cases}$

$\vec{S} = \vec{S}_e + \vec{S}_p \Rightarrow \vec{S}_e \cdot \vec{S}_p = \frac{1}{2}(S^2 - S_e^2 - S_p^2)$

$\Rightarrow \langle \vec{S}_e \cdot \vec{S}_p \rangle = \begin{cases} \frac{\hbar^2}{2}\left[1(1+1) - \frac{1}{2}\left(1+\frac{1}{2}\right) - \frac{1}{2}\left(1+\frac{1}{2}\right)\right] = \frac{\hbar^2}{4} \\ \frac{1/2\hbar^2}{2}\left[0(0+1) - \frac{3}{4} - \frac{3}{4}\right] = -\frac{3}{4}\hbar^2 \end{cases}$

17. C-G coefficients

$|j,m\rangle = \sum_{m_l, m_s} C^{j\ m}_{m_l\ m_s} |l, m_l\rangle |s, m_s\rangle$

Griffiths P188 Tab. 4.8 How to read?

关洪《量子力学基础》 Chap 10.2 Formulas

Recap of chap 7 Variational Principle

1. Estimate of upper bound of ground-state energy
2. Steps ① Normalized trial wave function
   ② $\langle H \rangle$ as a function of variational parameter
   ③ Minimized $\langle H \rangle$

3. Helium (Many-body wave function)

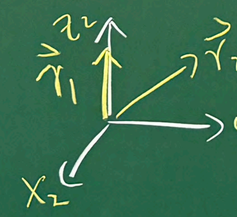
$H = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - \frac{e^2}{4\pi\epsilon_0}\left(\frac{2}{r_1} + \frac{2}{r_2} - \frac{1}{|\vec{r}_1 - \vec{r}_2|}\right)$ [7.14]

Trial wave function coordinates

$\psi_0(\vec{r}_1, \vec{r}_2) \equiv \psi_{100}(\vec{r}_1)\psi_{100}(\vec{r}_2) = \frac{1}{\pi a^3} e^{-\frac{2(r_1+r_2)}{a}}$ [7.17]

$\psi_1(\vec{r}_1, \vec{r}_2) \equiv \frac{z^3}{\pi a^3} e^{-\frac{z(r_1+r_2)}{a}}$ $1 < z < 2$

Mathematical trick



put $\vec{r}_1$ along z_2

4. Hydrogen molecule ion (one-particle wavefunction)

$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r_1} + \frac{1}{r_2}\right)$

$\psi = A[\psi_0(r_1) + \psi_0(r_2)]$, $\psi_0 \equiv \frac{1}{\sqrt{\pi a^3}} e^{-\frac{r}{a}}$

r_1, r_2: distance

Recap of chap 8 WKB approximation

1. The idea 1D slowly varying potential
2. Three regions $\begin{cases} E > V & \text{Bound state} \\ E < V & \text{Tunneling} \\ E \sim V & \text{Turning point} \leftarrow \text{Connection formulas} \end{cases}$
3. $\psi = Ae^{ikx} \rightarrow A(x)e^{i\phi(x)}$
4. $E > V \Rightarrow \psi_{WKB} \cong \frac{C_+}{\sqrt{p(x)}} e^{\frac{i}{\hbar}\int p(x)dx} + \frac{C_-}{\sqrt{p(x)}} e^{-\frac{i}{\hbar}\int p(x)dx}$

Chap 9 Time-dependent perturbation theory

Schrödinger eqn. $H(\vec{r},t)\Psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t)$

where $H = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t)$ (kinetic, potential)

If $V(\vec{r},t) \to V(\vec{r})$ time indepent, we can solve the equation by using the separation of variables

$$\Psi(\vec{r},t) = \psi(\vec{r})\varphi(t) \Rightarrow \begin{cases} \frac{\partial\Psi}{\partial t} = \psi(\vec{r})\frac{d\varphi}{dt} \\ \nabla^2\Psi = (\nabla^2\psi)\varphi \end{cases}$$

$$\Rightarrow i\hbar\psi(\vec{r})\frac{d\varphi(t)}{dt} = \left(-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi\right)\varphi$$

Divided on both sides by $\psi\varphi$

$$\Rightarrow i\hbar\frac{1}{\varphi}\frac{d\varphi}{dt} = \frac{1}{\psi}\left(-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi\right) = \text{Constant} = E$$

Because ψ and $\varphi(t)$ are of different degrees of freedom.

$$\Rightarrow i\hbar\frac{1}{\varphi}\frac{d\varphi}{dt} = E \Rightarrow \frac{d\varphi}{\varphi} = -i\frac{E}{\hbar}dt$$

Integrate on both sides

$$\Rightarrow \ln\varphi = -i\frac{E}{\hbar}t \quad \text{up to a constant}$$

$$\Rightarrow \varphi = e^{-i\frac{E}{\hbar}t}$$

$$\left(-\frac{\hbar^2}{2m}\nabla + V\right)\psi_n = E_n\psi_n \quad \text{Stationary Schrödinger eqn.}$$

$\Rightarrow$ If $V(\vec{r},t) \to V(\vec{r})$, the wave function

$$\Psi(\vec{r},t) = \sum_n C_n \psi_n(\vec{r}) e^{-i\frac{E_n}{\hbar}t}$$

C_n: superposition coefficients determined by initial conditions

↑ 投影背景墙面，注意保护，严禁书写！ ↑

If a time-dependent $V(\vec{r},t)$ is weak, we can treat it as perturbation

9.1 Two-level system

E_b ——

E_a ——

The unperturbed Hamiltonian

$$H^{(0)}\psi_a = E_a\psi_a, \quad H^{(0)}\psi_b = E_b\psi_b, \quad \langle\psi_a|\psi_b\rangle = \delta_{ab}$$ (orthonormal)

In this Hilbert space spanned by $\{\psi_a, \psi_b\}$ (basis), any states can be expressed as

$$\Psi(t=0) = C_a\psi_a + C_b\psi_b$$

Its time dependence, or the full solution

$$\Psi(t) = C_a\psi_a e^{-i\frac{E_a}{\hbar}t} + C_b\psi_b e^{-i\frac{E_b}{\hbar}t}$$

$|C_a|^2 + |C_b|^2 = 1$ time-independent

9.1.1 Perturbation $H'(t)$ time-dependent

Assumption $\Psi(t) = C_a(t)\psi_a e^{-i\frac{E_a}{\hbar}t} + C_b(t)\psi_b e^{-i\frac{E_a}{\hbar}t}$

The problem turns to solve $C_a(t)$ and $C_b(t)$

Put the trial wave function into $H\Psi = i\hbar\frac{\partial}{\partial t}\Psi$

where $H = H^{(0)} + H'(t)$

$$\text{left} = [H^{(0)} + H'(t)]\left[C_a(t)\psi_a e^{-i\frac{E_a}{\hbar}t} + C_b(t)\psi_b e^{-i\frac{E_b}{\hbar}t}\right]$$

$$= C_a(t)H^{(0)}\psi_a e^{-i\frac{E_a}{\hbar}t} + C_b(t)H^{(0)}\psi_b e^{-i\frac{E_b}{\hbar}t}$$

$$+ C_a(t)H'\psi_a e^{-i\frac{E_a}{\hbar}t} + C_b(t)H'\psi_b e^{-i\frac{E_b}{\hbar}t}$$

$H^{(0)}\psi_a = E_a\psi_a$, $H^{(0)}\psi_b = E_b\psi_b$

$$\text{Right} = i\hbar\frac{\partial}{\partial t}\left[C_a(t)\psi_a e^{-i\frac{E_a}{\hbar}t} + C_b(t)\psi_b e^{-i\frac{E_b}{\hbar}t}\right]$$

$$= i\hbar\left[\dot{C}_a \psi_a e^{-i\frac{E_a}{\hbar}t} + \dot{C}_b \psi_b e^{-i\frac{E_b}{\hbar}t} + C_a\psi_a(-i\tfrac{E_a}{\hbar})e^{-i\frac{E_a}{\hbar}t} + C_b\psi_b(-i\tfrac{E_b}{\hbar})e^{-i\frac{E_b}{\hbar}t}\right]$$

$$\Rightarrow C_a H'\psi_a e^{-i\frac{E_a}{\hbar}t} + C_b H'\psi_b e^{-i\frac{E_b}{\hbar}t} = i\hbar\left[\dot{C}_a\psi_a e^{-i\frac{E_a}{\hbar}t} + \dot{C}_b\psi_b e^{-i\frac{E_b}{\hbar}t}\right]$$

[Trick] Inner product $\langle\psi_a|$ (time independent)

$$\Rightarrow C_a\langle\psi_a|H'|\psi_b\rangle e^{-i\frac{E_a}{\hbar}t} + C_b\langle\psi_a|H'|\psi_b\rangle e^{-i\frac{E_b}{\hbar}t} = i\hbar\left[\dot{C}_a\underbrace{\langle\psi_a|\psi_a\rangle}_{=1} e^{-i\frac{E_a}{\hbar}t} + \dot{C}_b\underbrace{\langle\psi_a|\psi_b\rangle}_{=0} e^{-i\frac{E_b}{\hbar}t}\right]$$

Define $H'_{ij} = \langle\psi_i|H'(t)|\psi_j\rangle$ (time dependent; time independent)

$$\Rightarrow C_a H'_{aa} e^{-i\frac{E_a}{\hbar}t} + C_b H'_{ab} e^{-i\frac{E_b}{\hbar}t} = i\hbar\dot{C}_a e^{-i\frac{E_a}{\hbar}t}$$

Multiply on both sides by $-\frac{i}{\hbar}e^{i\frac{E_a}{\hbar}t}$

$$\Rightarrow \dot{C}_a = -\frac{i}{\hbar}\left[C_a H'_{aa} + C_b H'_{ab} e^{-i\frac{(E_b-E_a)}{\hbar}t}\right]$$

Similarly, Inner product $\langle\psi_b|$

$$\Rightarrow \dot{C}_b = -\frac{i}{\hbar}\left[C_b H'_{bb} + C_a H'_{ba} e^{i\frac{E_b-E_a}{\hbar}t}\right]$$

[Approximation] $H'_{aa} = H'_{bb} = 0$ ⟸ Light $-e\vec{E}\cdot\vec{r}$ (Integral of odd function)

$$\Rightarrow \begin{cases} \frac{d}{dt}C_a = -\frac{i}{\hbar}H'_{ab}e^{-i\omega_0 t}C_b \\ \frac{d}{dt}C_b = -\frac{i}{\hbar}H'_{ba}e^{i\omega_0 t}C_a \end{cases} \quad [9.13]$$

where $\omega_0 \equiv \frac{E_b - E_a}{\hbar} > 0$, we assume $E_a > E_a$ a ——— b

9.1.2 Time-dependent perturbation theory

Initial conditions

$C_a(t=0) = 1$, $C_b(t=0) = 0$,

Zeroth order

$C_a^{(0)} = 1$, $C_b^{(0)} = 0$ Iteration 迭代法

1st order

$$[9.13] \Rightarrow \dot{C}_a^{(1)} = -\frac{i}{\hbar}H'_{ab}(t)e^{-i\omega_0 t}C_b^{(0)} = 0$$

Which means that $C_a^{(1)}$ does not change with time

$$C_a^{(1)} = C_a^{(0)} = 1$$

Similarly

$$\frac{dC_b^{(1)}}{dt} = \dot{C}_b^{(1)} = -\frac{i}{\hbar}H'_{ba}e^{i\omega_0 t}C_a^{(0)} = -\frac{i}{\hbar}H'_{ba}(t)e^{i\omega_0 t}$$

$$\Rightarrow dC_b^{(1)} = -\frac{i}{\hbar}H'_{ba}(t)e^{i\omega_0 t}dt$$

Integrate on both sides (dumb variable)

$$C_b^{(1)}(t) - C_b^{(1)}(t=0) = -\frac{i}{\hbar}\int_0^t dt' H'_{ba}(t)e^{i\omega_0 t'}$$

(upper bound; lower bound)

$$\because C_b^{(0)}(t=0) = 0$$

$$\Rightarrow \boxed{C_b^{(1)}(t) = -\frac{i}{\hbar}\int_0^t dt' H'_{ba}(t')e^{i\omega_0 t'}} \quad [9.17]$$

2nd order

$$\dot{C}_a^{(2)} = -\frac{i}{\hbar}H'_{ab}e^{-i\omega_0 t}C_b^{(1)}$$

⬆ 投影背景墙面，注意保护，严禁书写！⬆

$\Rightarrow \frac{d}{dt}C_a^{(2)}(t) = -\frac{1}{i\hbar^2} H'_{ab}(t) e^{-i\omega_0 t} \int_0^t dt' H'_{ba}(t') e^{i\omega_0 t'}$

$\Rightarrow dC_a^{(2)} = \cdots\cdots dt$ Integrate on both sides

$\Rightarrow C_a^{(2)}(t) - C_a^{(2)}(0) = -\frac{1}{i\hbar^2}\int_0^t dt' H'_{ab}(t') e^{-i\omega_0 t'} \times \int_0^{t'} dt'' H'_{ba}(t'') e^{i\omega_0 t''}$

$C_a^{(2)}(0) = C_a^{(1)}(0) = 1$

$\Rightarrow C_a^{(2)}(t) = 1 - \frac{1}{i\hbar^2}\int_0^t dt' H'_{ab}(t') e^{-i\omega_0 t'} \times \int_0^{t'} dt'' H'_{ba}(t'') e^{i\omega_0 t''}$

We stop at this order

About P345 "However, $|C_a^{(1)}(t)|^2 + |C_b^{(1)}(t)|^2 = 1$ to first order in H', read "Hack QM II"

9.1.3. Sinusoidal Perturbation

$H'(\vec{r}, t) = V(\vec{r}) \cos\omega t$

$\vec{r}$ means no time dependence

So that

$H'_{ab} \equiv \langle \psi_a(\vec{r}) | H'(\vec{r}, t) | \psi_b(\vec{r}) \rangle$

$= \langle \psi_a(\vec{r}) | V(\vec{r}) \cos\omega t | \psi_b(\vec{r}) \rangle$

$= \langle \psi_a(\vec{r}) | V(\vec{r}) | \psi_b(\vec{r}) \rangle \cos\omega t$

$\equiv V_{ab} \cos\omega t = V_{ab} \frac{1}{2}(e^{i\omega t} + e^{-i\omega t})$

Eq. [9.17] $\Rightarrow C_b^{(1)}(t) \simeq -\frac{i}{\hbar}\int_0^t dt' V_{ab} \cos\omega t' e^{i\omega_0 t}$

$= -\frac{i}{2\hbar} V_{ba} \int_0^t dt' \left[e^{i(\omega+\omega_0)t'} + e^{i(\omega_0-\omega)t'} \right]$ ($H'_{ab}(t')$)

$\Rightarrow C_b(t) = -\frac{V_{ba}}{2\hbar}\left[\frac{e^{i(\omega_0+\omega)t} - 1}{\omega+\omega_0} + \frac{e^{i(\omega_0-\omega)t} - 1}{\omega_0-\omega} \right]$

[Approximation] Resonance $\omega_0 \sim \omega \sim 10^{15}$ Hz

b ——— $\hbar\omega_0$

a ———

$\Rightarrow \omega_0 + \omega >> |\omega_0 - \omega|$, so we drop the 1st term

$\Rightarrow$ Transition Coefficient $C_b(t) \simeq -\frac{V_{ba}}{2\hbar} \frac{e^{i(\omega_0-\omega)t} - 1}{\omega_0 - \omega}$

$= -\frac{V_{ba}}{2\hbar} \frac{e^{i(\omega_0-\omega)t/2}}{\omega_0-\omega} \left[e^{i(\omega_0-\omega)t/2} - e^{-i(\omega_0-\omega)t/2} \right]$

$2i \sin\frac{(\omega_0-\omega)t}{2}$

$P = |C|^2$

Transition probability $P_{a\to b} \equiv |C_b(t)|^2 \simeq \frac{|V_{ab}|^2}{\hbar^2} \frac{\sin^2(\frac{\omega_0-\omega}{2}t)}{(\omega_0-\omega)^2}$ [9.28]

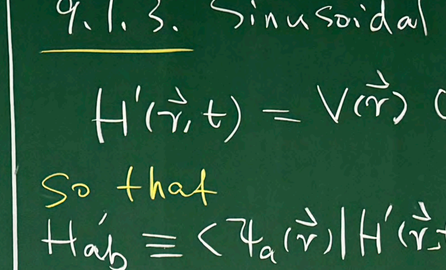
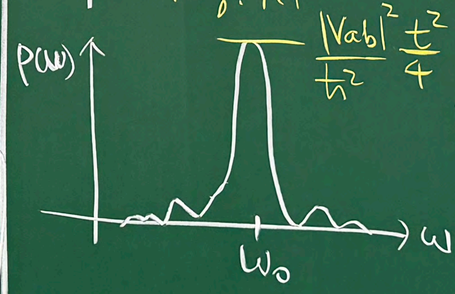


Fig. 9.1



Let $\omega_0 - \omega = x$, $\frac{t}{2} = a$

$\lim_{x\to 0} \frac{\sin^2(ax)}{x^2} = \lim_{x\to 0} \frac{2a \sin ax \cos ax}{2x}$

$= \lim_{x\to 0} \frac{a}{2} 2a \frac{\cos(2ax)}{1} = a^2 = \frac{t^2}{4}$

[Note]: Problem 9.7 very important

"Rotating wave approximation"

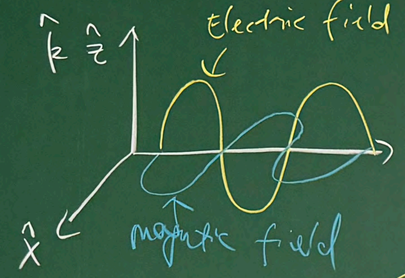
"Rabi frequency"

SUSTech

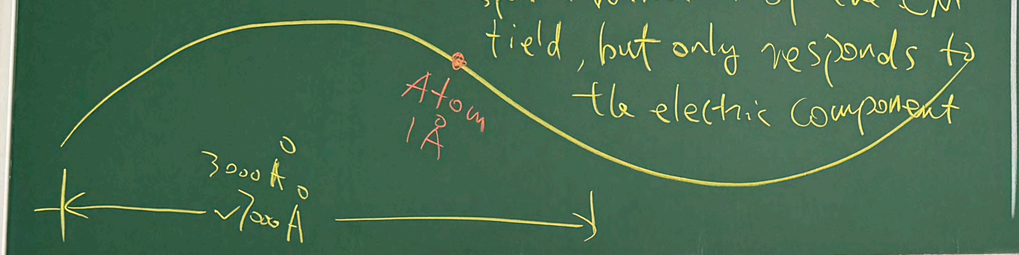
9.2. Emission and absorption of radiation

9.2.1 Electromagnetic waves

Light = transverse EM wave



The atom cannot "see" the spatial variation of the EM field, but only responds to the electric component



The electric field of a monochromatic light (single frequency)

$$\vec{\mathcal{E}} = \mathcal{E}_0 \cos\omega t \, \hat{k}$$ ← direction of polarization

Perturbation Hamiltonian

$$H' = \underbrace{-q\mathcal{E}_0 z}_{\text{spatial part}} \underbrace{\cos\omega t}_{\text{time dependence}}$$

The electric field drags the electron

Then $H'_{ba} \equiv \langle \psi_b | H'(t) | \psi_a \rangle$ (ψ_a: time-independent; $H'(t)$: time-dependent)

$$= -q\mathcal{E}_0 \langle \psi_b | z | \psi_a \rangle \cos\omega t \equiv -\mathcal{P}\mathcal{E}_0 \cos\omega t$$ ($\mathcal{P}$: dipole)

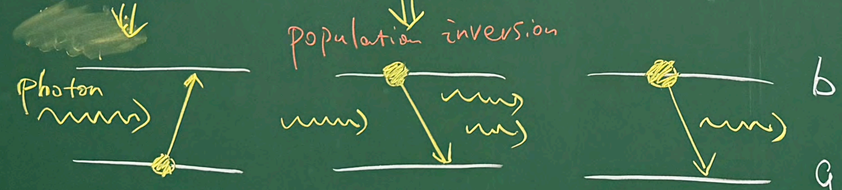
where $\mathcal{P} = q\langle \psi_b | z | \psi_a \rangle$

$\neq 0$ if { ψ_a is odd or even; ψ_b is even or odd } function of z

Therefore, $H'_{aa} = H'_{bb} = 0$ = integral $\int |\psi|^2 z \, d\tau$ (odd function)

9.2.2 Absorption, Stimulated emission, Spontaneous emission

Fig 9.4



(a) Absorption

The probability of a transition from the "lower" to "higher" state

$$[9.28] \Rightarrow P_{a\to b}(t) = \left(\frac{\mathcal{P}\mathcal{E}_0}{\hbar}\right)^2 \frac{\sin^2\left[\frac{(\omega_0-\omega)t}{2}\right]}{(\omega_0-\omega)^2} \quad [9.36]$$

Absorb a "photon", although we use "classical" light

(b) Stimulated emission

We can solve Eq. [9.13] using the initial condition $C_a(t=0)=0$, $C_b(t=0)=1$

Then probability $P_{b\to a}(t) \equiv |C_a^{(1)}(t)|^2$ (Coefficient) $= [9.28]$

Predicted by Einstein astonishingly

LASER = Light Amplification by Stimulated Emission of Radiation

(c) Spontaneous emission

No external perturbation (Really?)

9.2.3. Incoherent Perturbation

相干 coherent $|\psi_1+\psi_2|^2 = |\psi_1|^2+|\psi_2|^2+\psi_1^*\psi_2+\psi_1\psi_2^*$

不相干 incoherent $|\psi_1|^2+|\psi_2|^2$

Interference 干涉

Consider lights of different frequencies contribute independently (Summation of probabilities, instead of coefficients) Incoherent

We need to consider a distribution of lights as a function of frequency (weight)

Consider the energy density of EM field

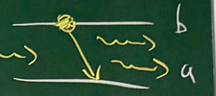
$$u = \left(\frac{\varepsilon_0}{2}\right) E_0^2$$

(Griffiths, Electrodynamics Eq. (9.21))

energy density; ε_0 ← vacuum dielectric constant; E_0 ← amplitude of electric field

$$[9.36] \Rightarrow P_{b\to a}(t) = \frac{|p|^2 E_0^2}{\hbar^2} \frac{\sin^2\left[\frac{(\omega_0-\omega)t}{2}\right]}{(\omega_0-\omega)^2}$$

$$E_0^2 = \frac{2u}{\varepsilon_0} \rightarrow = \frac{|p|^2}{\hbar^2}\frac{2u}{\varepsilon_0}\frac{\cdots}{\cdots}$$



Single frequency ⟶ Energy density in the frequency range $d\omega$

$$u \longrightarrow \rho(\omega)d\omega$$

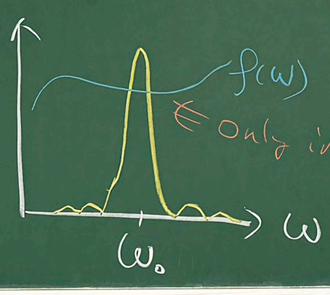
$$\Rightarrow P_{a\to b}(t) = \frac{2|p|^2}{\hbar^2\varepsilon_0}\int d\omega\, \rho(\omega) \left[\frac{\sin^2\left[\frac{(\omega_0-\omega)t}{2}\right]}{(\omega_0-\omega)^2}\right]$$

u

$P_{a\to b}(\omega)$

[Approximation] $\rho(\omega) \longrightarrow \rho(\omega_0)$ Resonance

$P(\omega)$ $a\to b$



look like $\int f(x)\,\delta(x-x_0)\,dx = f(x_0)$

$\rho(\omega)$ ∈ only important in this vicinity

$$\Rightarrow P_{a\to b}(t) = \frac{2|p|^2}{\hbar^2\varepsilon_0}\rho(\omega_0)\int_0^\infty d\omega \frac{\sin^2\left[\frac{(\omega_0-\omega)t}{2}\right]}{(\omega_0-\omega)^2}$$

let $x \equiv \frac{(\omega_0-\omega)t}{2} \Rightarrow d\omega = -\frac{2}{t}dx,\ \omega_0-\omega = \frac{2x}{t}$

$$\int_0^\infty \frac{\sin^2\left[\frac{(\omega_0-\omega)t}{2}\right]}{(\omega_0-\omega)^2}d\omega = t^2\int_{\frac{\omega_0 t}{2}}^{-\infty}\frac{\sin^2 x}{4x^2}\left(-\frac{2}{t}\right)dx$$

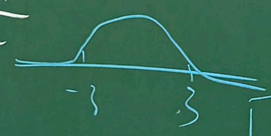
White light; ∞

$$= \frac{2t^2}{4t}\int_{-\infty}^{\infty}\frac{\sin^2 x}{x^2}dx = \frac{t\pi}{2}$$

$= \pi$

$$\int_{x_0-\delta x_0}^{x_0+\delta x_0}\delta(x-x_0)dx = 1$$

$$= \int_{-a}^{a}$$



Transition Probability

$$P_{b\to a}(t) \cong \frac{2|p|^2}{\varepsilon_0\hbar^2}\rho(\omega_0)\frac{\pi}{2}t$$

Transition rate

$$R_{b\to a} \equiv \frac{dP_{b\to a}}{dt} = \frac{\pi}{\varepsilon_0\hbar^2}|p|^2\rho(\omega_0) \quad [9.43]$$

How about 2D?

$\frac{1}{2\pi}\int_0^{2\pi}\cos^2\varphi\,d\varphi = \frac{1}{2}$

Polar angle

Lights coming from all directions

(Average over the solid angle)

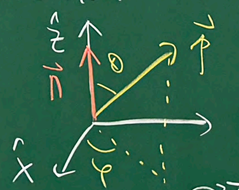
dipole $|p|^2 \longrightarrow |\vec{p}\cdot\hat{n}|^2$, where $\vec{p} \equiv q\langle\psi_b|\vec{r}|\psi_a\rangle$

$\hat{n}$ ← polarization

Light is a transverse wave

Average over propagation direction = Average over polarization direction

[Trick]



$\vec{p}\cdot\hat{n} = p\cos\theta$

$$|\vec{p}\cdot\hat{n}|^2_{\text{average}} = \frac{\int_0^{2\pi}d\varphi\int_0^{\pi}\sin\theta\,d\theta\; p^2\cos^2\theta}{\int_0^{2\pi}d\varphi\int_0^{\pi}\sin\theta\,d\theta = 4\pi}$$

$= \frac{2\pi}{4\pi}p^2\int_0^{\pi}\sin\theta d\theta\cos^2\theta = \frac{1}{2}|p|^2\left(-\frac{1}{3}\cos^3\theta\right)\Big|_0^{\pi} = \frac{1}{3}|p|^2$

"3" from three-dimensions

$$[9.43] \Rightarrow R_{b\to a} = \frac{\pi}{3\varepsilon_0\hbar^2}|p|^2 \rho(\omega_0) \quad [9.47]$$

Transition rate for stimulated emission from state b to a, under ① incoherent, ② unpolarized light, incident from all directions

Matrix element of the electric dipole moment (parameter)

energy density per unit frequency at $\omega_0 = \frac{E_b - E_a}{\hbar}$

9.3 Spontaneous emission

Goal: To derive the transition rate of the spontaneous emission

9.3.1 Einstein's A and B coefficients

$$R_{\substack{b\to a\\ a\to b}} = \underbrace{\frac{\pi}{3\varepsilon_0\hbar^2}|p|^2}_{\text{B coefficient}} \rho(\omega_0) \Rightarrow \text{Rate} \quad R_{b\to a} = B_{ba}\rho(\omega_0), \quad R_{a\to b} = B_{ab}\rho(\omega_0)$$

Consider the population on level b (N_b) changes with time

$$\frac{dN_b}{dt} = \underbrace{N_a}_{\text{population on level a}} B_{ab}\rho(\omega_0) - N_b B_{ba}\rho(\omega_0) - A N_b$$

Absorption, Stimulated, Spontaneous

Thermal equilibrium $\Rightarrow \frac{dN_b}{dt} = 0$



$$\Rightarrow N_b A = \rho(\omega_0)(N_a B_{ab} - N_b B_{ba})$$

$$\Rightarrow \rho(\omega_0) = \frac{N_b A}{N_a B_{ab} - N_b B_{ba}} = \frac{A}{\frac{N_a}{N_b}B_{ab} - B_{ba}}$$

The population satisfies the Boltzmann distribution

$$\frac{N_a}{N_b} = \frac{e^{-E_a/k_BT}}{e^{-E_b/k_BT}} = e^{\hbar\omega_0/k_BT}, \quad \omega_0 \equiv \frac{E_b - E_a}{\hbar}$$

$$\Rightarrow \rho(\omega_0) = \frac{A}{e^{\hbar\omega_0/k_BT}B_{ab} - B_{ba}}$$

Meanwhile, Planck's blackbody formula (A measurement of temperature)

$$\rho(\omega) = \frac{\hbar}{\pi^2 c^3}\frac{\omega^3}{e^{\hbar\omega/k_BT} - 1}$$



Compare them $\Rightarrow$

$$B_{ba} = B_{ab}, \quad A = \frac{\omega_0^3\hbar}{\pi^2 c^3}B_{ba} = \frac{\omega_0^3\hbar}{\pi^2 c^3}\frac{\pi}{3\varepsilon_0\hbar^2}|p|^2$$

$$= \frac{\omega_0^3|p|^2}{3\pi\varepsilon_0\hbar c^3} \quad [9.56]$$

Transition rate of the spontaneous emission

9.3.2 Lifetime

No radiation, only spontaneous emission

$$\Rightarrow \frac{dN_b}{dt} = -A N_b \Rightarrow \frac{dN_b}{N_b} = -A\,dt$$

Integrate on both sides

$$\ln N_b = -At + \text{const.}$$

$$\text{or } N_b = Ce^{-At} = N_b(t=0)e^{-At} = Ce^{-t/\tau}$$

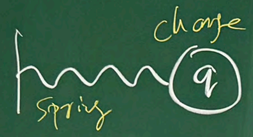
Define lifetime $\tau \equiv \frac{1}{A}$ The time it takes for $N_b(t)$ to reach $1/e \approx 0.368$ of its initial value

Additional Rules

$$\frac{1}{\tau} = \frac{1}{\tau_1} + \frac{1}{\tau_2} + \frac{1}{\tau_3} + \dots$$ from different mechanisms

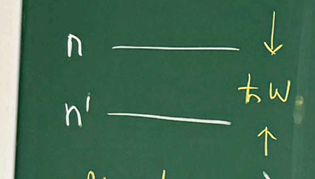
↑ 投影背景墙面，注意保护，严禁书写！ ↑

Example 9.1 Radiation from a charged harmonic oscillator



Charge q attached to a spring oscillating along the x direction. Starting from state $|n\rangle$ it decays by spontaneous emission to $|n'\rangle$

Einstein's coefficient A



dipole $\vec{p} = q\langle n|\hat{x}|n'\rangle\hat{i}$ ($\hat{x}$: operator)

where Problem 3.33 ⇒

$$\langle n|x|n'\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n'}\,\delta_{n,n'-1} + \sqrt{n}\,\delta_{n',n-1}\right)$$

[2.47] + [2.66] ↗

[2.47] $a_\pm \equiv \frac{1}{\sqrt{2\hbar\omega m}}(\mp ip + m\omega x)$

$\Rightarrow x = \frac{a_+ + a_-}{\sqrt{2m\omega/\hbar}}$ [2.66] ⇒ $a_+|n\rangle = \sqrt{n+1}\,|n+1\rangle$, $a_-|n\rangle = \sqrt{n}\,|n-1\rangle$

We consider only emission, so $n' < n$

$$\Rightarrow \vec{p} = q\sqrt{\frac{n\hbar}{2m\omega}}\,\delta_{n',n-1}\,\hat{i}$$

Spontaneous emission rate Eq. [9.56] ⇒

$$A = \frac{\omega_0^2|\vec{p}|^2}{3\pi\varepsilon_0\hbar c^3} = \frac{\omega^2 q^2 n\hbar}{3\pi\varepsilon_0\hbar c^3 2m\omega} = \frac{nq^2\omega^2}{6\pi\varepsilon_0 mc^3}$$

Lifetime $\tau \equiv \frac{1}{A}$

Radiation power $P \equiv A\hbar\omega = \frac{nq^2\omega}{6\pi\varepsilon_0 mc^3}\hbar\omega$

$E_n = (n+\frac{1}{2})\hbar\omega \Rightarrow n\hbar\omega = E_n - \frac{1}{2}\hbar\omega$ ⇒

$$P = \frac{q^2\omega^2}{6\pi\varepsilon_0 mc^3}\left(E_n - \tfrac{1}{2}\hbar\omega\right)$$

Compasion with the classical case

$$P = \frac{q^2\omega^2}{6\pi\varepsilon_0 mc^3}E$$ No zero-point energy $\frac{1}{2}\hbar\omega$

9.3.3 Selection Rules (选择定则)

The calculation of spontaneous emission rate is to evaluate $\langle\psi_b|\vec{r}|\psi_a\rangle$ (arbitrary) Most of them = 0

We need to know which two states can be coupled by light

Hydrogen Matrix elements of dipole $\langle n'\ell'm'|\vec{r}|n\ell m\rangle$ ($\vec{r}$: x, y, z; $\langle z$, $\langle z$)

Selection Rules involving m and m'

Note that $\hat{L}_z|n\ell m\rangle = \hbar m|n\ell m\rangle$

$\vec{L} \equiv \vec{r}\times\vec{p}$, $\hat{L}_z = xp_y - yp_x$

$[L_z, x] = [xp_y - yp_x, x] = [xp_y, x] - [yp_x, x]$ ($[p_y, x] = 0$, $[y, x]\,p_x = 0$)

$= 0 - y[p_x, x] = -y(-i\hbar) = i\hbar y$

$[L_z, y] = [xp_y - yp_x, y] = x[p_y, y] - 0 = -i\hbar x$

$[L_z, z] = [xp_y - yp_x, z] = 0$

Using $0 = [L_z, z]$ ⇒

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

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

$0 = \hbar(m'-m)\langle n'\ell'm'|z|n\ell m\rangle \Rightarrow \langle n'\ell'm'|z|n\ell m\rangle$

If $m = m'$, could be nonzero

Using $[L_z, x] = i\hbar y \Rightarrow$

$\langle n'l'm'|[L_z,x]|nlm\rangle = i\hbar\langle n'l'm'|y|nlm\rangle$

($L_z x - x L_z$)

$\Rightarrow \hbar(m'-m)\langle n'l'm'|x|nlm\rangle = i\hbar\langle n'l'm'|y|nlm\rangle$ [9.70]

Using $[L_z, y] = -i\hbar x \Rightarrow$

$\hbar(m'-m)\langle n'l'm'|y|nlm\rangle = -i\hbar\langle n'l'm'|x|nlm\rangle$ [9.71]

Combine [9.70] and [9.71] $\Rightarrow$

$\hbar(m'-m)\langle n'l'm'|x|nlm\rangle = i\hbar\langle n'l'm'|y|nlm\rangle$

$= i\hbar(-i\hbar)\langle n'l'm'|x|nlm\rangle$ $\frac{1}{\hbar(m'-m)}$

$\Rightarrow (m-m')^2\langle n'l'm'|x|nlm\rangle = \langle n'l'm'|x|nlm\rangle$

$\Rightarrow [(m-m')^2 - 1]\langle n'l'm'|\underset{y}{x}|nlm\rangle = 0$

Only when $m' = m \pm 1$, $\langle n'l'm'|\underset{y}{x}|nlm\rangle$ could be nonzero

[Summary]: Selection Rules for m

No transition unless $\Delta m = \pm 1$ or 0

$m - m'$; x, y ; z

Selection Rules involving l and l'

Problem [9.12] $\Rightarrow$ $[L^2, [L^2, \vec{r}]] = 2\hbar^2(\vec{r}L^2 + L^2\vec{r})$ (Left, Right)

$\text{Left} = \langle n'l'm'|[L^2,[L^2,\vec{r}]]|nlm\rangle$

$= \langle n'l'm'|L^2[L^2,\vec{r}] - [L^2,\vec{r}]L^2|nlm\rangle$

($\hbar^2 l'(l'+1)$, $\hbar^2 l(l+1)$)

$= \hbar^2[l'(l'+1) - l(l+1)]\langle n'l'm'|L^2\vec{r} - \vec{r}L^2|nlm\rangle$

$= [\hbar^2[l'(l'+1) - l(l+1)]]^2\langle n'l'm'|\vec{r}|nlm\rangle$

$\text{Right} = 2\hbar^2\hbar^2[l'(l'+1) + l(l+1)]\langle n'l'm'|\vec{r}|nlm\rangle$

$\text{Left} = \text{Right} \Rightarrow [l'(l'+1) - l(l+1)]^2 = 2[l'(l'+1) + l(l+1)]$

We can check

$\sqrt{\text{Left}} = l'(l'+1) - l(l+1)$

$= [l'(l'+1) + ll'] - [l(l+1) + ll']$

$= l'(l + l' + 1) - l(l' + l + 1)$

$= (l' - l)(l + l' + 1)$ [9.76a]

$\text{Right} = 2[l(l+1) + l'(l'+1)] = 2[l^2 + l + (l')^2 + l']$

Also, we can check

$(l' + l + 1)^2 + (l' - l)^2 - 1 = (l')^2 + l^2 + 1 + 2ll' + 2l + 2l' + 2l' + (l')^2 + l^2 - 2ll' - 1$

$= 2[(l')^2 + l^2 + l + l'] = \text{Right}$

$\text{Left} = \text{Right} \Rightarrow (l' - l)^2(l' + l + 1)^2 = (l' + l + 1)^2 + (l' - l)^2 - 1$

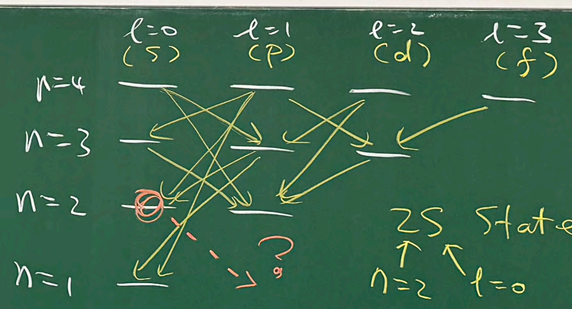
$\Rightarrow [(l' - l)^2 - 1][(l' + l + 1)^2 - 1] = 0$

No transition unless $\Delta l = \pm 1$

cannot be zero unless $l = l' = 0$

$\langle n00|\vec{r}|n00\rangle = 0$ odd integral

Fig. 9.6



Chap 10. Adiabatic Approximation

(Topological physics 101)

Nobel Prize 1985, 1998, 2016

10.1 Adiabatic theorem

10.1.1 Adiabatic process

$T_e \gg T_i$

T_i Internal time $\Leftrightarrow$ Period

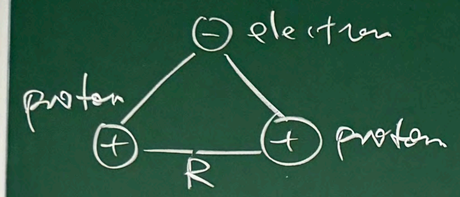
T_e External time, time scale of changing L

Pendulum Period $T = 2\pi\sqrt{\frac{L(t)}{g}}$

Gradual change of the external conditions defines an adiabatic process

↑ 投影背景墙面，注意保护，严禁书写！ ↑

Hydrogen molecule ion



Fix R, Solve the electron part

Minimize $\langle H \rangle$ as a function of R (Born-Oppenheimer approximation)

Infinite square well

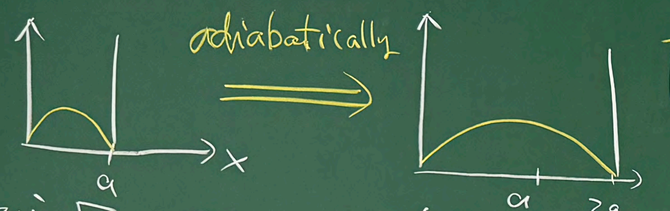
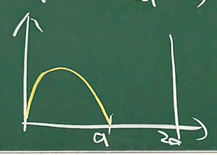


Fig 10.2

$$\psi^i = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi}{a}x\right) \Longrightarrow \psi^f = \sqrt{\frac{2}{2a}} \sin\left(\frac{\pi}{2a}x\right)$$

Abrupt change



10.1.2 Adiabatic theorem

In an adiabatic process, if we start from the nth eigen state of H^i (initial), we end up at the nth state of H^f (final)

parameters of Hamiltonian changes slowly (adiabatically), but no transition to other states

In sharp contrast to "time-dependent perturbation", where $\omega \sim \omega_0$ ($T_e \sim T_i$), light induces transitions

Proof of adiabatic theorem

If Hamiltonian is time-independent

$$H\psi_n = E_n \psi_n$$

We start at the nth state, its time evolution simply picks up a phase (相位)

$$\Psi_n(t) = \psi_n e^{-iE_n t/\hbar}$$

If Hamiltonian changes with time adiabatically, then the eigen energies and eigen states are "time-dependent"

$$H(t)\psi_n(t) = E_n(t)\psi_n(t)$$ Instantaneous solution

↑ Here, t is not time, but a parameter

and $\langle \psi_n(t) | \psi_m(t) \rangle = \delta_{n,m}$

$\psi_n(t)$ are complete, so the general solution to the time-dependent Schrödinger eqn.

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

can be expressed as

$$\Psi(t) = \sum_n C_n(t)\psi_n(t) e^{i\theta_n(t)} \quad [10.2]$$

$C_n(t)$: parameter

where $\theta(t) = -\frac{1}{\hbar}\int_0^t E_n(t')dt'$ → if E_n is constant → $-\frac{1}{\hbar}E_n t$

phase accumulated from t' to $t'+dt'$

The job is to determine $C_n(t)$

↑ 投影背景墙面，注意保护，严禁书写！↑

Proof of adiabatic theorem

The "time"-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\underline{\Psi}(t) = H(t)\underline{\Psi}(t) \quad [10,11]$$

($H(t)$: treated as a parameter)

Trial Solution $\underline{\Psi}(t) = \sum_n C_n(t)\psi_n(t)e^{i\theta_n(t)}$ [10,12]

where $\theta(t) = -\frac{1}{\hbar}\int_0^t E_n(t')dt' \xrightarrow{E_n \text{ is constant}} -\frac{E_n t}{\hbar}$

Put [10,12] into [10,11] $\Rightarrow$

$$i\hbar\frac{\partial}{\partial t}\sum_n C_n(t)\psi_n(t)e^{i\theta_n(t)} = H(t)\sum_n C_n(t)\psi_n(t)e^{i\theta_n(t)}$$

$$\Rightarrow i\hbar\sum_n\left[\dot{C}_n\psi_n e^{i\theta_n} + C_n\dot{\psi}_n e^{i\theta_n} + iC_n\psi_n e^{i\theta_n}\dot{\theta}_n\right]$$

$$= \sum_n C_n H\psi_n e^{i\theta_n} \quad (H\psi_n = E_n\psi_n)$$

$\dot{\theta}_n = -\frac{1}{\hbar}E_n(t)$

where $H(t)\psi_n(t) = E_n(t)\psi_n(t)$ (Instantaneous solution) $\quad \langle\psi_m(t)|\psi_n(t)\rangle = \delta_{n,m}$

$$\Rightarrow \sum_n \dot{C}_n\psi_n e^{i\theta_n} = -\sum_n C_n\dot{\psi}_n e^{i\theta_n}$$

Take the inner product $\langle\psi_m(t)|$

$$\sum_n \dot{C}_n\underbrace{\langle\psi_m(t)|\psi_n(t)\rangle}_{\delta_{m,n}}e^{i\theta_n} = -\sum_n C_n\langle\psi_m|\dot{\psi}_n\rangle e^{i\theta_n}$$

($\langle\psi_m|\dot{\psi}_n\rangle$: never seen before)

$$\Rightarrow \dot{C}_m e^{i\theta_m} = -\sum_n C_n\langle\psi_m|\dot{\psi}_n\rangle e^{i\theta_n}$$

$$\Rightarrow \dot{C}_m = -\sum_n C_n\langle\psi_m|\dot{\psi}_n\rangle e^{i(\theta_n-\theta_m)} \quad [10,16]$$

To calculate $\langle\psi_m|\dot{\psi}_n\rangle$, differentiate $H(t)\psi_n(t) = E_n(t)\psi_n(t)$ with respect to t $\Rightarrow$

$$\frac{d}{dt}[H(t)\psi_n(t)] = \frac{d}{dt}[E_n(t)\psi_n(t)]$$

$$\Rightarrow \dot{H}\psi_n + H\dot{\psi}_n = \dot{E}_n\psi_n + E_n\dot{\psi}_n$$

Inner product $\langle\psi_m(t)|$

$$\langle\psi_m|\dot{H}|\psi_n\rangle + \underbrace{\langle\psi_m|H}_{E_m\langle\psi_m|}|\dot{\psi}_n\rangle = \dot{E}_n\underbrace{\langle\psi_m|\psi_n\rangle}_{\delta_{m,n}} + E_n\langle\psi_m|\dot{\psi}_n\rangle$$

For $m \neq n$

$$\langle\psi_m|\dot{H}|\psi_n\rangle = (E_n - E_m)\langle\psi_m|\dot{\psi}_n\rangle$$

$$\Rightarrow \langle\psi_m|\dot{\psi}_n\rangle = \frac{\langle\psi_m|\dot{H}|\psi_n\rangle}{E_n - E_m}$$

[10,16] $\Rightarrow \dot{C}_m = -C_m\langle\psi_m|\dot{\psi}_m\rangle - \sum_{n(\neq m)} C_n\frac{\langle\psi_m|\dot{H}|\psi_n\rangle}{E_n - E_m}e^{i(\theta_n-\theta_m)}$

So far, it is exact.

Now, we apply the adiabatic approximation

$\dot{H}$ means the change of H with time, which is extremely small in an adiabatic process, so we drop the second term on the right.

$$\Rightarrow \dot{C}_m(t) = -C_m\langle\psi_m|\dot{\psi}_m\rangle$$

$$\Rightarrow \frac{d}{dt}C_m(t) = -C_m\langle\psi_m|\dot{\psi}_m\rangle$$

$$\Rightarrow \frac{dC_m}{C_m} = -\langle\psi_m|\dot{\psi}_m\rangle dt$$

$$\Rightarrow \ln C_m = -\int dt'\langle\psi_m|\frac{d}{dt'}\psi_m\rangle + \text{const.}$$

$$\Rightarrow C_m(t) = C_m(t=0)\,e^{-\int_0^t dt'\langle\psi_m(t')|\frac{d}{dt'}\psi_m(t')\rangle}$$

or $C_m(t) = C_m(0)\,e^{i\gamma_m(t)}$

where $\gamma_m(t) \equiv i\int_0^t\langle\psi_m(t')|\frac{d}{dt'}\psi_m(t')\rangle dt'$

[Note] γ_m is real, because $\frac{d}{dt}\langle\psi_m|\psi_m\rangle = 0$

$$= \langle\psi_m|\dot{\psi}_m\rangle + \langle\dot{\psi}_m|\psi_m\rangle = 2\,\mathrm{Re}\langle\psi_m|\dot{\psi}_m\rangle = 0$$

We have assumed that $\underline{\Psi}(t) = \sum_n C_n(t)\psi_n(t)e^{i\theta_n(t)}$

If we start with $C_n(t=0) = 1$, $C_{m\neq n}(t=0) = 0$

$$\underline{\Psi}_n(t) = \psi_n(t)e^{i\theta_n(t)}e^{i\gamma_n(t)}$$

$$\Psi_n(t) = \psi_n(t)\, e^{i\theta_n(t)}\, e^{i\gamma_n(t)}$$

Still on the nth eigen state — Dynamic phase — Pick up an extra geometric phase

10.2. Berry phase

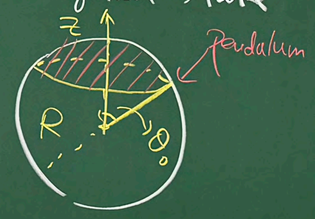
10.2.1 Nonholonomic process

Its state depends on the path taken in order to achieve it.

A system does not return to its original state when transported around a loop

Classical geometric phase

Foucault pendulum



The rotation of earth carries a pendulum to do an adiabatic transport around a loop, the change of the angle of the pendulum plane = the solid angle of the closed loop

$$\Theta = \frac{A_{enc}}{R^2} = \Omega = \int_0^{\theta_0} \sin\theta\, d\theta \int_0^{2\pi} d\varphi = 2\pi(-\cos\theta)\Big|_0^{\theta_0}$$
$$= 2\pi(1-\cos\theta_0)$$

10.2.2. Quantum geometric phase

For an adiabatic process, if we start from the nth eigen state of $H(t=0)$, we remain on the nth eigen state of $H(t)$, pick up only a time-dependent factor

$$\Psi(t) = e^{i[\theta_n(t)+\gamma_n(t)]}\psi_n(t)$$, where $H(t)\psi_n(t) = E_n(t)\psi_n(t)$

parameter — Instantaneous solution

Dynamic phase $\theta_n(t) \equiv -\frac{1}{\hbar}\int_0^t E_n(t')\,dt'$ — $E_n(t')$: Instantaneous eigen energy

If $E_n(t) \to E_n$, $\theta_n \to -\frac{1}{\hbar}E_n t$

Geometric phase $\gamma_n(t) \equiv i\int_0^t \langle \psi_n(t') \left| \frac{d}{dt'} \psi_n(t') \right\rangle dt'$

$\psi_n(t)$ depends on t because some parameters $R(t)$ in the Hamiltonian are changing with time

$$\frac{\partial \psi_n}{\partial t} = \frac{\partial \psi_n}{\partial R}\frac{dR}{dt}$$

$$\Rightarrow \gamma_n(t) = i\int_0^t \langle \psi_n \left| \frac{\partial \psi_n}{\partial R} \right\rangle \frac{dR}{dt'} dt' = i\int_{R_i}^{R_f} \langle \psi_n(R) \left| \frac{\partial \psi_n}{\partial R} \right\rangle dR$$

Where $R_f = R(t)$, $R_i = R(0)$

If there is only one parameter, the Hamiltonian returns to its initial state

Period: $\gamma_n(T) = 0 = \int_{R_i}^{R_f = R_i} \cdots$

However, if there are N parameters.

$\vec{R} = [R_1, R_2, \ldots, R_N]$ to form a vector of parameters (parameter space)

$$\frac{\partial \psi_n}{\partial t} = \frac{\partial \psi_n}{\partial R_1}\frac{dR_1}{dt} + \frac{\partial \psi_n}{\partial R_2}\frac{dR_2}{dt} + \cdots + \frac{\partial \psi_n}{\partial R_N}\frac{dR_N}{dt}$$
$$= (\nabla_R \psi_n)\cdot\frac{d\vec{R}}{dt} \quad [10.43]$$

$$\Rightarrow \gamma_n(t) = i\int_{\vec{R}_i}^{\vec{R}_f} \langle \psi_n | \nabla_R \psi_n \rangle \cdot d\vec{R}$$ path integral

What can be a parameter space?

$\vec{R} = (x, y, z)$ real space

$\vec{R} = (k_x, k_y, k_z)$ wave vectors

$\vec{R} = (B_x, B_y, B_z) = (B, \theta, \varphi)$ magnetic field

⬆ 投影背景墙面，注意保护，严禁书写！⬆

Berry phase = geometric phase of a complete cycle (closed loop)

$$\gamma_n(T) = i\oint \langle \psi_n | \nabla_R \psi_n \rangle \cdot d\vec{R} \quad [10.45]$$

M. V. Berry, Proc. R. Soc. Lond. A 392, 45 (1984)

Pancharatnam 1956

Berry connection $\vec{A}$, Berry curvature $\vec{B}$, Berry phase

P381 of Griffiths (Second Version) Everything is important

Recall: The magnetic field $\vec{B}$ can be written in terms of vector potential $\vec{A}$, $\vec{B} = \nabla \times \vec{A}$

Using the stokes' theorem, the magnetic flux Φ

$$\Phi = \int_S \vec{B}\cdot d\vec{a} = \int_S (\nabla\times\vec{A})\cdot d\vec{a} = \oint_C \vec{A}\cdot d\vec{r}$$

Area integral = loop integral

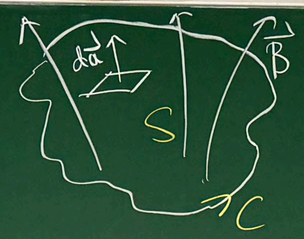


Fig 10.8

Compare with [10.45]

Berry connection $\vec{A} \equiv i\langle \psi_n | \nabla_R \psi_n \rangle$ "vector potential"

Berry curvature $\vec{B} \equiv i\nabla_R \times \langle \psi_n | \nabla_R \psi_n \rangle$ "magnetic field"

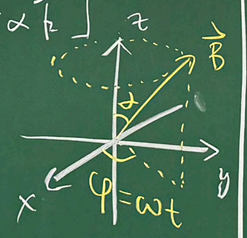
Berry phase $\gamma_n(T) = \oint \vec{A}\cdot d\vec{R} = \int \vec{B}\cdot d\vec{a}$ "flux"

loop integral = Area integral

or $\gamma_n(T) = i\int [\nabla_R \times \langle \psi_n | \nabla_R \psi_n \rangle \cdot d\vec{a}$ [10.51]

☆ **Example 10.2** Berry phase of a spin in a slowly rotating magnetic field

$$\vec{B}(t) = B_0\left[\sin\alpha\cos\omega t\,\hat{i} + \sin\alpha\sin\omega t\,\hat{j} + \cos\alpha\,\hat{k}\right]$$



The Hamiltonian

$$H(t) = \frac{e}{m}\vec{B}\cdot\vec{S} = \frac{e\hbar B_0}{2m}\left[\sin\alpha\cos\omega t\,\sigma_x + \sin\alpha\sin\omega t\,\sigma_y + \cos\alpha\,\sigma_z\right]$$

($\vec{S} = \frac{\hbar}{2}\vec{\sigma}$)

$$= \frac{\hbar\omega_1}{2}\begin{pmatrix} \cos\alpha & e^{-i\omega t}\sin\alpha \\ e^{i\omega t}\sin\alpha & -\cos\alpha \end{pmatrix}$$

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

where $\omega_1 \equiv \frac{eB_0}{m}$ (Internal time)

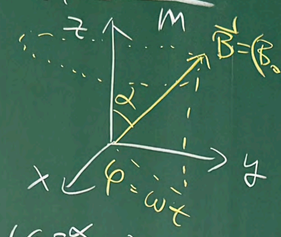
The eigen energies $E_\pm = \pm\frac{\hbar\omega_1}{2}$ Instantaneous solution

eigen states $\chi_+(t) = \begin{pmatrix} \cos\frac{\alpha}{2} \\ e^{i\omega t}\sin\frac{\alpha}{2} \end{pmatrix}$, $\chi_-(t) = \begin{pmatrix} \sin\frac{\alpha}{2} \\ -\cos\frac{\alpha}{2}e^{i\omega t} \end{pmatrix}$

SUSTech

Example 10.2 Berry phase of a spin in a slowly (adiabatically) rotating magnetic field

$$H(t)=\frac{\hbar\omega_1}{2}\begin{pmatrix}\cos\alpha & e^{-i\omega t}\sin\alpha\\ e^{i\omega t}\sin\alpha & -\cos\alpha\end{pmatrix},\quad \omega_1\equiv\frac{eB_0}{m}$$



Internal time $T_i\sim 1/\omega_1$

External time $T_e\sim 1/\omega$

Eigen energies $E_\pm=\pm\frac{\hbar\omega_1}{2}$

Instantaneous eigen states $\chi_+=\begin{pmatrix}\cos\frac{\alpha}{2}\\ \sin\frac{\alpha}{2}e^{i\omega t}\end{pmatrix}$, $\chi_-=\begin{pmatrix}\sin\frac{\alpha}{2}\\ -\cos\frac{\alpha}{2}e^{i\omega t}\end{pmatrix}$

Suppose the initial state $\chi(t=0)=\chi_+(t=0)=\begin{pmatrix}\cos\frac{\alpha}{2}\\ \sin\frac{\alpha}{2}\end{pmatrix}$

the exact solution to $i\frac{\partial}{\partial t}\chi(t)=H(t)\chi(t)$ is

$$\chi(t)=\begin{pmatrix}\left[\cos\frac{\lambda t}{2}-i\frac{\omega_1-\omega}{\lambda}\sin\frac{\lambda t}{2}\right]\cos\frac{\alpha}{2}e^{-i\omega t/2}\\ \left[\cos\frac{\lambda t}{2}-i\frac{\omega_1+\omega}{\lambda}\sin\frac{\lambda t}{2}\right]\sin\frac{\alpha}{2}e^{i\omega t/2}\end{pmatrix}\quad[10.32]$$

where $\lambda\equiv\sqrt{\omega^2+\omega_1^2-2\omega\omega_1\cos\alpha}$

or it can be expressed as a linear combination

$$|\chi(t)\rangle=\underbrace{\left[|\chi_+(t)\rangle\langle\chi_+(t)|+|\chi_-(t)\rangle\langle\chi_-(t)|\right]}_{=1}|\chi(t)\rangle$$

$$=\underbrace{\langle\chi_+(t)|\chi(t)\rangle}_{\text{superposition coefficients}}|\chi_+(t)\rangle+\langle\chi_-(t)|\chi(t)\rangle|\chi_-(t)\rangle$$

$$\langle\chi_+(t)|\chi(t)\rangle=\left(\cos\tfrac{\alpha}{2},\sin\tfrac{\alpha}{2}e^{-i\omega t}\right)\begin{pmatrix}1\times 2\\ 2\times 1\end{pmatrix}$$

$$\langle\chi_-(t)|\chi(t)\rangle=\left(\sin\tfrac{\alpha}{2},-\cos\tfrac{\alpha}{2}e^{-i\omega t}\right)\begin{pmatrix}1\times 2\\ 2\times 1\end{pmatrix}$$

$$\Rightarrow|\chi(t)\rangle=\left[\cos\frac{\lambda t}{2}-i\frac{\omega_1-\omega\cos\alpha}{\lambda}\sin\frac{\lambda t}{2}\right]e^{-i\frac{\omega t}{2}}|\chi_+(t)\rangle+i\left[\frac{\omega}{\lambda}\sin\alpha\sin\frac{\lambda t}{2}\right]e^{i\frac{\omega t}{2}}|\chi_-(t)\rangle\quad[10.33]$$

So we have projected the exact solution onto the basis formed by the instantaneous eigen states.

↑ 投影背景墙面，注意保护，严禁书写！ ↑

Let's check the adiabatic limit of the exact solution ($\omega\ll\omega_1$)

$$\lambda=\omega_1\sqrt{1-2\frac{\omega}{\omega_1}\cos\alpha+\left(\frac{\omega}{\omega_1}\right)^2}\approx\omega_1\left(1-\frac{\omega}{\omega_1}\cos\alpha\right)$$

($\sqrt{1-x}\approx 1-\frac{1}{2}x$)

$$\approx\omega_1-\omega\cos\alpha\quad[10.52]$$

$[10.33]\Rightarrow$

$$\chi(t)\cong\left\{\cos\left[\frac{t}{2}(\omega_1-\omega\cos\alpha)\right]-i\frac{\omega_1-\omega\cos\alpha}{\omega_1-\omega\cos\alpha}\sin\frac{t}{2}(\omega_1-\omega\cos\alpha)\right\}e^{-i\frac{\omega t}{2}}|\chi_+(t)\rangle$$

$$+i\left\{\frac{\omega}{\omega_1-\omega\cos\alpha}\sin\alpha\sin\left[\frac{t}{2}(\omega_1-\omega\cos\alpha)\right]\right\}e^{i\frac{\omega t}{2}}|\chi_-(t)\rangle$$

($\frac{\omega}{\omega_1-\omega\cos\alpha}\to 0$, as $\frac{\omega}{\omega_1}\to 0$)

$$=\left[\cos\frac{t}{2}(\omega_1-\omega\cos\alpha)-i\sin\frac{t}{2}(\omega_1-\omega\cos\alpha)\right]e^{-i\frac{\omega t}{2}}|\chi_+(t)\rangle$$

$$=e^{-i\frac{t}{2}(\omega_1-\omega\cos\alpha)}e^{-i\frac{\omega t}{2}}|\chi_+(t)\rangle$$

$$=e^{-i\frac{\omega_1 t}{2}}e^{i\frac{t\omega\cos\alpha}{2}}e^{-i\frac{\omega t}{2}}|\chi_+(t)\rangle$$

$$=e^{-i\frac{\omega_1 t}{2}}e^{-i\frac{t\omega}{2}(1-\cos\alpha)}|\chi_+(t)\rangle\quad[10.53]$$

Dynamic phase — Geometric phase

which is of the form of [10.23]

$$\psi(t)=e^{i\theta_n(t)}e^{i\gamma_n(t)}\psi_n(t)$$

The dynamic phase

$[10.29]\Rightarrow\theta_+(t)=-\frac{1}{\hbar}\int_0^t E_+(t')dt'=-\frac{\omega_1 t}{2}$ ($E_+=\frac{\hbar\omega_1}{2}$)

The geometric phase, compare with [10.53], it should be

$$\gamma_+(t)=\frac{\omega t}{2}(\cos\alpha-1)\quad[10.56]$$

$|\chi_+(t)\rangle$ For a complete cycle, we can have the Berry phase

$$\gamma_+(T)=\frac{\omega T}{2}(\cos\alpha-1)=\frac{2\pi}{2}(\cos\alpha-1)=\pi(\cos\alpha-1)$$

Now, we calculate the Berry phase

$$[10.51]\Rightarrow\gamma_n(T)\equiv i\int\nabla_R\times\langle\psi_n|\nabla_R\psi_n\rangle]\cdot d\vec{a}$$

($\psi_n\to\chi_+$; $\vec{R}=\vec{B}=(B_0,\theta,\phi)$; ①, ②, ③, ④)

The parameter space $\vec{B} = (B_0, \theta, \phi)$ Spherical coordinates ($\theta = \omega t$)

① $\nabla \chi_+ = \frac{\partial \chi_+}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial \chi_+}{\partial \theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial \chi_+}{\partial \phi}\hat{\phi}$ ($\frac{\partial}{\partial r}$: B_0)

$\chi_+ = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} e^{i\phi} \end{pmatrix}$ ($\phi = \omega t$)

$\Rightarrow \nabla\chi_+ = \frac{1}{r}\begin{pmatrix} -\frac{1}{2}\sin\frac{\theta}{2} \\ e^{i\phi}\cos\frac{\theta}{2} \end{pmatrix}\hat{\theta} + \frac{1}{r\sin\theta}\begin{pmatrix} 0 \\ i e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix}\hat{\phi}$

② $\langle \chi_+ | \nabla \chi_+ \rangle = \begin{pmatrix} \cos\frac{\theta}{2}, e^{-i\phi}\sin\frac{\theta}{2} \end{pmatrix}\begin{pmatrix} ① \\ ② \end{pmatrix}$

$= \frac{1}{r}\left(-\frac{1}{2}\cos\frac{\theta}{2}\sin\frac{\theta}{2} + \frac{1}{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2}\right)\hat{\theta} + \frac{1}{r\sin\theta}\left(0 + i\sin^2\frac{\theta}{2}\right)\hat{\phi}$

$= i\frac{\sin^2\frac{\theta}{2}}{r\sin\theta}\hat{\phi} = (\underbrace{0}_{v_r}, \underbrace{0}_{v_\theta}, \underbrace{i\frac{\sin^2\frac{\theta}{2}}{r\sin\theta}}_{v_\phi})$

③ $\nabla \times$ ②, for $\vec{v} = (v_r, v_\theta, v_\phi)$

$\nabla \times \vec{v} = \frac{1}{r\sin\theta}\left[\frac{\partial}{\partial\theta}(\sin\theta\, v_\phi) - \frac{\partial v_\theta}{\partial\phi}\right]\hat{r}$

$+ \frac{1}{r}\left[\frac{1}{\sin\theta}\frac{\partial v_r}{\partial\phi} - \frac{\partial}{\partial r}(r v_\phi)\right]\hat{\theta}$

$+ \frac{1}{r}\left[\frac{\partial}{\partial r}(r v_\theta) - \frac{\partial v_r}{\partial\theta}\right]\hat{\phi}$

$\Rightarrow \nabla \times \langle \chi_+ | \nabla \chi_+ \rangle = \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\left(i\frac{\sin^2\frac{\theta}{2}}{r\sin\theta}\right)\right]\hat{r}$

$= \frac{i}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin^2\frac{\theta}{2}\right)\hat{r} = \frac{i}{2r^2}\hat{r}$ "Monopole" "Electric field of a charge"

④ $\gamma_+(T) = i\int_S \nabla \times \langle \chi_+ | \nabla \chi_+ \rangle \cdot d\vec{a}$

where $d\vec{a} = r^2 \underbrace{d\Omega}_{\text{Solid angle}}\hat{r} = r^2 \sin\theta\, d\theta\, d\phi\, \hat{r}$

$\Rightarrow \gamma_+(T) = -i\int_S \frac{i}{2r^2}\hat{r}\cdot r^2 d\Omega\, \hat{r} = -\frac{1}{2}\int_S d\Omega = -\frac{1}{2}\Omega$ ← Solid angle enclosed by one cycle of rotation of the magnetic field

$\boxed{\Omega = 2\pi(1-\cos\theta_0)}$

Recall the classical geometric phase of the pendulum on earth



$\Rightarrow \gamma_+(T) = -\frac{1}{2}2\pi(1-\cos\alpha) = \pi(\cos\alpha - 1)$

Exactly the adiabatic limit of the exact solution

10.2.3 Aharonov-Bohm effect

scalar potential φ and vector potential $\vec{A}$

Electric field $\vec{E} = -\nabla\varphi - \frac{\partial \vec{A}}{\partial t}$, $\vec{B} = \nabla \times \vec{A}$

Gauge Invariance

We can do a gauge transformation

$\varphi \to \varphi' = \varphi - \frac{\partial \Lambda}{\partial t}$ (Λ is a function of $\vec{r}$ and t (Lambda))

$\vec{A} \to \vec{A}' = \vec{A} + \nabla\Lambda$

which has no influence on $\vec{E}$ and $\vec{B}$

$\vec{E} = -\nabla\left(\varphi - \frac{\partial\Lambda}{\partial t}\right) - \frac{\partial}{\partial t}\left[\vec{A} + \nabla\Lambda\right]$

$= -\nabla\varphi + \nabla\frac{\partial}{\partial t}\Lambda - \frac{\partial}{\partial t}\vec{A} - \frac{\partial}{\partial t}\nabla\Lambda = -\nabla\varphi - \frac{\partial}{\partial t}\vec{A}$

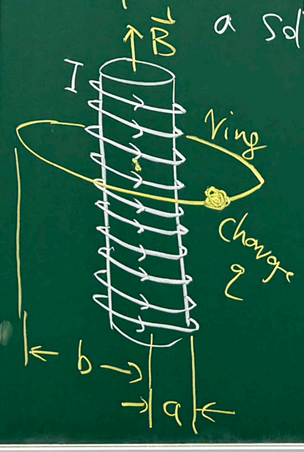
$\vec{B} = \nabla \times \left[\vec{A} + \nabla\Lambda\right] = \nabla\times\vec{A} + \underbrace{\nabla\times\nabla\Lambda}_{=0}$

In classical theory: No electromagnetic influences in the region where $\vec{E} = \vec{B} = 0$

In Quantum mechanics: Things are different,

For example: A-B effect

Example A charge constrained to move in a ring around a solenoid



If the solenoid is infinitely, the magnetic field inside is uniform, outside is zero. But, the vector potential $\vec{A}$ is not zero outside.

Let's derive $\vec{A}$ (Griffiths EM Example 5.12)

⬆ 投影背景墙面，注意保护，严禁书写！⬆

Find the vector potential $\vec{A}$ of an infinite solenoid, with n turns per unit length, radius a, current I

[Solution]



Ampere's law: $\oint \vec{B}\cdot d\vec{\ell} = \mu_0 I$ (μ_0: magnetic permittivity)

$Bx = \mu_0 I n x \Rightarrow B = \mu_0 n I$

Note that $\oint_C \vec{A}\cdot d\vec{\ell} = \int_S (\nabla\times\vec{A})\cdot d\vec{a} = \int_S \vec{B}\cdot d\vec{a} = \Phi$ (Stokes's theorem; Φ: magnetic flux)

Inside the solenoid

$A\,2\pi r = \mu_0 n I\,\pi r^2$ (C: circle, S: disk)

$\Rightarrow \vec{A} = \frac{\mu_0 n I}{2} r\,\hat{\phi}$ for $r < a$ (cylindrical coordinates)

Outside the solenoid

$A\,2\pi r = \mu_0 n I\,\pi a^2$

$\Rightarrow \vec{A} = \frac{\mu_0 n I \pi a^2}{2\pi r}\hat{\phi}$, for $r > a$

Outside Solenoid, $\vec{B}=0$, but $\vec{A}\neq 0$

Hamiltonian in magnetic field

$H = \frac{1}{2m}\left(\frac{\hbar}{i}\nabla - q\vec{A}\right)^2$ — Minimal Substitution, Peierls replacement

($\frac{\hbar}{i}\nabla$: momentum; q: charge; $\vec{A}$: vector potential of $\vec{B} = \nabla\times\vec{A}$)

$H = \frac{1}{2m}\left[-\hbar^2\nabla^2 + q^2A^2 + iq\hbar\nabla\cdot\vec{A} + iq\hbar\vec{A}\cdot\nabla\right]\psi$ (ψ: wave function (scalar))

$\in \nabla\cdot(\vec{A}\psi) = \vec{A}\cdot\nabla\psi$

where we have used $\nabla\cdot(f\vec{A}) = f(\nabla\cdot\vec{A}) + \vec{A}\cdot\nabla f$ (f: scalar, $\vec{A}$: vector; $\nabla\cdot\vec{A} = 0$)

In cylindrical coordinates $\begin{cases}\nabla\cdot\vec{A} = \frac{1}{r}\frac{\partial}{\partial r}(rA_r) + \frac{1}{r}\frac{\partial A_\phi}{\partial\phi} + \frac{\partial A_z}{\partial z}\\ \vec{A} = \frac{\mu_0 n I \pi a^2}{2\pi r}\hat{\phi} = \frac{\Phi}{2\pi r}\hat{\phi}\end{cases}$

$\Rightarrow H = \frac{1}{2m}\left[-\hbar^2\nabla^2 + q^2A^2 + i\,2q\hbar\vec{A}\cdot\nabla\right]\psi$

$\nabla^2\psi = \nabla\cdot\nabla\psi$

In cylindrical coordinates $\nabla^2\psi = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\phi^2} + \frac{\partial^2\psi}{\partial z^2}$

$\nabla\psi = \frac{\partial\psi}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial\psi}{\partial\phi}\hat{\phi} + \frac{\partial\psi}{\partial z}\hat{z}$

for fixed r and z of the charge on the ring

$\Rightarrow H\psi = \frac{1}{2m}\left[-\hbar^2\frac{1}{r^2}\frac{\partial^2\psi}{\partial\phi^2} + q^2\left(\frac{\Phi}{2\pi r}\right)^2 + i\,2\hbar q\left(\frac{\Phi}{2\pi r}\frac{1}{r}\frac{\partial\psi}{\partial\phi}\right)\right]$

where the magnetic flux $\Phi = \mu_0 n I \pi a^2$

The radius of the ring is b, $r\to b$

$\Rightarrow H\psi = \frac{1}{2m}\left[-\hbar^2\frac{1}{b^2}\frac{\partial^2\psi}{\partial\phi^2} + q^2\left(\frac{\Phi}{2\pi b}\right)^2\psi + i\hbar q\frac{\Phi}{\pi b^2}\frac{\partial\psi}{\partial\phi}\right]$

$= E\psi$ ← 0th; 2nd; 0th; 1st

Eigen equation

This differential equation can be written as

$\frac{d^2\psi}{d\phi^2} - i\,2\beta\frac{d\psi}{d\phi} + \varepsilon\psi = 0$, where $\beta \equiv \frac{q\Phi}{2\pi\hbar}$, $\varepsilon = \frac{2mb^2E}{\hbar^2} - \beta^2$

To solve it, assume the trial solution

$\psi = Ae^{i\lambda\phi}$

$\Rightarrow \frac{d^2}{d\phi^2}\left(Ae^{i\lambda\phi}\right) - i\,2\beta\frac{d}{d\phi}\left(Ae^{i\lambda\phi}\right) + \varepsilon Ae^{i\lambda\phi} = 0$

$\Rightarrow \left(-\lambda^2 + 2\beta\lambda + \varepsilon\right)Ae^{i\lambda\phi} = 0$

$\Rightarrow \lambda = \frac{2\beta \pm \sqrt{4\beta^2 + 4\varepsilon}}{2} = \beta \pm \sqrt{\beta^2 + \varepsilon}$

Periodic boundary conditions:

$e^{i\lambda\phi} = e^{i\lambda(\phi + 2\pi)} = e^{i\lambda\phi}e^{i\lambda 2\pi} \Rightarrow e^{i\lambda 2\pi} \in 1 \Rightarrow \lambda$ is an integer n

$\Rightarrow \beta \pm \sqrt{\beta^2 + \varepsilon} = n \Rightarrow \beta \pm \sqrt{\beta^2 + \frac{2mb^2E}{\hbar} - \beta^2} = n$

$\Rightarrow E_n = \frac{\hbar^2}{2mb^2}(\beta - n)^2$, $n = 0, \pm1, \pm2, \ldots$

The energy is corrected by the flux, although $\vec{B}=0$ outside the solenoid

$\beta \equiv \frac{q\Phi}{2\pi\hbar} = \frac{\Phi}{\hbar/q}$ ← flux; ← flux quantum

SUSTech

↑ 投影背景墙面，注意保护，严禁书写！↑

Effect of magnetic field on wave function

Suppose in a region $\vec{B}=0$, so that $\nabla\times\vec{A}=0$, but $\vec{A}\neq 0$. (Imagine the solenoid case)

The Schrödinger eqn. (potential)

$$\left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla-q\vec{A}\right)^2+V\right]\Psi=i\hbar\frac{\partial\Psi}{\partial t} \quad [10.75]$$

Minimal coupling

[Conclusion]: The effect of $\vec{A}$ can be absorbed in terms of $\Psi=e^{ig}\Psi'$, where

$$g(\vec{r})\equiv\frac{q}{\hbar}\int_{\mathcal{O}}^{\vec{r}}\vec{A}(\vec{r}')\cdot d\vec{r}', \quad \text{path integral of } \vec{A}$$

$\mathcal{O}$ ← some reference point

$$i\hbar\frac{\partial}{\partial t}\Psi'=H\Psi' \quad \text{where no } \vec{A} \text{ in } H$$

[Proof]: We put $\Psi=e^{ig}\Psi'$ into [10.75]

$$\nabla\Psi=\nabla(e^{ig}\Psi')=e^{ig}(i\nabla g)\Psi'+e^{ig}\nabla\Psi'$$

gradient; Scalar

$$\nabla g=\frac{q}{\hbar}\nabla\int_{\mathcal{O}}^{\vec{r}}\vec{A}(\vec{r}')\cdot d\vec{r}'=\frac{q}{\hbar}\vec{A}(\vec{r})$$

$$=e^{ig}i\frac{q}{\hbar}\vec{A}(\vec{r})\Psi'+e^{ig}(\nabla\Psi')$$

$$=i\frac{q}{\hbar}\vec{A}(\vec{r})\Psi+e^{ig}(\nabla\Psi')$$

$$\Rightarrow\frac{\hbar}{i}\nabla\Psi=q\vec{A}+\frac{\hbar}{i}e^{ig}(\nabla\Psi')$$

$$\Rightarrow\left(\frac{\hbar}{i}\nabla-q\vec{A}\right)\Psi=\frac{\hbar}{i}e^{ig}(\nabla\Psi') \quad [10.78]$$

Act $\left(\frac{\hbar}{i}\nabla-q\vec{A}\right)$ on [10.78]

Vector

$$\Rightarrow\left(\frac{\hbar}{i}\nabla-q\vec{A}\right)^2\Psi=\left(\frac{\hbar}{i}\nabla-q\vec{A}\right)\frac{\hbar}{i}e^{ig}(\nabla\Psi')$$

$$=-\hbar^2\nabla(e^{ig}\nabla\Psi')-\frac{q\hbar}{i}\vec{A}e^{ig}\nabla\Psi'$$

$$=-\hbar^2\left(ie^{ig}(\nabla g)\nabla\Psi'+e^{ig}\nabla^2\Psi'\right)-\frac{q\hbar}{i}\vec{A}e^{ig}\nabla\Psi'$$

$$=-\hbar^2e^{ig}\nabla^2\Psi' \quad [10.79]$$

Put [10.79] into [10.75] $\Rightarrow$

$$\left[-\frac{\hbar^2}{2m}e^{ig}\nabla^2\Psi'+Ve^{ig}\Psi'\right]=i\hbar\frac{\partial}{\partial t}\Psi'e^{ig}$$

$$\Rightarrow-\frac{\hbar^2}{2m}\nabla^2\Psi'+V\Psi'=i\hbar\frac{\partial}{\partial t}\Psi' \Leftrightarrow H\Psi'=i\frac{\partial}{\partial t}\Psi'$$

no $\vec{A}$ in H

In other words, the effect of magnetic field (in terms of the vector potential $\vec{A}$) is to add a phase factor e^{ig}, $g(\vec{r})=\int_{\mathcal{O}}^{\vec{r}}\vec{A}(\vec{r}')\cdot d\vec{r}'$

Aharonov-Bohm phase [Physical Review 115, 485 (1959)]

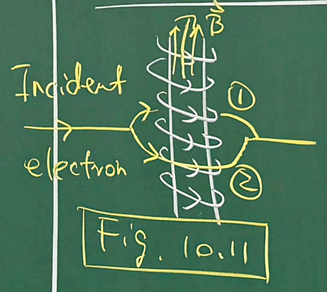


Fig. 10.11

Outside solenoid

$\vec{B}=0$, $\vec{A}\neq 0$

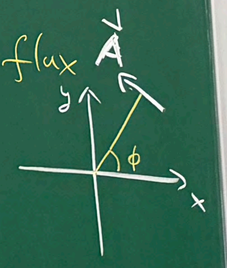
A beam of electron is split in two, the two beams arrive with different phases $\Rightarrow$ phase difference ?

Using [10.77] and [10.66]

$$\vec{A}=\frac{\Phi}{2\pi r}\hat{\phi}$$ ← Polar angle direction

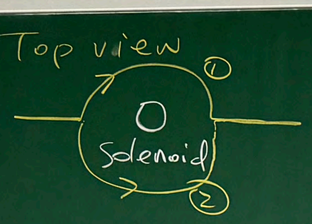
Φ magnetic flux

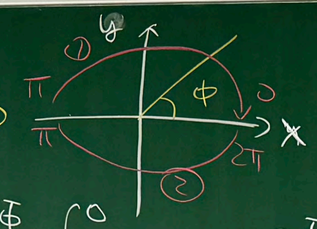
$$g=\frac{q}{\hbar}\int\vec{A}\cdot d\vec{r}=\frac{q\Phi}{2\pi\hbar}\int\frac{1}{r'}\hat{\phi}\cdot r'd\phi\,\hat{\phi}$$



$$=\frac{q\Phi}{2\pi\hbar}\int_{?}^{?}d\phi$$

Top view





For path ①, $g_1 = \frac{q\Phi}{2\pi\hbar}\int_{\pi}^{0} d\phi = -\frac{q\Phi}{2\hbar}$

For path ②, $g_2 = \frac{q\Phi}{2\pi\hbar}\int_{\pi}^{2\pi} d\phi = \frac{q\Phi}{2\hbar}$

The phase difference $g_2 - g_1$

$$\frac{q\Phi}{2\pi\hbar}\left(\int_{\pi}^{2\pi} - \int_{\pi}^{0}\right)d\phi = \frac{q\Phi}{2\pi\hbar}\left(\int_{\pi}^{2\pi} + \int_{0}^{\pi}\right)d\phi$$

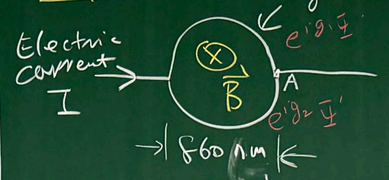
$$= \frac{q\Phi}{2\pi\hbar}\int_{0}^{2\pi} d\phi = \frac{q\Phi}{2\pi\hbar}\oint d\phi$$ loop integral around the solenoid

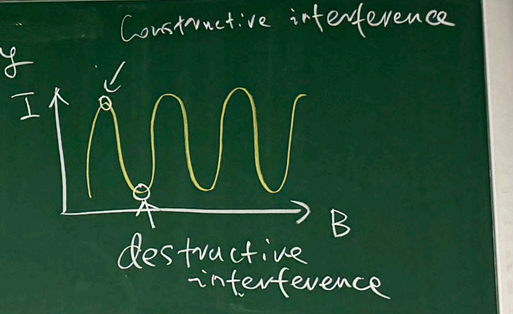
This is the AB phase

$$\frac{q\Phi}{\hbar} = \frac{q\Phi}{h/2\pi} = 2\pi\frac{\Phi}{h/q}$$ ← magnetic flux enclosed by the loop

h/q ← flux quantum

Experiment — gold ring





$$|e^{ig_1}\Psi' + e^{ig_2}\Psi'|^2$$

$$|e^{ig_1} + e^{ig_2}|^2 = (e^{ig_1} + e^{ig_2})(e^{-ig_1} + e^{-ig_2}) = \underbrace{2\cos(g_1 - g_2)}_{\text{Interference}} + \underbrace{2}_{\text{Incoherent}}$$

[Washburn & Webb, PRL 54, 2696 (1985)]

A-B phase is a geometric phase [Berry 1984]

Suppose a charge is confined in a box

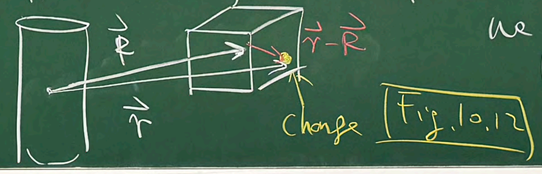


Fig. 10.12

We will transport the box around the solenoid

Eigen equation — potential inside the box

$$\left\{\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - q\vec{A}(\vec{r})\right)^2 + V(\vec{r}-\vec{R})\right\}\psi_n = E_n\psi_n$$

parameter dependent

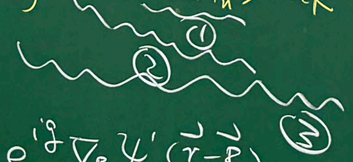
let $\psi_n = e^{ig}\psi_n'$, $g \equiv \frac{q}{\hbar}\int_{\vec{R}}^{\vec{r}} \vec{A}(\vec{r}')\cdot d\vec{r}'$ ← For convenience, so that g is a function of $\vec{r}-\vec{R}$

So that ψ_n' satisfies

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}-\vec{R})\right)\psi_n' = E_n\psi_n'$$ ← a function of $\vec{r}-\vec{R}$

Recall Eq. [10.45] $\gamma_n(T) = i\oint \langle\psi_n|\nabla_R\psi_n\rangle\cdot d\vec{R}$

$\vec{R}$ is the parameter space



① $\nabla_R\psi_n = \nabla_R\left(e^{ig}\psi_n'(\vec{r}-\vec{R})\right)$

$= e^{ig} i(\nabla_R g)\psi_n'(\vec{r}-\vec{R}) + e^{ig}\nabla_R\psi_n'(\vec{r}-\vec{R})$

$\frac{q}{\hbar}\nabla_R\int_{\vec{R}}^{\vec{r}}\vec{A}(\vec{r}')\cdot d\vec{r}' = -\frac{q}{\hbar}\vec{A}(\vec{R})$

$\Rightarrow \nabla_R\psi_n = e^{ig}\left[-i\frac{q}{\hbar}\vec{A}(\vec{R})\right]\psi_n'(\vec{r}-\vec{R}) + e^{ig}\nabla_R\psi_n'(\vec{r}-\vec{R})$

$= e^{ig}\left[-i\frac{q}{\hbar}\vec{A}(\vec{R})\psi_n'(\vec{r}-\vec{R}) + \nabla_R\psi_n'(\vec{r}-\vec{R})\right]$

② $\langle\psi_n|\nabla_R\psi_n\rangle = \int d^3\vec{r}\, e^{-ig}\left[\psi_n'(\vec{r}-\vec{R})\right]^* e^{ig}$

$\times\left[-i\frac{q}{\hbar}\vec{A}(\vec{R})\psi_n'(\vec{r}-\vec{R}) + \nabla_R\psi_n'(\vec{r}-\vec{R})\right]$

Note that the integrand is a function of $\vec{r}-\vec{R}$,

So $\boxed{\nabla_R \to -\nabla_r}$

$\Rightarrow \langle\psi_n|\nabla_R|\nabla_r\psi_n\rangle = \int d^3\vec{r}\left[\psi_n'(\vec{r}-\vec{R})\right]^*\left[-i\frac{q}{\hbar}\vec{A}(\vec{R})\psi_n'(\vec{r}-\vec{R}) + \nabla\psi_n'(\vec{r}-\vec{R})\right]$

$= \int d^3\vec{r}\left(-i\frac{q}{\hbar}\vec{A}(\vec{R})\right)|\psi_n'(\vec{r}-\vec{R})|^2$

$+ \int d^3\vec{r}\left[\psi_n'(\vec{r}-\vec{R})\right]^*\nabla\psi_n'(\vec{r}-\vec{R})$

~ expectation value of $\langle\vec{p}\rangle$, odd integral = 0

$= -i\frac{q}{\hbar}\vec{A}(\vec{R})$

③ $\gamma_n(T) = i\oint\langle\psi_n|\nabla_R\psi_n\rangle\cdot d\vec{R} = \frac{q}{\hbar}\oint_C\vec{A}\cdot d\vec{R}$

$= \frac{q}{\hbar}\iint_S(\nabla\times\vec{A})\cdot d\vec{a} = \frac{q\Phi}{\hbar}$ which is the AB phase

⬆ 投影背景墙面，注意保护，严禁书写！⬆

Chap 12. Landau levels (Harmonic Oscillator)

The energy quantization of cyclotron motion of a charged particle in magnetic field

[Reference] = Chap XV of "Quantum Mechanics non-relativistic theory" 2nd ed. by Landau & Lifshitz

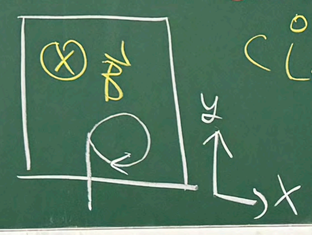
2D Electron gas

$H = \frac{p^2}{2m}$ → Apply a magnetic field → $H = \frac{\hbar^2}{2m}(\vec{k} - \frac{q}{\hbar}\vec{A})^2 - \vec{\mu}\cdot\vec{B}$

Minimal coupling (Peierls substitution)

$p^2 = p_x^2 + p_y^2 = \vec{p}\cdot\vec{p} = (p_x\hat{i} + p_y\hat{j})\cdot(p_x\hat{i} + p_y\hat{j})$

① Orbital effect on charge (Lorentz force) ② Zeeman effect on spin (magnetic moment)



q charge, $q = -e$ for electron, $e = 1.6\times10^{-19}$ Coulomb

$\vec{A}$ vector potential, $\vec{B} = \nabla\times\vec{A}$

$\vec{B} = (0,0,B)$ Assume a magnetic field along the $\hat{z}$ direction

$= B\hat{z}$

How about the vector potential $\vec{A}$ of $\vec{B}$?

Landau gauges $\vec{A} = \begin{cases} (-yB, 0, 0) \\ (0, xB, 0) \end{cases}$

We can check

$$\nabla\times\vec{A} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \partial_x & \partial_y & \partial_z \\ -yB & 0 & 0 \end{vmatrix} = \begin{matrix} \hat{x}(0-0) \\ +\hat{y}(0-0) \\ +\hat{z}(0-(-B)) \end{matrix} = B\hat{z}$$

$$\begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \partial_x & \partial_y & \partial_z \\ 0 & xB & 0 \end{vmatrix}$$

Any linear combination of the two Landau gauges can define the same $\vec{B}$

Symmetric gauge $\vec{A} = (-\frac{1}{2}yB, \frac{1}{2}xB, 0)$

(Important for Fractional quantum Hall effect)

We focus on the "orbital effect"

$$H = \frac{\hbar^2}{2m}(\vec{k} + \frac{e}{\hbar}\vec{A})^2 = \frac{\hbar^2}{2m}\left[(k_x - \frac{e}{\hbar}yB)^2 - \partial_y^2\right]$$

(k_x, k_y) (A_x, A_y) A_x $k_y \to -i\partial_y$

Now, the Hamiltonian is an explicit function of y

Because $[y, k_y] = i$, $[H, k_y] \neq 0$, so we need to write $\hat{k}_y$ → k_y good quantum number $[k_y, H] = 0$

→ $-i\partial_y$, $[k_y, H] \neq 0$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{\hbar^2}{}$$

Landau levels

The "orbital part" of an electron in a magnetic field (-e) z-direction

$$H = \frac{\hbar^2}{2m}\left(\vec{k} + \frac{e}{\hbar}\vec{A}\right)^2 = \frac{\hbar^2}{2m}\left[\left(k_x - \frac{e}{\hbar}yB\right)^2 - \partial_y^2\right]$$

Landau gauge $\vec{A} = (-yB, 0, 0)$

$$\left.\begin{matrix} H(y) \\ [y, k_y] = i \end{matrix}\right\} \Rightarrow k_y \longrightarrow -i\partial_y$$

We define the magnetic length

$$l_B \equiv \sqrt{\frac{\hbar}{eB}} \approx \frac{25.6\,\text{nm}}{\sqrt{B}}$$

B: induction; Strength of magnetic in units of Tesla

$B = 1$ Tesla, $l_B \approx 25.6$ nm

$B = 100$ Tesla, $l_B \approx 2.56$ nm

$$\Rightarrow H = \frac{\hbar^2}{2m}\left[\left(k_x - \frac{y}{l_B^2}\right)^2 - \partial_y^2\right] = \frac{\hbar^2}{2m}\frac{1}{l_B^2}\left[\left(\frac{y - y_0}{l_B}\right)^2 - (l_B\partial_y)^2\right]$$

$y_0 \equiv l_B^2 k_x$

Define the ladder operators

$$a = -\frac{1}{\sqrt{2}}\left(\frac{y - y_0}{l_B} + l_B\partial_y\right)$$

$$a^\dagger = -\frac{1}{\sqrt{2}}\left(\frac{y - y_0}{l_B} - l_B\partial_y\right)$$ ← dagger

Commutative relation of Boson

Use $[\hat{x}, \hat{P}_x] = i\hbar$, we can check $[a, a^\dagger] = 1$

$[x, P_y] = 0$

[check] $[x, P_x] = i\hbar \Rightarrow [x, -i\hbar\partial_x] = i\hbar$

$\Rightarrow [x, -\partial_x] = [\partial_x, x] = 1$ F○

$$[a, a^\dagger] = \left[-\frac{1}{\sqrt{2}}\left(\frac{y - y_0}{l_B} + l_B\partial_y\right), -\frac{1}{\sqrt{2}}\left(\frac{y - y_0}{l_B} - l_B\partial_y\right)\right]$$

(Commutation ⇐) Exchange to ⇒ $\left[\frac{y - y_0}{l_B}, \frac{y - y_0}{l_B}\right] = 0$

$[X, Y] \equiv XY - YX$

$$= \frac{1}{2}\left(\left[\frac{y - y_0}{l_B}, -l_B\partial_y\right] + \left[l_B\partial_y, \frac{y - y_0}{l_B}\right]\right)$$

$[y_0, \partial_y] \sim [k_x^2, \partial_y] = 0$

$$= \frac{1}{2}\left(\left[y, -\partial_y\right] + \left[\partial_y, y\right]\right) = \frac{1}{2}(1 + 1) = 1$$

$$\Rightarrow \frac{1}{\sqrt{2}}(a + a^\dagger) = -\frac{y - y_0}{l_B}, \quad \frac{1}{\sqrt{2}}(a - a^\dagger) = -l_B\partial_y$$

$$\Rightarrow H = \frac{\hbar^2}{2m}\frac{1}{l_B^2}\left[\left(\frac{y - y_0}{l_B}\right)^2 - (l_B\partial_y)^2\right]$$

$$= \frac{\hbar^2}{2m}\frac{1}{2l_B^2}\left[(a + a^\dagger)^2 - (a - a^\dagger)^2\right]$$

$$= \frac{\hbar^2}{2m}\frac{1}{2l_B^2}\left(aa + aa^\dagger + a^\dagger a + a^\dagger a^\dagger - (aa - aa^\dagger - a^\dagger a + a^\dagger a^\dagger)\right)$$

$$= \frac{\hbar^2}{2m}\frac{1}{l_B^2}\left[aa^\dagger + a^\dagger a\right]$$

$[a, a^\dagger] = 1$

$\Rightarrow aa^\dagger - a^\dagger a = 1$

$\Rightarrow aa^\dagger = a^\dagger a + 1$

$$= \frac{\hbar^2}{2m}\frac{1}{l_B^2}\left[a^\dagger a + 1 + a^\dagger a\right]$$

$$= \frac{\hbar^2}{m}\frac{1}{l_B^2}\left(a^\dagger a + \frac{1}{2}\right)$$

Define the cyclotron frequency $\omega \equiv \frac{eB}{m} = \frac{\hbar/l_B^2}{\hbar/eB}$

$$= \frac{\hbar}{m}\frac{1}{l_B^2}$$

$\Rightarrow H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$ "Harmonic oscillator" in the y direction

Center of the oscillator $y_0 = l_B^2 k_x$ (Guiding center) depends on the wave vector in the x direction

Recall chap 2.3 Harmonic oscillator

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$$

Eigen energies $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$, $n = 0, 1, 2, \ldots$

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

$\xi \equiv \sqrt{\frac{m\omega}{\hbar}}\,x$

Hermite polynomials

Orthogonality $\int_{-\infty}^{\infty} d\xi\, H_\nu(\xi)H_\mu(\xi)e^{-\xi^2} = \sqrt{\pi}\,2^\nu \nu!\,\delta_{\mu,\nu}$

⇒ The eigen energies of a charged particle in a strong magnetic field

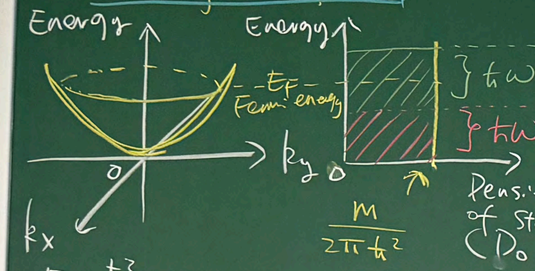
$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$, $n = 0, 1, 2, \ldots$

Wave function

$$\psi_{n,k_x}(y) = \left(\frac{e^{-ik_x x}}{\sqrt{L_x}}\right)\frac{1}{\sqrt{n!\,2^n\, l_B\sqrt{\pi}}}e^{-\frac{\xi^2}{2}}H_n(\xi), \quad \xi = \frac{(y - l_B^2 k_x)/l_B}$$

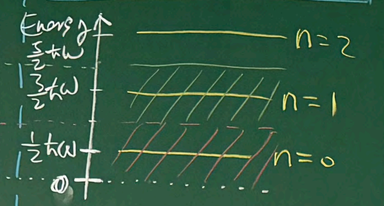
Degeneracy of Landau levels

No magnetic field



$E = \frac{\hbar^2}{2m}(k_x^2 + k_y^2)$

In strong magnetic field

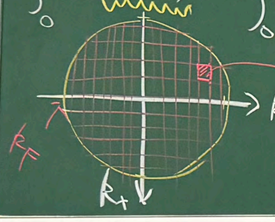


$E_n = (n+\frac{1}{2})\hbar\omega$, $n = 0, 1, 2, \ldots$

Number of states on a single Landau level
$N_L = \hbar\omega \cdot \frac{m}{2\pi\hbar^2}$

Derivation of density of states $D(E)$ (per unit area)

$$\int_0^{E_F} dE\, D(E) = \int_0^{k_F} \frac{k\,dk}{(2\pi)^2} \int_0^{2\pi} d\phi = \frac{1}{2\pi}\int k\,dk = \frac{1}{2\pi}\int \frac{m}{\hbar^2} dE$$



$E = \frac{\hbar^2}{2m}k^2 \Rightarrow dE = \frac{\hbar^2}{2m} 2k\,dk$

$\Rightarrow D(E) = \frac{m}{2\pi\hbar^2}$ Constant does not depend on E

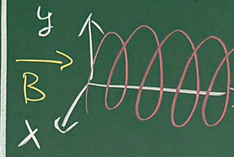
Landau degeneracy = number of states on each Landau level

$$N_L = \hbar\omega \cdot \frac{m}{2\pi\hbar^2} = \hbar \frac{eB}{m} \frac{m}{2\pi\hbar^2} = \frac{eB}{2\pi\hbar} = \frac{1}{2\pi l_B^2}$$

3D Electron gas

$\vec{k} = (k_x, k_y, k_z)$, $\vec{B} = (0, 0, B)$, $\vec{A} = (-yB, 0, 0)$

$$H = \frac{\hbar^2}{2m}\left(\vec{k} + \frac{e}{\hbar}\vec{A}\right)^2 = \frac{\hbar^2}{2m}\left[\left(k_x - \frac{y}{l_B^2}\right)^2 - \partial_y^2 + k_z^2\right]$$



= cyclotron motion in the x-y plane + (plane wave along the z direction)

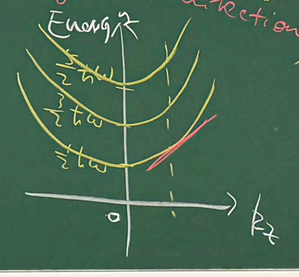
Still a good quantum number

$\Rightarrow H = \hbar\omega(a^\dagger a + \frac{1}{2}) + \frac{\hbar^2}{2m}k_z^2$

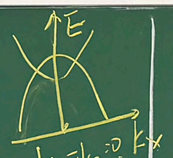
$\Rightarrow$ Eigen energies $E_{n,k_z} = (n+\frac{1}{2})\hbar\omega + \frac{\hbar^2}{2m}k_z^2$

wave function

$$\psi_{n,k_x,k_z}(y,z) = \frac{e^{ik_x x}}{\sqrt{L_x}}\left(\frac{e^{ik_z z}}{\sqrt{L_z}}\right)|\ldots\rangle$$



Topological Weyl Semimetal



$$H(\vec{k}) = \begin{bmatrix} M_k & Ak_- \\ Ak_+ & -M_k \end{bmatrix}$$, where $k_\pm \equiv k_x \pm ik_y$

$M_k \equiv M_0 - M_1(k_x^2 + k_y^2 + k_z^2)$

A, M_0, M_1 are parameters

Apply $\vec{B} = (0, 0, B)$, $\vec{A} = (-yB, 0, 0)$

$k_x^2 + k_y^2 \longrightarrow a^\dagger a + \frac{1}{2}$,

$k_+ = k_x + ik_y \longrightarrow k_x - \frac{y}{l_B} + i(-i\partial_y)$

$$= -\frac{1}{l_B}\left(\frac{y - l_B^2 k_x}{l_B} - l_B\partial_y\right) = \frac{\sqrt{2}}{l_B}a^\dagger$$

$k_- = k_x - ik_y \longrightarrow k_x - \frac{y}{l_B^2} - i(-i\partial_y)$

$$= -\frac{1}{l_B^2}\left(\frac{y - l_B^2 k_x}{l_B} + l_B\partial_y\right) = \frac{\sqrt{2}}{l_B}a$$

Minimal coupling: $\vec{k} \to \vec{k} + \frac{e}{\hbar}\vec{A}$

$H(\vec{k}) \longrightarrow H(a, a^\dagger, k_z) = \begin{bmatrix} M_a & \eta a \\ \eta a^\dagger & -M_a \end{bmatrix}_{2\times 2}$

where $M_a = M_0 - M_1 k_z^2 - \omega(a^\dagger a + \frac{1}{2})$,

$\omega = \frac{2M_1}{l_B^2}$, $\eta = \frac{\sqrt{2}A}{l_B}$, $l_B = \sqrt{\frac{\hbar}{eB}}$

How to diagonalize the Hamiltonian?

Assume the trial wave function $\begin{bmatrix} c_1|\nu-1\rangle \\ c_2|\nu\rangle \end{bmatrix}$ (some coefficients)

where $a^\dagger|\nu\rangle = \sqrt{\nu+1}|\nu+1\rangle$, $a|\nu\rangle = \sqrt{\nu}|\nu-1\rangle$

$a^\dagger a|\nu\rangle = a^\dagger\sqrt{\nu}|\nu-1\rangle = \sqrt{\nu}\sqrt{(\nu-1)+1}|\nu-1+1\rangle = \nu|\nu\rangle$

For $\nu \geq 1$

$$\begin{bmatrix} M_a & \eta a \\ \eta a^\dagger & -M_a \end{bmatrix}\begin{bmatrix} c_1|\nu-1\rangle \\ c_2|\nu\rangle \end{bmatrix} = E\begin{bmatrix} c_1|\nu-1\rangle \\ c_2|\nu\rangle \end{bmatrix}$$

↑ 投影背景墙面，注意保护，严禁书写！↑

$$\Rightarrow \begin{cases} M_a c_1|\nu-1\rangle + \eta a^\dagger c_2|\nu\rangle = \epsilon c_1|\nu-1\rangle \\ \eta a^\dagger c_1|\nu-1\rangle - M_a c_2|\nu\rangle = \epsilon c_2|\nu\rangle \end{cases}$$

where $M_a|\nu-1\rangle = \left[M_0 - M_1 k_z^2 - \omega(a^\dagger a + \frac{1}{2})\right]|\nu-1\rangle$

$= M_0 - M_1 k_z^2 - \omega(\nu - 1 + \frac{1}{2})\Big]|\nu-1\rangle$

$M_a|\nu\rangle = \left[M_0 - M_1 k_z^2 - \omega(\nu + \frac{1}{2})\right]|\nu\rangle$

$$\Rightarrow \begin{cases} (M_\nu + \frac{\omega}{2} - \epsilon)|\nu-1\rangle c_1 + \eta\sqrt{\nu}\,|\nu-1\rangle c_2 = 0 \\ \eta\sqrt{\nu}\,|\nu\rangle c_1 + \left[-M_\nu + \frac{\omega}{2} - \epsilon\right]|\nu\rangle c_2 = 0 \end{cases}$$

$M_\nu \equiv M_0 - M_1 k_z^2 - \omega\nu$

$\Rightarrow$ Matrix form

$$\begin{bmatrix} M_\nu + \frac{\omega}{2} - \epsilon & \eta\sqrt{\nu} \\ \eta\sqrt{\nu} & -M_\nu + \frac{\omega}{2} - \epsilon \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = 0 \quad \Longleftrightarrow H_\nu \psi = E\psi$$

H_ν: 2×2 Matrix

For nontrivial solution of c_1 and c_2

$$\det \begin{vmatrix} M_\nu - \frac{\omega}{2} - \epsilon & \eta\sqrt{\nu} \\ \eta\sqrt{\nu} & -M_\nu + \frac{\omega}{2} - \epsilon \end{vmatrix} = 0$$

$$\Rightarrow \epsilon^{\nu\pm}_{k_z} = \frac{\omega}{2} \pm \sqrt{M_\nu^2 + \eta^2\nu}, \quad \nu \geq 1$$

(k_z, ν)

For $\nu = 0$, trial state $\begin{bmatrix} 0 \\ |0\rangle \end{bmatrix}$ ← nothing

The lowest state of Hamonic oscillator

There is only one equation

$(-M_0 + \frac{\omega}{2} - \epsilon)|0\rangle = 0$

$\Rightarrow \epsilon = -M_0 + \frac{\omega}{2}$

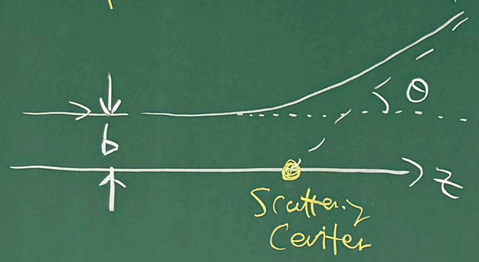
$M_{\nu=0}$

⬆ 投影背景墙面，注意保护，严禁书写！ ⬆

Chap 11 Scattering

11.1 classical scattering theory

Definition of the problem



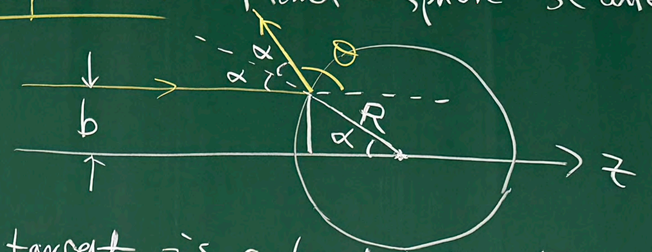
A particle with energy E incident on a scattering center with impact parameter b, and it emerges at a scattering angle Θ

Given the impact parameter, calculate the scattering angle

We can expect: The smaller the impact parameter, the greater the scattering angle

[Note]: We have assumed that the scattering center is azimuthally symmetrical, so trajectory remains in one plane

Example 11.1 Hard-sphere Scattering



The target is a hard ball of radius R, the scattering is elastic (No energy loss)

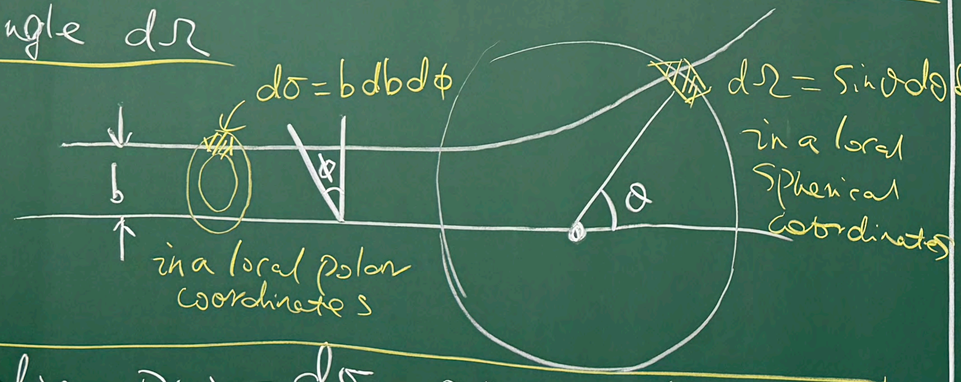
The impact parameter $b = R\sin\alpha$

Scattering angle $\Theta = \pi - 2\alpha \Rightarrow \alpha = \frac{\pi}{2} - \frac{\Theta}{2}$

$$\Rightarrow b = R\sin\left(\frac{\pi}{2} - \frac{\Theta}{2}\right) = R\cos\frac{\Theta}{2}$$

$$\Rightarrow \Theta = \begin{cases} 2\cos^{-1}\left(\frac{b}{R}\right), & \text{if } b \le R \\ 0, & \text{if } b > R \end{cases}$$

More generally, particles incident with an infinitesmal patch of cross-sectional area $d\sigma$ will scatter into an infinitesmal solid angle $d\Omega$



Refine $D(\Theta) \equiv \frac{d\sigma}{d\Omega}$ Differential (Scattering) cross-section

or $d\sigma = D(\Theta)\,d\Omega$ [11.3]

D is neither differential nor a cross-section

In terms of the impact parameter b and the azimuthal angle ϕ

$$d\sigma = b\,db\,d\phi, \quad d\Omega = \sin\Theta\,d\Theta\,d\phi$$

$$\Rightarrow D(\Theta) = \frac{b\,db\,d\phi}{\sin\Theta\,d\Theta\,d\phi} = \frac{b}{\sin\Theta}\left|\frac{db}{d\Theta}\right|$$

The absolute value is also a part of the definition, because Θ is supposed to decrease with b

Example 11.2 Hard-sphere scattering (with $\frac{d\sigma}{d\Omega}$)

$$b = R\cos\frac{\Theta}{2} \Rightarrow \frac{db}{d\Theta} = -\frac{R}{2}\sin\frac{\Theta}{2}$$

$$\Rightarrow D(\Theta) = \frac{b}{\sin\Theta}\left|\frac{db}{d\Theta}\right| = \frac{R\cos\frac{\Theta}{2}}{2\sin\Theta}\frac{R}{2}\sin\frac{\Theta}{2} = \frac{R^2}{4}$$

Here, the differential cross-section is independent of Θ

The total cross-section

$$\sigma \equiv \int D(\theta)\, d\Omega \qquad [11.7]$$

It is the total area of incident beam that is scattered by the target

For hard spons, $\sigma = \frac{R^2}{4}\int d\Omega = \frac{R^2}{4} 4\pi = \pi R^2$

which is the cross-sectional area of the sphere

Measurement A beam of incident particles with uniform intensity of luminosity $\mathcal{L}$ (number of incident particles per unit area, per unit time)

The number of particles entering the area $d\sigma$ per unit time

$dN = \mathcal{L}\, d\sigma = \mathcal{L} D(\theta) d\Omega \Rightarrow D(\theta) = \frac{1}{\mathcal{L}}\frac{dN}{d\Omega}$

We count the number dN received by a detector into a solid angle $d\Omega$ per unit time

11.1.2 Quantum Scattering theory

Everything is about wave function

Incident plane wave $\psi(z) = Ae^{ikz}$ $\quad k \equiv \frac{\sqrt{2mE}}{\hbar}$

Scattering spherical wave $\sim \frac{e^{ikr}}{r}$

(Assuming target is azimuthally symmetrical)

$$\psi(r,\theta) \simeq A\left\{e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right\} \text{ for large } r$$

The factor $\frac{1}{r}$ is to make sure that $|\psi|^2$ goes like $\frac{1}{r^2}$ to conserve probability

$f(\theta)$ Scattering amplitude = is a function of θ (and also ϕ)

The problem now turns to determine $f(\theta)$

The probability that the incident particle, at speed v, through the area $d\sigma$, in time period dt, is $dp = |\psi_{incident}|^2 dV = |A|^2 v\, dt\, d\sigma$

which is equal to the probability that the particle scatters into the corresponding solid angle $d\Omega$

$$dp = |\psi_{scattered}|^2 dV = \frac{|A|^2|f|^2}{r^2} v\, dt\, r^2 d\Omega$$
$$= |A|^2 |f|^2 v\, dt\, d\Omega$$

$\Rightarrow |A|^2 v\, dt\, d\sigma = |A|^2 |f|^2 v\, dt\, d\Omega$

$\Rightarrow d\sigma = |f|^2 d\Omega$

$\Rightarrow$ Experimentally measurable $D(\theta) = \frac{d\sigma}{d\Omega} = |f(\theta)|^2$ ← To be calculated by two approaches ① Partial wave ② Born approximation

11.2 Partial wave analysis 分波法

11.2.1 Formalism

Chap 4 $\Rightarrow$ For a spherically symmetrical potential $V(r)$ (e.g. Hydrogen atom), the wave function

$$\psi(r,\theta,\phi) = R(r) Y_l^m(\theta,\phi)$$

where Y_l^m spherical harmonics

$u(r) \equiv rR(r)$ satisfies the radial equation

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

① Radiation Zone

At very large r, $V(r) \to 0$, $\frac{1}{r^2} \to 0$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} \simeq Eu \Rightarrow \frac{d^2u}{dr^2} \simeq -k^2 u \qquad k \equiv \frac{\sqrt{2mE}}{\hbar}$$

↑ 投影背景墙面，注意保护，严禁书写！↑

Assume $u = e^{\lambda r} \Rightarrow \lambda^2 e^{\lambda r} = -k^2 e^{\lambda r}$

$\Rightarrow \lambda = \pm ik \Rightarrow$ General solution $u(r) = Ce^{ikr} + De^{-ikr}$ (Outgoing / Incoming)

For scattered wave $D = 0$

Then, at very large r, $R(r) = \frac{e^{ikr}}{r}$

② Intermediate region

$V(r) \to 0$ only

$\Rightarrow \frac{d^2u}{dr^2} - \frac{l(l+1)}{r^2}u = -k^2 u$

$\Rightarrow \frac{d^2u}{dr^2} + \left[k^2 - \frac{l(l+1)}{r^2}\right]u = 0$ [11.17]

and the general solution is a linear combination of Spherical Bessel functions (Neumann)

$rR(r) \equiv u(r) = Ar j_l(kr) + Br n_l(kr)$ [11.18]

"Hack QM II" — 1st Kind — 2nd Kind

j_l Sin-like, n_l Cos-like

But, we need e^{ikr}, so we introduce the Spherical Hankel functions

$h_l^{(1)}(x) \equiv j_l(x) + in_l(x)$, $h_l^{(2)} \equiv j_l(x) - in_l(x)$

Tab. 11.1 $\Rightarrow \begin{cases} h_l^{(1)}(kr) \to \frac{e^{ikr}}{r} \\ h_l^{(2)}(kr) \to \frac{e^{-ikr}}{r} \end{cases}$ at larger r

So for outgoing wave, we need Spherical Hankel function of the 1st kind $R(r) \sim h_l^{(1)}(kr)$

Then, the wave function outside the scattering region (in the intermediate region $V(r) = 0$)

$\psi(r,\theta,\phi) = A\left\{e^{ikz} + \sum_{l,m} C_{lm} h_l^{(1)}(kr) Y_l^m(\theta,\phi)\right\}$ [11.21]

Incident — Scattered

Also, we assume a spherically symmetrical potential so ψ does not depend on ϕ, or $m = 0$ in Y_l^m

[4.27] [4.32] $Y_l^0(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta)$ [11.22]

(P_l: the lth Legendre polynomial)

For convenience, we define

$C_{l0} \equiv i^{l+1} k \sqrt{4\pi(2l+1)}\, a_l$

[11.21] + [11.22] $\Rightarrow$

$\psi(\theta,r) = A\left\{e^{ikz} + \sum_l i^{l+1} k\sqrt{4\pi(2l+1)}\, a_l h_l^{(1)}(kr)\sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta)\right\}$

$= A\left\{e^{ikz} + k\sum_{l=0}^{\infty} i^{l+1}(2l+1) a_l h_l^{(1)}(kr) P_l(\cos\theta)\right\}$ [11.23]

(a_l: the lth partial wave amplitude)

Tab. 11.1 $\Rightarrow h_l^{(1)} \to (-i)^{l+1}\frac{e^{ikr}}{kr}$

[11.23] $\Rightarrow \psi(r,\theta) = A\left\{e^{ikz} + k\sum_{l=0}^{\infty}(2l+1)a_l \frac{e^{ikr}}{kr} P_l(\cos\theta)\right\}$

$= A\left\{e^{ikz} + \frac{e^{ikr}}{r}\sum_{l=0}^{\infty}(2l+1)a_l P_l(\cos\theta)\right\}$ (a_l: unknown)

$\equiv A\left\{e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right\}$, where $f(\theta) = \sum_{l=0}^{\infty}(2l+1)a_l P_l(\cos\theta)$

The differential cross-section

$D(\theta) = |f(\theta)|^2 = \left(\sum_{l=0}^{\infty}(2l+1)a_l^* P_l(\cos\theta)\right)\left(\sum_{l'=0}^{\infty}(2l'+1)a_{l'} P_{l'}(\cos\theta)\right)$

$= \sum_l \sum_{l'} (2l+1)(2l'+1)\, a_l^* a_{l'} P_l(\cos\theta) P_{l'}(\cos\theta)$

The total cross-section $\sigma = \int D(\theta)\, d\Omega$

$\sigma = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \sum_{l,l'} (2l+1)(2l'+1)\, a_l^* a_{l'} P_l(\cos\theta) P_{l'}(\cos\theta)$

($\int_0^{2\pi} d\phi = 2\pi$; $\int_0^{\pi} d\theta \sin\theta = -\int_1^{-1} d(\cos\theta)$)

where $\int_{-1}^{1} P_l(x) P_{l'}(x)\, dx = \frac{2}{2l+1}\delta_{l,l'}$ ($x \equiv \cos\theta$)

$\Rightarrow \sigma = \sum_l \sum_{l'} (2l+1)(2l'+1)\, a_l^* a_{l'} 2\pi \frac{2}{2l+1}\delta_{l,l'}$

$= \sum_l (2l+1)\, |a_l|^2 4\pi$ (a_l to be determined)

11.2.2 Spherical wave expansion

① Expand e^{ikz} into spherical waves (incident plane wave)

② Match boundary condition to determine a_l

SUSTech

↑ 投影背景墙面，注意保护，严禁书写！↑

Chap 11 Scattering

11.2 Partial wave analysis

$$\psi(r,\theta) = A\left\{e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right\}$$

e^{ikz}: Incident plane wave; $f(\theta)\frac{e^{ikr}}{r}$: Outgoing spherical wave

Differential Scattering Cross-section $D(\theta) = |f(\theta)|^2$ ← Measurable

$$f(\theta) = \sum_{l=0}^{\infty}(2l+1)a_l P_l(\cos\theta)$$

a_l: Partial-wave amplitude

$$\Rightarrow D(\theta) = \sum_{l,l'}(2l+1)(2l'+1)a_l^* a_{l'} P_l(\cos\theta)P_{l'}(\cos\theta)$$

Total cross-section $\sigma = 4\pi\sum_l (2l+1)|a_l|^2$

11.2.2 Strategy (Spherical wave expansion)

We need to determine a_l by matching the solution of Schrödinger eqn. with $V(r)\neq 0$ (Intermediate region) to Eq. [11.23], using boundary conditions

We need to express e^{ikz} in terms of Spherical waves (Spherical wave expansion)

Rayleigh's formula ("Mathematical Methods for Physicists" Arfken & Weber)

$$e^{ikz} = \sum_{l=0}^{\infty} i^l (2l+1)\hat{j}_l(kr)P_l(\cos\theta) \quad [11.28]$$

[11.23] + [11.28] ⇒

$$\psi(r,\theta) = A\left\{e^{ikz} + k\sum_{l=0}^{\infty} i^{l+1} a_l h_l^{(1)}(kr)P_l(\cos\theta)\right\}$$

$$= A\left\{\sum_{l=0}^{\infty} i^l(2l+1)\hat{j}_l(kr)P_l(\cos\theta) + \sum_{l=0}^{\infty} i^{l+1}(2l+1)k a_l h_l^{(1)}(kr)P_l(\cos\theta)\right\}$$

$$= A\sum_{l=0}^{\infty} i^l(2l+1)\left[\hat{j}_l(kr) + ik a_l h_l^{(1)}(kr)\right]P_l(\cos\theta) \quad [11.29]$$

Next step: Boundary conditions

Example 11.3 Quantum Hard sphere

$$V(r) = \begin{cases}\infty, & r \le R \text{ (Radius of sphere)}\\ 0, & r > R\end{cases}$$

Boundary conditions $\psi(r=R,\theta) = 0$ (Legendre polynomials)

[11.29] ⇒

$$\sum_{l=0}^{\infty} i^l(2l+1)\left[\hat{j}_l(kR) + ik a_l h_l^{(1)}(kR)\right]P_l(\cos\theta) = 0 \quad [11.32]$$

using $\int_{-1}^{1} dx\, P_l(x)P_{l'}(x) = \frac{2\delta_{l,l'}}{2l+1}$

$$\int_0^{2\pi} d\theta \sin\theta\, P_{l'}(\cos\theta)\,[11.32] = 0$$

$$\Rightarrow \sum_{l=0}^{\infty} i^l(2l+1)\left[\hat{j}_l(kR) + ik a_l h_l^{(1)}(kR)\right]\int_0^{\pi} d\theta \sin\theta P_{l'}(\cos\theta)P_l(\cos\theta) = 0$$

$$\Rightarrow \sum_{l=0}^{\infty} 2\delta_{l,l'} i^{-l}\left[\hat{j}_l(kR) + ik a_l h_l^{(1)}(kR)\right] = 0$$

$$\Rightarrow \hat{j}_{l'}(kR) + ik a_{l'} h_{l'}^{(1)}(kR) = 0$$

$$\Rightarrow a_l = i\frac{\hat{j}_l(kR)}{k\, h_l^{(1)}(kR)}$$

[11.27] ⇒ (Exact Result)

$$\sigma = 4\pi\sum_{l=0}^{\infty}(2l+1)|a_l|^2 = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\left|\frac{\hat{j}_l(kR)}{h_l^{(1)}(kR)}\right|^2 \quad [11.34]$$

Low-energy (Long-wave) limit

$kR \ll 1$ or $\frac{2\pi}{\lambda}R \ll 1 \Rightarrow \lambda \gg 2\pi R$

(k: wave vector, $k = \sqrt{2mE}/\hbar$; λ: wave length; R: sphere radius)

$$\frac{\hat{j}_l(z)}{h_l^{(1)}(z)} \xrightarrow{z\ll 1} z^{2l+1} \quad \text{"Hack QM II"}$$

For $l=0$, $z \sim 0.1$

$l=1$, $z^3 \sim 0.001$ (Much smaller)

⇒ Keep only $l=0$ term in Eq. [11.34]

[11.34] $kR \ll 1 \longrightarrow \sigma \approx \frac{4\pi}{k^2}\left|\frac{j_0(kR)}{h_0^{(1)}(kR)}\right|^2$

Tab. 11.1 $\Rightarrow h_0^{(1)}(x) \longrightarrow -i\frac{e^{ix}}{x}$

$e^{ix} = \cos x + i\sin x$

$j_0(x) = \frac{h_0^{(1)} + h_0^{(2)}}{2} = \frac{-ie^{ix} + ie^{-ix}}{2x} = \frac{\sin x}{x}$

$\Rightarrow \sigma \approx \frac{4\pi}{k^2}\left|\frac{\frac{\sin(kR)}{kR}}{-i\frac{e^{ikR}}{kR}}\right|^2 = 4\pi\frac{\sin^2(kR)}{k^2}$

$kR \to 0 \longrightarrow 4\pi\frac{(kR)^2}{k^2} = 4\pi R^2$ Solid angle

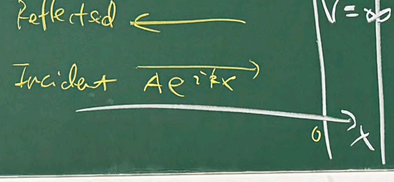
long wave

Scatters Center

11.3 phase shift 相移

Alternative way to express a_ℓ

Hard-wall reflection



$\psi(0)=0 \Rightarrow A = -B$

$\psi(x) = A(e^{ikx} - e^{-ikx})$

or it can be written as

$\psi(x) = A(e^{-ikx} + e^{i\pi}e^{-ikx})$

We can view the change of amplitude as a phase shift.

For partial-wave amplitude a_ℓ (phase shift)

$a_\ell = \frac{1}{2ik}(e^{2i\delta_\ell} - 1) = \frac{1}{k}e^{i\delta_\ell}\sin(\delta_\ell)$

[11.25] $\Rightarrow f(\theta) = \sum_{\ell=0}^{\infty}(2\ell+1)a_\ell P_\ell(\cos\theta) = \frac{1}{k}\sum_\ell(2\ell+1)e^{i\delta_\ell}\sin(\delta_\ell)P_\ell(\cos\theta)$

[11.27] $\Rightarrow \sigma = 4\pi\sum_\ell(2\ell+1)|a_\ell|^2 = \frac{4\pi}{k^2}\sum_{\ell=0}(2\ell+1)\sin^2\delta_\ell$

11.4 Green function and Born approximation

11.4.1 Integral form of Schrödinger eqn.

Tim-independent Schrödinger eqn.

$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$ can be written as

$(-\frac{\hbar^2}{2m}\nabla^2 - E)\psi = -V\psi$

$\Rightarrow (\nabla^2 + \frac{2mE}{\hbar^2})\psi = \frac{2mV}{\hbar^2}\psi \Rightarrow (\nabla^2+k^2)\psi = Q$

where $k \equiv \frac{\sqrt{2mE}}{\hbar}$, $Q \equiv \frac{2m}{\hbar^2}V\psi$

Inhomogeneous term

Superficial ($Q \neq 0$) form of Helmholtz eqn.

Suppose we can find a function $G(\vec{r})$ that solves the Helmholtz eqn. with a delta "source"

$(\nabla^2+k^2)G(\vec{r}) = \delta^3(\vec{r})$ [11.52] $\delta^3(\vec{r}) \equiv \delta(x)\delta(y)\delta(z)$

then we can express ψ as an integral

$\psi(\vec{r}) = \int G(\vec{r}-\vec{r}_0)\,Q(\vec{r}_0)\,d^3\vec{r}_0$

Convolution; Scattering potential

[Proof]: $(\nabla^2+k^2)\psi(\vec{r}) = (\nabla^2+k^2)\int G(\vec{r}-\vec{r}_0)Q(\vec{r}_0)d^3\vec{r}_0$

$= \int(\nabla^2+k^2)G(\vec{r}-\vec{r}_0)\,Q(\vec{r}_0)\,d^3\vec{r}_0$

[11.52] $\Rightarrow = \int\delta^3(\vec{r}-\vec{r}_0)\,Q(\vec{r}_0)\,d^3\vec{r}_0$

$= Q(\vec{r})$ //

$G(\vec{r})$ Green's function for the Helmholtz equation.

In general, the Green's function for a differential equation represents the "response" to a delta source

↑ 投影背景墙面，注意保护，严禁书写！↑

Our task = Solve $G(\vec{r})$

[Trick]: Fourier transformation, which turns the differential eqn. into algebraic eqn.

Let $G(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \int e^{i\vec{s}\cdot\vec{r}}\, g(\vec{s})\, d^3\vec{s}$ [11.54]

(could be different in different books)

Then [11.52] $\Rightarrow$

$$\delta^3(\vec{r}) = (\nabla^2 + k^2)\, G(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \int (\nabla^2 + k^2) e^{i\vec{s}\cdot\vec{r}}\, g(\vec{s})\, d^3\vec{s}$$

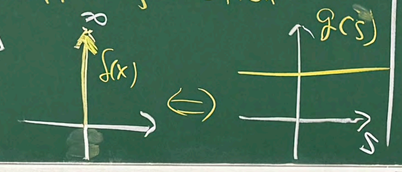
where $\nabla^2 e^{i\vec{s}\cdot\vec{r}} = \nabla\cdot\nabla e^{i\vec{s}\cdot\vec{r}} = i\nabla\cdot\vec{s}\, e^{i\vec{s}\cdot\vec{r}}$ (Divergence, Gradient)

$= (i)^2 \vec{s}\cdot\vec{s}\, e^{i\vec{s}\cdot\vec{r}} = -s^2 e^{i\vec{s}\cdot\vec{r}}$

and use the definition of the delta function

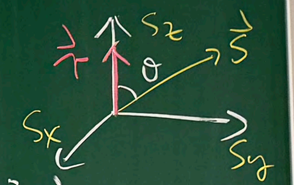
$$\delta^3(\vec{r}) = \frac{1}{(2\pi)^3} \int e^{i\vec{s}\cdot\vec{r}}\, d^3\vec{s} \quad [2.144]$$

To make sure $\int \delta^3(\vec{r})\, d^3\vec{r} = 1$



$$\Rightarrow \frac{1}{(2\pi)^3} \int e^{i\vec{s}\cdot\vec{r}}\, d^3\vec{s} = \frac{1}{(2\pi)^{3/2}} \int (-s^2 + k^2) e^{i\vec{s}\cdot\vec{r}}\, g(\vec{s})\, d^3\vec{s}$$

$$\Rightarrow g(\vec{s}) = \frac{1}{(2\pi)^{3/2}(k^2 - s^2)}$$



[11.54] $\Rightarrow$

$$G(\vec{r}) = \frac{1}{(2\pi)^3} \int e^{i\vec{s}\cdot\vec{r}} \frac{1}{k^2 - s^2}\, d^3\vec{s}$$

$$= \frac{1}{(2\pi)^3} \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \int_0^{\infty} ds\, s^2 e^{i\vec{s}\cdot\vec{r}} \frac{1}{k^2 - s^2}$$

where $\vec{s}\cdot\vec{r} = sr\cos\theta$

$$\Rightarrow G(\vec{r}) = \frac{1}{(2\pi)^3} 2\pi \int_0^{\infty} ds\, s^2 \frac{1}{k^2 - s^2} \int_0^{\pi} d\theta \sin\theta\, e^{isr\cos\theta}$$

where $\int_0^{\pi} d\theta \sin\theta\, e^{isr\cos\theta} = \int_{-1}^{1} d(\cos\theta)\, e^{isr\cos\theta}$

$$= \frac{1}{isr} e^{isr\cos\theta}\Big|_{\cos\theta=-1}^{1} = \frac{1}{isr}\left(e^{isr} - e^{-isr}\right)$$

$$\Rightarrow G(\vec{r}) = \frac{1}{(2\pi)^2} \int_0^{\infty} ds\, s^2 \frac{1}{k^2 - s^2} \frac{1}{isr}\left(e^{isr} - e^{-isr}\right)$$

$$= -\frac{i}{4\pi^2 r} \int_0^{\infty} \frac{s}{k^2 - s^2}\left(e^{isr} - e^{-isr}\right) ds \quad [11.60]$$

which can be written as (Analytic continuation)

$$G(\vec{r}) = (-)\frac{i}{8\pi^2 r} \int_{-\infty}^{\infty} ds\, \frac{s\left(e^{isr} - e^{-isr}\right)}{k^2 - s^2 + i0^+}$$

Integral of even function: $\int_0^{\infty} = \frac{1}{2}\int_{-\infty}^{\infty}$

Pos. infinitesmal to prevent the divergence of the integrand

$$\Rightarrow G(\vec{r}) = \frac{i}{8\pi^2 r} \int_{-\infty}^{\infty} \frac{s\left(e^{isr} - e^{-isr}\right)}{(s + k + i0^+)(s - k - i0^+)}$$

where we can check

$$(s + k + i0^+)(s - k - i0^+) = (s + k)(s - k) - i0^+(s + k) + i0^+(s - k)$$

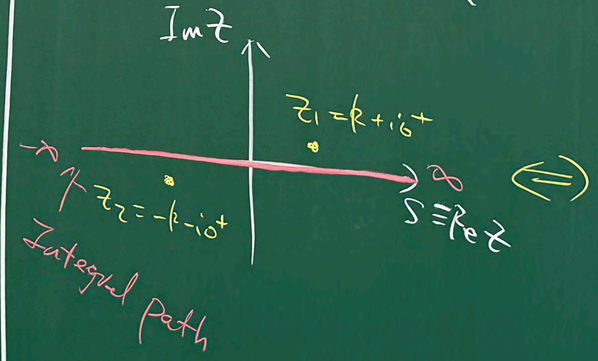
$$= (s + k)(s - k) - i0^+ 2k = (s + k)(s - k) - i0^+$$

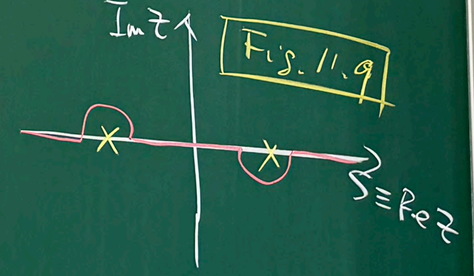
[11.60] becomes

$$G(\vec{r}) = \frac{i}{8\pi^2 r}\left[\underbrace{\int_{-\infty}^{\infty} \frac{s e^{isr} ds}{(s - k - i0^+)(s + k + i0^+)}}_{I_1} - \underbrace{\int_{-\infty}^{\infty} \frac{s e^{-isr} ds}{(s - k - i0^+)(s + k + i0^+)}}_{I_2}\right]$$

$$\equiv \frac{i}{8\pi r}(I_1 - I_2)$$

So we have two poles $\begin{cases} z_1 = k + i0^+ \\ z_2 = -k - i0^+ \end{cases}$





↑ 投影背景墙面，注意保护，严禁书写！↑

11.4 Green function technique and Born approximation

Suppose $(\nabla^2+k^2)G(\vec{r}) = \delta(\vec{r})$ ← delta source

$\Rightarrow \psi(\vec{r}) = \int G(\vec{r}-\vec{r}_0)\, Q(\vec{r}_0)\, d^3\vec{r}_0$

where $k \equiv \frac{\sqrt{2mE}}{\hbar}$, $Q(\vec{r}) \equiv \frac{2m}{\hbar^2} V(\vec{r})\psi(\vec{r})$

(Scattering) potential

Our task: Find $G(\vec{r})$

Fourier transformation $G(\vec{r}) = \frac{1}{(2\pi)^{3/2}}\int e^{i\vec{s}\cdot\vec{r}} g(\vec{s})\, d^3\vec{s}$

where $g(\vec{s}) = \frac{1}{(2\pi)^{3/2}} \frac{1}{(k^2-s^2)}$

$\Rightarrow G(\vec{r}) = \frac{1}{(2\pi)^3}\int e^{i\vec{s}\cdot\vec{r}} \frac{1}{k^2-s^2} d^3\vec{s}$ ($s \equiv |\vec{s}|$)

Analytic continuation ↓

$= \frac{1}{8\pi^3 r}\left[\underbrace{\int_{-\infty}^{\infty} \frac{s e^{isr} ds}{(s-k-i0^+)(s+k+i0^+)}}_{I_1} - \underbrace{\int_{-\infty}^{\infty} \frac{s e^{-isr} ds}{(s-k-i0^+)(s+k+i0^+)}}_{I_2} \right]$

Integrals of ϕ and θ

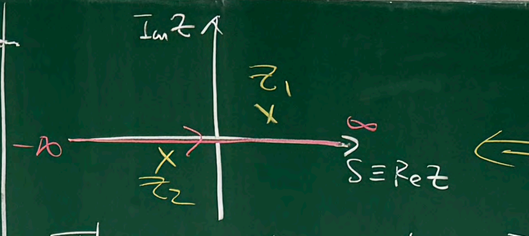


Fig 11.9

There are two poles $z_1 = k+i0^+$, $z_2 = -k-i0^+$

The idea is to turn $\int_{-\infty}^{\infty} ds$ into an contour integral on the complex plane ($S \equiv Re z$, $Im z$), then we can use the Residue theorem (Cauchy's integral formula)

$$\oint \frac{f(z)}{(z-z_0)} dz = i2\pi f(z_0)$$

Pole enclosed by the contour

We need to choose a contour so that the integrand goes to zero as z goes to infinity

---

$I_1 + \underbrace{\text{Imaginary path}}_{\text{to } 0} = I_1$

① $I_1 \equiv \int_{-\infty}^{\infty} ds \frac{s e^{isr}}{(s-k-i0^+)(s+k+i0^+)}$

If positive ↓

$e^{isr} \longrightarrow e^{i(Re z + i Im z)r} = e^{iRe z\, r} e^{-Im z\, r}$

So if $Im z$ is positive, the integrand goes to zero as $Im z \to \infty$, which means that the Contour is on the upper plane.

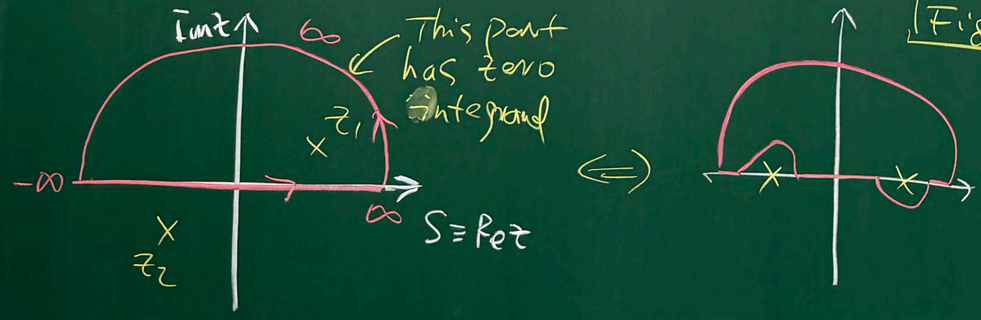


Fig 11.10 (R)

$I_1 = \int_{-\infty}^{\infty} ds \ldots \longrightarrow \oint dz$ on the upper plane

On the upper plane, there is only one pole z_1

$I_1 = \oint \underbrace{\frac{z e^{izr}}{(z+k+i0^+)[z-(k+i0^+)]}}_{f(z)} = i2\pi f(z_1)$ ($z_1 = k+i0^+$)

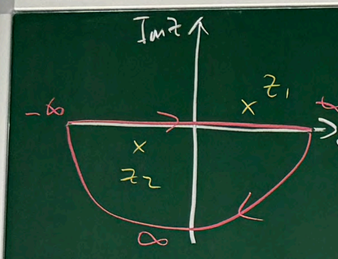
$= i2\pi \frac{(k+i0^+)e^{i(k+i0^+)r}}{k+i0^+ + k+i0^+} = i2\pi \frac{(k+i0^+)e^{ikr}e^{0}}{2(k+i0^+)}$

$= i\pi e^{ikr}$

② $I_2 = \int_{-\infty}^{\infty} \frac{s e^{-isr} ds}{[s-(k+i0^+)][s-(-k-i0^+)]}$

where $e^{-isr} \longrightarrow e^{-i(Re z + i Im z)r} = e^{-iRe z\, r} e^{Im z\, r}$ (has to be negative)

$Im z$ has to be negative, so that the integrand $\to 0$ as $z \to \infty$, so the Contour is on the lower plane



$\Longleftrightarrow$

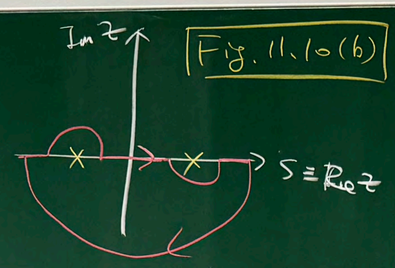


Fig. 11.10(b)

The contour is defined "right-handed", so there is an extra minus sign

$$I_2 = \int_{-\infty}^{\infty} ds \cdots \longrightarrow -\oint dz \underbrace{\frac{z e^{-izr}}{z-(k+i0^+)}}_{f(z)} \frac{1}{z-z_2}$$

Use the Residue theorem

$$I_2 = -i2\pi f(z_2) = -i2\pi \frac{(-k-i0^+)\, e^{-i(-k-i0^+)r}}{-k-i0^+-(k+i0^+)}$$

$$= -i2\pi \frac{(-k-i0^+)e^{-ikr}e^{0}}{2(-k-i0^+)} = -i\pi e^{-ikr}$$

[11.61] $\Rightarrow$ $G(\vec{r}) = \frac{z}{8\pi^2 r}(I_1 - I_2) = \frac{z}{8\pi^2 r}(i\pi e^{ikr} + i\pi e^{ikr})$

$$\Rightarrow G(\vec{r}) = -\frac{e^{ikr}}{4\pi r}$$ looks like a spherical wave decaying from the origin

This is the Green function for the Helmholtz equation

Also, the homogeneous Helmholtz equation. ($Q \neq 0$)

$$(\nabla^2 + k^2) G_0(\vec{r}) = 0 \leftarrow Q(\vec{r}) = 0 \quad [11.66]$$

Definition of Green function $(\nabla^2 + k^2) G(\vec{r}) = \delta^3(\vec{r})$ [11.52]

[11.52] + [11.66] $\Rightarrow (\nabla^2 + k^2)\underline{[G_0(\vec{r}) + G(\vec{r})]} = \delta(\vec{r})$

According to [11.53]

$$\psi(\vec{r}) = \int G(\vec{r}-\vec{r}_0) Q(\vec{r}_0) d^3\vec{r}_0$$

$$= \int [G_0(\vec{r}-\vec{r}_0) + G(\vec{r}-\vec{r}_0)] Q(\vec{r}_0) d^3\vec{r}_0$$

$$= \underbrace{\int G_0(\vec{r}-\vec{r}_0) Q(\vec{r}_0) d^3\vec{r}_0}_{\text{Which is the wave function } \psi_0 \text{ for free electron}} + \int G(\vec{r}-\vec{r}_0) Q(\vec{r}_0) d^3\vec{r}_0$$

because $(\nabla^2 + k^2) \int G_0(\vec{r}-\vec{r}_0) Q(\vec{r}_0) d^3\vec{r}_0 = 0$

Definition of ψ_0 (plane wave for free electron)

$\uparrow$ $V(\vec{r}) = 0$, $Q(\vec{r}) = 0$

$$\Rightarrow \psi(\vec{r}) = \psi_0(\vec{r}) + \int G(\vec{r}-\vec{r}_0) Q(\vec{r}_0) d^3\vec{r}_0$$

G: $-\frac{e^{ik|\vec{r}-\vec{r}_0|}}{4\pi|\vec{r}-\vec{r}_0|}$; Q: $\frac{2m}{\hbar^2} V(\vec{r}_0)\psi(\vec{r}_0)$

$$\Rightarrow \psi(\vec{r}) = \psi_0(\vec{r}) - \int \frac{e^{ik|\vec{r}-\vec{r}_0|}}{4\pi|\vec{r}-\vec{r}_0|} \frac{2m}{\hbar^2} V(\vec{r}_0)\psi(\vec{r}_0) d^3\vec{r}_0$$

$$\Rightarrow \boxed{\psi(\vec{r}) = \psi_0(\vec{r}) - \frac{m}{2\pi\hbar^2} \int d^3\vec{r}_0 \frac{e^{ik|\vec{r}-\vec{r}_0|}}{|\vec{r}-\vec{r}_0|} V(\vec{r}_0)\psi(\vec{r}_0)}$$

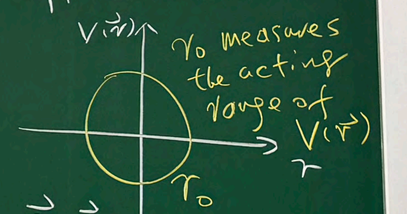
Integral form of Schrödinger equation [11.67]

It is a self-consistent iteration equation

If we know ψ, we know ψ

11.4.2 The First-order Born approximation

$$|\vec{r}-\vec{r}_0|^2 = r^2 + r_0^2 - 2\vec{r}\cdot\vec{r}_0 \approx r^2\left(1 - 2\frac{\vec{r}\cdot\vec{r}_0}{r^2}\right)$$



$$|\vec{r}-\vec{r}_0| \approx r\sqrt{1 - 2\frac{\vec{r}\cdot\vec{r}_0}{r^2}} \approx r\left(1 - \frac{1}{2}2\frac{\vec{r}\cdot\vec{r}_0}{r^2}\right)$$

$$= r - \hat{r}\cdot\vec{r}_0$$ ($\hat{r}$: unit vector of $\vec{r}$)

Let $\vec{k} \equiv k\hat{r}$, $e^{ik|\vec{r}-\vec{r}_0|} = e^{ikr} e^{-i\vec{k}\cdot\vec{r}_0}$

then $\frac{e^{ik|\vec{r}-\vec{r}_0|}}{|\vec{r}-\vec{r}_0|} \approx \frac{e^{ikr}}{r} e^{-i\vec{k}\cdot\vec{r}_0}$ ($|\vec{r}-\vec{r}_0| \approx r$)

Incident wave $\psi_0(\vec{r}) = A e^{ikz}$ [11.74]

[11.67] + [11.73] + [11.74] $\Rightarrow$

$$\psi(\vec{r}) = A e^{ikz} - \frac{m}{2\pi\hbar^2} \frac{e^{ikr}}{r} \int e^{-i\vec{k}\cdot\vec{r}_0} V(\vec{r}_0)\psi(\vec{r}_0) d^3\vec{r}_0$$

↑ 投影背景墙面，注意保护，严禁书写！↑

Which can be written as

$$\psi(\vec{r}) \equiv A\left[e^{ikz} + \frac{e^{ikr}}{r} f(\theta)\right]$$

where $f(\theta) \equiv -\frac{m}{2\pi\hbar^2 A}\int e^{-i\vec{k}\cdot\vec{r}_0} V(\vec{r}_0)\,\psi(\vec{r}_0)\,d^3\vec{r}_0$

Scattering amplitude

Born approximation $\psi(\vec{r}_0) \longrightarrow \psi_0(\vec{r}_0) = Ae^{ikz_0} \equiv Ae^{i\vec{k}'\cdot\vec{r}_0}$

where $\vec{k}' \equiv k\hat{z}$ along the z direction

$$\Rightarrow f(\theta) = -\frac{m}{2\pi\hbar^2 A}\int e^{-i\vec{k}\cdot\vec{r}_0} V(\vec{r}_0)\,\psi_0(\vec{r}_0)\,d^3\vec{r}_0$$

$$\Rightarrow \boxed{f(\theta) = -\frac{m}{2\pi\hbar^2}\int e^{i(\vec{k}'-\vec{k})\cdot\vec{r}_0} V(\vec{r}_0)\,d^3\vec{r}_0}$$

For $r \gg r_0$, and under the Born approximation (11.79)

Scattered $\vec{k} = k\hat{r}$; Incident $\vec{k}' \equiv k\hat{z}$; $\vec{\kappa} \equiv \vec{k}' - \vec{k}$ Kappa

Low-energy (long-wave) scattering

$$e^{i(\vec{k}'-\vec{k})\cdot\vec{r}_0} \approx 1$$

$k = \frac{2\pi}{\lambda}$ $\quad \lambda \gg r_0$

$$\Rightarrow f(\theta) \approx -\frac{m}{2\pi\hbar^2}\int V(\vec{r})\,d^3\vec{r}$$

Example 11.4 low-energy soft sphere (radius of sphere)

$$V(\vec{r}) = \begin{cases} V_0, & \text{if } r \le a \\ 0, & \text{if } r > a \end{cases}$$

[Solution]:

$$f(\theta) = -\frac{m}{2\pi\hbar^2}\int_0^a V_0\,dr\,r^2\int_0^\pi \sin\theta\,d\theta\int_0^{2\pi} d\phi = -\frac{m}{2\pi\hbar^2}V_0\frac{4\pi}{3}a^3$$

Differential cross-section $\frac{d\sigma}{d\Omega} \equiv D(\theta) \equiv |f(\theta)|^2$

Total cross-section $\sigma \equiv \int D(\theta)\,d\Omega$

Spherically symmetrical potential $V(\vec{r}) = V(r)$

Not necessarily at low energy

Define $\vec{\kappa} = \vec{k}' - \vec{k}$ Momentum transfer between the incident and scattered waves

[Trick] = Let the polar axis of $\vec{r}_0$ lie along $\vec{\kappa}$, so

$$(\vec{k}'-\vec{k})\cdot\vec{r}_0 = \kappa r_0\cos\theta_0$$

$$\Rightarrow f(\theta) \approx -\frac{m}{2\pi\hbar^2}\int r_0^2\,dr_0\int_0^\pi d\theta_0\sin\theta_0\,e^{i\kappa r_0\cos\theta_0}\int_0^{2\pi} d\phi_0\,V(r)$$

$[11.59] \Rightarrow \frac{2\sin\kappa r_0}{\kappa r_0}$ $\qquad 2\pi$

$$\Rightarrow \boxed{f(\theta) \approx -\frac{2m}{\hbar^2\kappa}\int_0^\infty r\,V(r)\sin(\kappa r)\,dr}$$

For spherically symmetrical $V(r)$, where the θ dependence lies in $\kappa \equiv 2k\sin\frac{\theta}{2}$

Example 11.5 Yukawa potential $V(r) = \beta\frac{e^{-\mu r}}{r}$, μ and β are parameters

$$f(\theta) = -\frac{2m}{\hbar^2\kappa}\int_0^\infty r\beta\frac{e^{-\mu r}}{r}\sin(\kappa r)\,dr = -\frac{2m\beta}{\hbar^2\kappa}\int_0^\infty e^{-\mu r}\sin(\kappa r)\,dr$$

$$= -\frac{2m\beta}{\hbar^2(\mu^2+\kappa^2)}$$

$\kappa \equiv 2k\sin\frac{\theta}{2}$, $k \equiv \frac{\sqrt{2mE}}{\hbar}$

Example 11.6 Rutherford scattering ($\beta = \frac{q_1 q_2}{4\pi\varepsilon_0}$, $\mu = 0$ in Yukawa)

(Coulomb potential of two point charges)

$$f(\theta) = -\frac{2m\beta}{\hbar^2(\mu^2+\kappa^2)} = -\frac{q_1 q_2}{16\pi\varepsilon_0 E\sin^2\frac{\theta}{2}}$$

($\mu = 0$)

11.4.3. Born series

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \int g(\vec{r}-\vec{r}_0)V(\vec{r}_0)\psi_0(\vec{r})\,d^3\vec{r}_0$$

which can be simplified as

$$\Rightarrow \psi = \psi_0 + \int gV\psi = \psi_0\int gV[\psi_0 + \int gV\psi]$$

$$= \psi_0 + \int gV(\psi_0 + \int gV(\psi_0 + \int gV\psi]] + \cdots$$

$$= \psi_0 + \int gV\psi_0 + \iint gVgV\psi_0 + \iiint gVgVgV\psi_0 + \cdots$$

Born approximation

Feynman Diagrams

$$\psi = \psi_0 + \psi_0 + \psi_0 + \cdots$$

THE END

↑ 投影背景墙面，注意保护，严禁书写！↑

Recap of chaps 9-12

Fundamental principles, ideas, techniques, results

[Disclaimer]: These probably have nothing to do with the final exam.

Chap 9 Time-dependent perturbation theory

Time-dependent Schrödinger equation

$$H\Psi = i\hbar \frac{\partial \Psi}{\partial t} \qquad \Psi(\vec{r},t)$$

If $V(\vec{r},t) = V(\vec{r})$, we can solve it by using separation of variables (P24-26)

$$\Psi(\vec{r},t) = \sum_n c_n \psi_n(\vec{r})\, e^{-iE_n t/\hbar}, \quad H\psi_n = E_n\psi_n$$

(c_n: superposition coefficients)

What if $V(\vec{r},t)$ is time-dependent?

Two-level system

$\langle \psi_a | \psi_b \rangle = \delta_{a,b}$

Perturbation $H'(t)$

Assume $\Psi(\vec{r},t) = \sum_{n=1}^{2} c_n(t)\,\psi_n(\vec{r})\, e^{-iE_n t/\hbar}$

$$\Rightarrow \begin{cases} \dot{c}_a = -\frac{i}{\hbar}\left[c_a \underbrace{H'_{aa}}_{E_0} + c_b H'_{ab} e^{-i(E_b-E_a)t/\hbar}\right] \\ \dot{c}_b = -\frac{i}{\hbar}\left[c_b \underbrace{H'_{bb}}_{E_0} + c_a H'_{ba} e^{i(E_b-E_a)t/\hbar}\right] \end{cases}$$

$H'_{aa} = H'_{bb} = 0$ for light $\qquad H'_{ab} \equiv \langle \psi_a | H'(t) | \psi_b \rangle$

$$\Rightarrow \dot{c}_a = -\frac{i}{\hbar} H'_{ab} e^{-i\omega_0 t} c_b, \quad \dot{c}_b = -\frac{i}{\hbar} H'_{ba} e^{i\omega_0 t} c_a$$

$\omega_0 \equiv \frac{E_b - E_a}{\hbar} > 0$

Iteration with the initial conditions $\begin{cases} c_a(t=0) = 1 \\ c_b(t=0) = 0 \end{cases}$

$$\boxed{c_b^{(1)} = -\frac{i}{\hbar}\int_0^t H'_{ba}(t')\, e^{i\omega_0 t'}\, dt'} \quad [9.17]$$

($H'(t)$ could be time-independent)

Sinusoidal perturbation $H'(\vec{r},t) = V(\vec{r})\cos\omega t$

Resonance $\omega \sim \omega_0 \Rightarrow \omega_0 + \omega >> |\omega_0 - \omega|$

(ω: External time; ω_0: Internal time)

Transition Probability (Observable) $P_{a\to b} \equiv |c_b(t)|^2$ (coefficient)

assuming $\begin{cases} c_a(t=0) = 1 \\ c_b(t=0) = 0 \end{cases}$

Problem 9.7 Rotating wave approximation, Rabi frequency

Light = Electric field $E = E_0 \hat{\epsilon} \cos\omega t\, \hat{k}$ (Transverse wave)

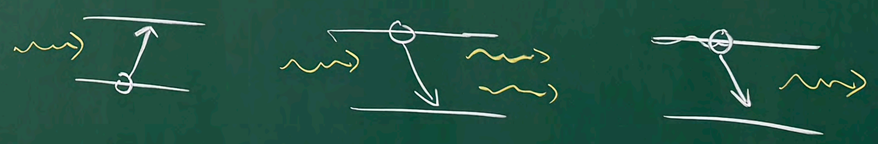
($300nm \sim 700nm$)

Polarization $\vec{\epsilon} \propto \hat{k}$ → Propagation

$$\Rightarrow H'(\vec{r},t) = -qE_0 z \cos\omega t \Rightarrow \begin{cases} H'_{aa} = H'_{bb} = 0 \\ H'_{ab},\ H'_{ba} \end{cases}$$

Three ways light interacts with two levels

① Absorption, ② Stimulated emission, ③ Spontaneous emission



Incoherent $|\psi_a|^2 + |\psi_b|^2$, Coherent $|\psi_a + \psi_b|^2 = |\psi_a|^2 + |\psi_b|^2 + \psi_a^* \psi_b + \psi_a \psi_b^*$ (Interference)

Transition Rate $R_{a\to b} \equiv \frac{dP_{a\to b}}{dt}$

Spontaneous emission rate [9.47], How is it derived? [9.48]

(Lights of all frequencies, incident from all directions)

Lifetime? $\sim e^{-t/\tau}$ (τ: lifetime)

$\begin{cases} a|n\rangle = \sqrt{n}\,|n-1\rangle \\ a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle \end{cases}$

Example 9.1 Charged Harmonic oscillator ($x \to a, a^\dagger$; $p \to a, a^\dagger$)

How to calculate emission rate

Selection Rules

Light ~ $\vec{r}$ (dipole) Evaluate (Non-zero) $\langle \psi_a | \vec{r} | \psi_a \rangle$

For Hydrogen $\langle n'l'm' | \vec{r} | nlm \rangle$

$\Rightarrow m - m' = 0, \pm 1$, $l - l' = \pm 1$

Chap 10 Adiabatic approximation

Adiabatic Process { Internal time T_i / External time T_e — Frequency $\omega_i \gg \omega_e$, $T_i \ll T_e$

Adiabatic approximation
- Born-Oppenheimer approximation

Adiabatic theorem

[10,23] $\psi_n(t) = e^{i\theta_n} e^{i\gamma_n} \psi_n(t)$ In an adiabatic process

Where $H_n(t)\psi_n(t) = E_n(t)\psi_n(t)$ t as a parameter

Instantaneon solution

[10,13] Dynamic phase $\theta_n(t) \equiv -\frac{1}{\hbar}\int_0^t E_n(t')\,dt'$

[10,22] Geometric phase $\gamma_n(t) \equiv i\int_0^t \langle \psi_n(t') | \frac{\partial}{\partial t'} \psi_n(t') \rangle dt'$

Example 10.1 Electron spin in rotating magnetic field

→ Zeeman effect

[10,25] Hamiltonian

[10,27] [10,28] Instantaneon solution $\chi_+ = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} e^{i\varphi} \end{pmatrix}$ $\chi_- = \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} e^{i\varphi} \end{pmatrix}$

Everything on Page 381 (2nd edition of Griffiths)

[10,45] Berry phase $\gamma_n(T) \equiv \oint \langle \psi_n | \nabla_R \psi_n \rangle \cdot d\vec{R}$ (T: period)

$= \oint \vec{A} \cdot d\vec{R}$ (loop integral)

Berry connection $\vec{A} \equiv i\langle \psi_n | \nabla_R \psi_n \rangle$

"Vector potential" of a "magnetic field" in the parameter space $\vec{R}$

Berry Curvature $\vec{B} \equiv \nabla \times \vec{A} \equiv i \nabla_R \times \langle \psi_n | \nabla_R \psi_n \rangle$

"magnetic field"

Berry phase $\gamma_n(T) \equiv \oint \vec{A} \cdot d\vec{R} \equiv \int \vec{B} \cdot d\vec{a}$ ("Flux")

Example 10.2. Berry phase of spin in rotating magnetic field [10,57] — [10,62]

Aharonov–Bohm effect (AB phase) is also a Berry phase

Gauge invariance

$B = 0$, but $\vec{A}$ could be nonzero. (Solenoid)

The path integral of $\vec{A}$ gives the AB phase

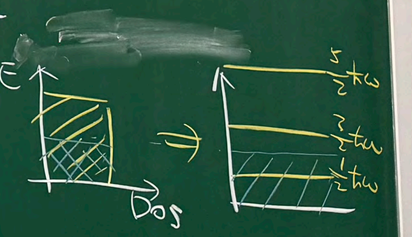
[10,81] $\theta_\pm = \frac{q}{\hbar}\int \vec{A} \cdot d\vec{r} = \pm \frac{q\Phi}{2\hbar}$ ← magnetic flux

[10,82] phase difference $\frac{q\Phi}{\hbar} = \frac{q\Phi}{h/2\pi} = 2\pi \frac{\Phi}{h/e}$ ← Flux quantum

[10,89] AB phase

Chap 12. Landau levels

① Calculation of the Landau levels in 2D
- Gauges, relations between $\vec{A}$ and $\vec{B} = \nabla \times \vec{A}$
- two Landau gauges, Symmetric gauge
- Definition of a and a^+
- Landau levels
- Degeneracy of Landau levels



② Generalization to 3D

2D $H = \frac{\hbar^2}{2m}(k_x^2 + k_y^2) \Rightarrow H = \hbar\omega(a^+a + \frac{1}{2})$

3D $H = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2) \Rightarrow H = \hbar\omega(a^+a + \frac{1}{2}) + \frac{\hbar^2}{2m}k_z^2$

③ Weyl fermion, a case of Matrix Hamiltonian

⬆ 投影背景墙面，注意保护，严禁书写！ ⬆

Chap 11 Scattering theory

[11.7] Total cross-section $\sigma = \int D(\theta) d\Omega$

[11.14] Differential cross-section $D(\theta) = |f(\theta)|^2$ ← measurable Experimentally

[11.12] $A\left[e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right]$ — e^{ikz}: Incident plane wave; $f(\theta)\frac{e^{ikr}}{r}$: Scattered spherical waves

To find $f(\theta)$ theoretically

— Partial wave analysis

— Green function technique + Born approximation

Partial-wave analysis

- Idea: Spherical wave expansion
- Spherical Bessel equation and functions
  — 1st and 2nd kind, ⇒ Spherical Hankel functions

How to find them: ① Handbooks, ② Wiki, ③ Wolfram Mathematica

[10.23] Wave function in terms of partial waves

$$\psi(r,\theta) = A\left\{e^{ikz} + f\sum_l i^{l+1}(2l+1)a_l h_l^{(1)}(kr)P_l(\cos\theta)\right\}$$

As $r \to$ infinity $f(\theta) = \sum_l (2l+1) a_l P_l(\cos\theta)$

[11.28] Rayleigh's formula (Expansion of e^{ikz} into spherical waves)

$$e^{ikz} = \sum_l i^l (2l+1) j_l(kr) P_l(\cos\theta)$$

Spherical Bessel of 1st kind; Legendre polynomials

- Long-wave (low-energy) limit $ka \ll 1$

  Wave vector $k \equiv \frac{\sqrt{2mE}}{\hbar}$, a radius of scattering center

  $\lambda = \frac{2\pi}{k} \Rightarrow \lambda \gg a$ (Wave length)

- Quantum hard sphere: $\sigma = 4\pi R^2$ (solid angle; R radius of sphere; long-wave limit)

  Classical Hard sphere $\sigma = \pi R^2$

- Problem 11.4, 11.5 $V(r) = \alpha\delta(\vec{r} - a)$ $ka \ll 1$

- Phase shift: Alternative description of partial-wave amplitudes

[11.46] Relation between a_l and δ_l (amplitude; phase shift)

$$a_l = \frac{1}{k} e^{i\delta_l} \sin\delta_l$$

Green function of Helmholtz equation

[11.52] $(\nabla^2 + k^2) G(\vec{r}) = \delta^3(\vec{r})$ ← delta source

$k \equiv \frac{\sqrt{2mE}}{\hbar}$; $G(\vec{r})$: Green function

[11.53] Wave function as a convolution

$$\psi(\vec{r}) = \int G(\vec{r} - \vec{r}_0) Q(\vec{r}_0) d^3\vec{r}$$

Scattering potential: $Q \equiv \frac{2m}{\hbar^2} V(\vec{r})\psi(\vec{r})$

[11.54]–[11.57] Strategy to calculate $G(\vec{r})$

— Fourier transformation to turn the differential equation into an algebraic equation

How [11.57] is derived?

— [11.58]–[11.65] Gauchy's integral

[11.67]–[11.68] Integral form of Schrödinger equation

[11.71] Born approximation ← $\psi \to \psi_0$ plane wave in the integral

[11.80] $f(\theta)$ in low-energy Born approximation

[11.88] $f(\theta)$ for spherically symmetrical potential

Example 11.4, 11.5

- Yukawa potential $\sim \frac{1}{r} e^{-\beta r}$
- Born Series (Feynman diagrams): $\psi = \psi_0 + \int g V \psi \Rightarrow \psi = \psi_0 + \int g V \psi_0 + \iint g V g V \psi_0 + \cdots$

SUSTech