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Part I Theory

1 The Wave Function

1.1 The Schrodinger Equation

Looking for Particle's wave function

$$\Psi(x, t)$$

by solving the Schrodinger equation

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

Planck's constant

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

1.2 The Statistical Interpretation

Born's statistical interpretation

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

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

1.3 Probability

1.3.1 Discrete Variables

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

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

The **variance** of the distribution

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

The **standard deviation**

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

1.3.2 Continuous Variables

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

$$P_{ab} = \int_a^b \rho(x) dx$$

Rules:

$$\begin{aligned} \int_{-\infty}^{\infty} \rho(x) dx &= 1 \\ \langle x \rangle &= \int_{-\infty}^{\infty} x \rho(x) dx \\ \langle f(x) \rangle &= \int_{-\infty}^{\infty} f(x) \rho(x) dx \end{aligned}$$

$$\sigma^2 \equiv \langle (\Delta x)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$$

1.4 Normalization

Normalizing the wave function (square-integrable)

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

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

$$\begin{aligned} \frac{\partial \Psi}{\partial t} &= \frac{i\hbar}{2m} \frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar} V \Psi, & \frac{\partial \Psi^*}{\partial t} &= -\frac{i\hbar}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar} V \Psi^* \\ &\downarrow \\ \frac{\partial}{\partial t} |\Psi|^2 &= \frac{\partial}{\partial t} (\Psi^* \Psi) = \Psi^* \frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^*}{\partial t} \Psi \\ &\downarrow \\ \frac{d}{dt} \int_{-\infty}^{\infty} |\Psi(x)|^2 dx &= \int_{-\infty}^{\infty} \frac{\partial}{\partial t} |\Psi(x)|^2 dx = 0 && \text{QED} \end{aligned}$$

1.5 Momentum

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

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

the expectation value of **momentum** is

$$\begin{aligned} \frac{d\langle x \rangle}{dt} &= \frac{i\hbar}{2m} \int x \frac{\partial}{\partial x} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \right) dx = -\frac{i\hbar}{m} \int \Psi^* \frac{\partial \Psi}{\partial x} dx \Rightarrow \\ \langle p \rangle &= m \frac{d\langle x \rangle}{dt} = -i\hbar \int \left(\Psi^* \frac{\partial \Psi}{\partial x} \right) dx = \int \Psi^* [-i\hbar(\partial/\partial x)] \Psi dx \end{aligned}$$

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

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

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

- **Ehrenfest's theorem**

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

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

1.6 The Uncertainty Principle

- de Broglie formula

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

- Heisenberg's **uncertainty principle**

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

2 Time-Independent Schrodinger Equation

2.1 Stationary States

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

$$\begin{aligned} \frac{d\varphi}{dt} &= -\frac{iE}{\hbar}\varphi \quad \rightarrow \quad \varphi(t) = e^{-iEt/\hbar} \\ -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi &= E\psi \quad \text{time-independent Schrodinger equation} \end{aligned}$$

Three Answers:

- stationary states

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

- *states of definite total energy*

- **Hamiltonian** : $H(x, p) = \frac{p^2}{2m} + V(x)$
- Hamiltonian *operator* :

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

- Rewrite time-independent S_e :

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

- expectation value of the total energy : $\langle H \rangle = E$ & $\langle H^2 \rangle = E^2$
- variance: $\sigma_H = 0$
- **linear combination** of separable solutions

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

- stationary states $\Psi_n(x, t) = \psi_n(x) e^{-iE_n t/\hbar}$
- $|c_n|^2$: *probability* that a measurement of the energy would return the value E_n

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

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

Four theorems

- For normalizable solutions, the separation constant E must be *real*
- $\psi(x)$ can always be taken to *real*; from any complex solution, we can $\psi = \frac{1}{2}[(\psi + \psi^*) - i(\psi - \psi^*)]$
- If $V(-x) = V(x)$ then $\psi(x)$ can always be taken to be either even or odd
- E must $> V_{min}$

2.2 The Infinite Square Well

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

Outside the well, $\psi(x) = 0$

Inside the well (**simple harmonic oscillator** equation)

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

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

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

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

$$\int \psi_m(x)^* \psi_n(x) dx = \delta_{mn}$$

- **complete**

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

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

$$\Rightarrow c_n = \int \psi_n(x)^* f(x) dx$$

• ★

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

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

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

2.3 The Harmonic Oscillator

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

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

2.3.1 Algebraic Method

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

$$\begin{aligned}
\hat{a}_{\pm} &\equiv \frac{1}{\sqrt{2\hbar m\omega}}(\mp i\hat{p} + m\omega x) \rightarrow \begin{cases} x = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_+ + \hat{a}_-) \\ \hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}(\hat{a}_+ - \hat{a}_-) \end{cases} \\
&\downarrow \\
\begin{cases} \hat{a}_+\hat{a}_- = \frac{1}{\hbar\omega}\hat{H} - \frac{1}{2} \\ \hat{a}_-\hat{a}_+ = \frac{1}{\hbar\omega}\hat{H} + \frac{1}{2} \end{cases} &\rightarrow \star \quad \begin{cases} \hbar\omega\left(\hat{a}_{\pm}\hat{a}_{\mp} \pm \frac{1}{2}\right)\psi = E\psi \\ [\hat{a}_-, \hat{a}_+] = 1 \end{cases} \\
&\downarrow \\
\hat{H}(\hat{a}_+\psi) &= (E + \hbar\omega)(\hat{a}_+\psi) \\
\hat{H}(\hat{a}_-\psi) &= (E - \hbar\omega)(\hat{a}_-\psi)
\end{aligned}$$

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

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

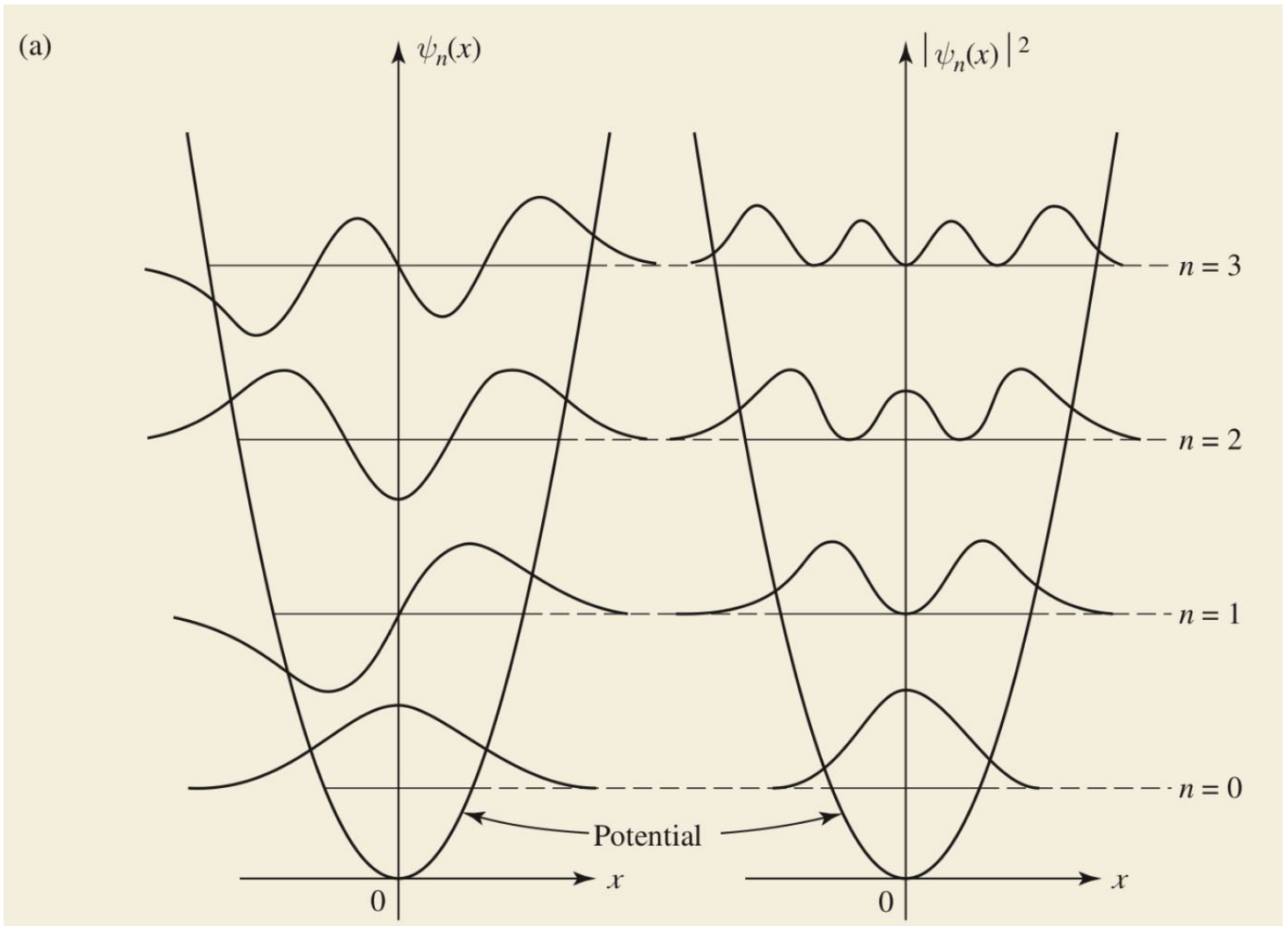
Excited states, increasing the energy by $\hbar\omega$ with each step:

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

Normalization algebraically

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

$$\begin{aligned}
&\int_{-\infty}^{\infty} f^*(\hat{a}_{\pm}g) dx = \int_{-\infty}^{\infty} (\hat{a}_{\mp}f)^* g dx \\
&\downarrow \\
\begin{cases} c_n = \sqrt{n+1} \\ d_n = \sqrt{n} \end{cases} &\leftarrow \begin{cases} \int_{-\infty}^{\infty} (\hat{a}_{\pm}\psi_n)^*(\hat{a}_{\pm}\psi_n) dx = \int_{-\infty}^{\infty} (\hat{a}_{\mp}\hat{a}_{\pm}\psi_n)^*\psi_n dx \\ \hat{a}_+\hat{a}_-\psi_n = n\psi_n, \quad \hat{a}_-\hat{a}_+\psi_n = (n+1)\psi_n \end{cases} \\
&\downarrow \\
\star \quad \psi_n &= \frac{1}{\sqrt{n!}}(\hat{a}_+)^n\psi_0(x)
\end{aligned}$$



2.3.2 Analytic Method

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

To begin with at very large ξ

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

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

In the form of *power series* in ξ

$$h(\xi) = \sum_{j=0}^{\infty} a_j \xi^j \quad \xrightarrow{\frac{dh}{d\xi}, \frac{d^2h}{d\xi^2}} \quad \sum_{j=0}^{\infty} [(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j] \xi^j = 0$$

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

For physically acceptable solutions:

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

$$\downarrow$$

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

Normalized stationary state

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

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

2.4 The Free Particle

$$V(x) = 0$$

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

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

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

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

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

This wave function is not normalizable

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

- Plancherel's theorem

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

Now *this* can be normalized

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

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

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

2.5 The Delta-Function Potential

2.5.1 Bound States and Scattering States

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

2.5.2 The Delta-Function Well

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

(1) bound state $E < 0$

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

$$\Downarrow$$

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

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

$$\psi(0) = B \Rightarrow \kappa = \frac{m\alpha}{\hbar^2}$$

Proof: ($\epsilon \rightarrow 0$)

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

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

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

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

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

(2) scattering state $E > 0$

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

$$\Downarrow$$

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

- Boundary conditions

$$F + G = A + B$$

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

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

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

When wave come from left:

A : amplitude of the incident wave

B : amplitude of the reflected wave

F : amplitude of the transmitted wave

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

The *relative* probability of reflection and transmission:

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

Discussion:

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

Fourier transform of $\delta(x)$

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

2.6 The Finite Square Well

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

(1) bound state $E < 0$

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

$$\begin{aligned} \frac{d^2\psi}{dx^2} &= \kappa^2\psi, \quad \text{where} \quad \kappa \equiv \frac{\sqrt{-2mE}}{\hbar} \\ &\Downarrow \\ \psi(x) &= Be^{\kappa x} \end{aligned}$$

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

$$\begin{aligned} \frac{d^2\psi}{dx^2} &= -l^2\psi, \quad \text{where} \quad l \equiv \frac{\sqrt{2m(E + V_0)}}{\hbar} \\ &\Downarrow \\ \psi(x) &= C \sin(lx) + D \cos(lx) \end{aligned}$$

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

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

- even solutions

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

- boundary condition at $x = a$

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

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

Discussion:

- Wide, deep well

$$z_0 \rightarrow \infty \Rightarrow z_n = n\pi/2 \Rightarrow$$

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

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

(2) scattering state $E > 0$

When wave come from left

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

Boundary conditions

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

Eliminate

$$B = i \frac{\sin(2la)}{2kl} (l^2 - k^2) F$$

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

Transmission coefficient

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

when $T = 1$

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

