Scattering Theory

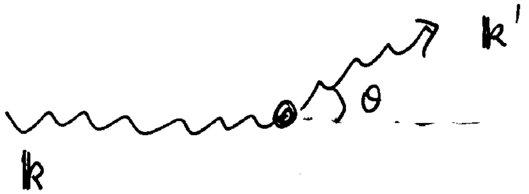
Contents :

1. Scattering in one dimension

$\boxed{\text{Scattering process}}$

$\Downarrow$

- This is not an eigenvalue problem.
- E is given. (Incident energy)



$$\left(E = \frac{k^2}{2m} \right)$$

- The observation of the outgoing particle in terms of <u>flux</u>

$$\begin{cases} \text{Incident flux} & \hat{j}_{in} \\ \text{Outgoing flux} & \hat{j}_{out} \end{cases}$$

<u>Probability</u>

$$\boxed{\underline{P} = \frac{\hat{j}_{out}}{\hat{j}_{in}}} \Longrightarrow \text{cross section.}$$

[Current density $\vec{j}$]

- current density $\vec{j}$ is defined as

$$\boxed{\vec{j} \equiv \frac{1}{2mi}\left(\psi^*(\nabla\psi) - (\nabla\psi^*)\psi\right)}$$

why?

$\updownarrow$

This is a conserved quantity.

(proof) Schrödinger equation.

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2m}\nabla^2\psi + V\psi$$

Thus, we find

$$-i\frac{\partial\psi^*}{\partial t} = -\frac{1}{2m}\nabla^2\psi^* + V\psi^*$$

We make

$$i\left(\frac{\partial\psi}{\partial t}\psi^* + \psi\frac{\partial\psi^*}{\partial t}\right)$$

$$= -\frac{1}{2m}(\nabla^2\psi)\psi^* + (V\psi)\psi^*$$

$$+ \frac{1}{2m}\psi(\nabla^2\psi^*) - \psi^* V\psi$$

Therefore, we find

$$i\,\frac{\partial(\psi^*\psi)}{\partial t} = -\frac{1}{2m}\nabla\left(\psi^*(\nabla\psi) - (\nabla\psi^*)\psi\right)$$

$$\therefore\ \boxed{\frac{\partial}{\partial t}(\psi^*\psi) + \frac{1}{2mi}\nabla\left\{\psi^*(\nabla\psi) - (\nabla\psi^*)\psi\right\} = 0}$$

Thus, we define

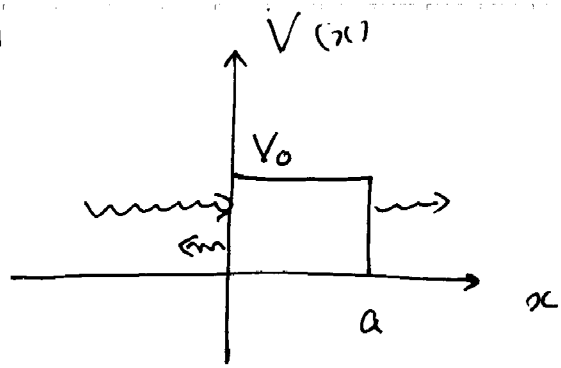
$$\boxed{\begin{aligned}\rho &\equiv \psi^*\psi \\ \mathbf{j} &\equiv \frac{1}{2mi}\left\{\psi^*(\nabla\psi) - (\nabla\psi^*)\psi\right\}\end{aligned}}$$

and this leads to

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{j} = 0$$

which is a current conservation.

[Example ①]



Potential: $V(x) = \begin{cases} 0 & x<0 \\ V_0 & 0<x<a \\ 0 & a<x \end{cases}$

- Schrödinger equation:

$$\left(-\frac{1}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x) = E\psi(x)$$

This is not an eigenvalue problem.

(1) Incident wave

E is given.

$$\boxed{E = \frac{k^2}{2m}}$$

Solution in $\underline{x<0}$

$$\boxed{\psi(x) = \frac{1}{\sqrt{V}} e^{ikx}} \qquad k = \sqrt{2mE}$$

$$\psi(x) = \frac{1}{\sqrt{V}} e^{ikx}$$ is an eigenstate of the momentum operator.

[Check:] $\hat{p} = -i \frac{\partial}{\partial x}$

$$\hat{p}\,\psi(x) = -i \frac{1}{\sqrt{V}} \frac{\partial}{\partial x} e^{ikx}$$

$$= k \frac{1}{\sqrt{V}} e^{ikx} = k\,\psi(x)$$ //

- Incident wave :

$$\psi_{in}(x) = \frac{1}{\sqrt{V}} e^{ikx}$$

We take $V = 1$, and then

$$\boxed{\psi_{in}(x) = e^{ikx}}$$

(2) Scattered wave

(a) Reflection: $\boxed{x<0}$

$$\boxed{\psi_R(x) = B e^{-ikx}}$$

(This particle is moving to the left-hand side.)

(b) Transmission $\boxed{x>a}$

$$\boxed{\psi_T(x) = C e^{ikx}}$$

(3) In between : $0<x<a$

Schrodinger equation

$$\left[\frac{d^2}{dx^2} + 2m(E-V_0) \right] \psi(x) = 0$$

By introducing κ as

$$\boxed{\kappa = \sqrt{2m(E-V_0)}}$$

$$\boxed{\psi(x) = C_1 \sin \kappa x + C_2 \cos \kappa x}$$

[Physical observables]

- Transmission probability

$$P_T = \frac{\hat{J}_T}{\hat{J}_{in}}$$

- Reflection probability

$$P_R = \frac{\hat{J}_R}{\hat{J}_{in}}$$

- Calculation of incident flux : $\hat{J}_{in}$

$$\hat{J}_{in} = \frac{1}{2mi}\left(\psi_{in}^* \frac{\partial \psi_{in}}{\partial x} - \left(\frac{\partial \psi_{in}^*}{\partial x}\right) \psi_{in} \right)$$

$$\underline{\psi_{in} = e^{ikx}}$$

$$\therefore \quad \hat{J}_{in} = \frac{1}{2mi}\left[ikx + ikx \right] = \frac{k}{m}$$

$$\boxed{\hat{J}_{in} = \frac{k}{m}}$$

- Calculation of reflection flux : $\hat{J}_R$

$$\hat{J}_R = \frac{1}{2mi}\left(\psi_R^* \frac{\partial \psi_R}{\partial x} - \left(\frac{\partial \psi_R^*}{\partial x}\right) \psi_R \right)$$

$$\psi_R = B\, e^{-ikx}$$

Thus, we find

$$\hat{J}_R = |B|^2 \frac{1}{2mi}\left[(-ik) - (ik)\right] = -\frac{k}{m}|B|^2$$

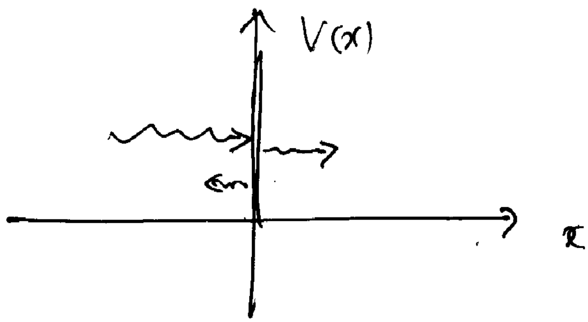
$$\therefore \quad \boxed{\hat{J}_R = -\frac{k}{m}|B|^2}$$

- Calculation of transmitted wave : $\hat{J}_T$

$$\boxed{\hat{J}_T = |C|^2 \frac{k}{m}}$$

[Example ②] δ-function potential

$$\boxed{V(x) = V_0\,\delta(x)}$$



- Schrödinger equation

$$\left[-\frac{1}{2m}\frac{\partial^2}{\partial x^2} + V_0\,\delta(x)\right]\psi(x) = E\,\psi(x)$$

$$k = \sqrt{2mE} \qquad (E > 0)$$

Solutions :

$$\begin{cases} \text{(i)} \quad x<0 & \psi = \underbrace{e^{ikx}}_{\psi_{in}} + \underbrace{A\,e^{-ikx}}_{\psi_R} \\ \text{(ii)} \quad x>0 & \underline{\psi_t = B\,e^{ikx}} \end{cases}$$

$$\begin{cases} \psi_{in} = e^{ikx} \\ \psi_R = A\,e^{-ikx} \end{cases}$$

- Continuation of wave function at $x=0$

(a) $\psi_{in}(0) = \psi_t(0)$

$$\therefore \boxed{1 + A = B}$$

(b) Derivative of the wave function

$$\int_{-\epsilon}^{\epsilon} -\frac{1}{2m}\frac{d^2\psi}{dx^2}\,dx + \int_{-\epsilon}^{\epsilon} V_0\,\delta(x)\psi(x)\,dx$$

$$= E\int_{-\epsilon}^{\epsilon}\psi\,dx \qquad (\epsilon \to 0)$$

$$\therefore -\frac{1}{2m}\left[\frac{d\psi}{dx}\right]_{-\epsilon}^{\epsilon} + V_0\psi(0) = 0$$

$$-\frac{1}{2m}\Big(ikB - \big(ik + A(-ik)\big)\Big) + V_0 B = 0$$

By making use of $1+A=B$,

we find

$$\boxed{B = \frac{ik}{mV_0}A}$$

Thus, we find

$$\boxed{\begin{aligned} A &= \frac{1}{-1 + \frac{ik}{mV_0}} \\ B &= \frac{ik}{mV_0} \cdot \frac{1}{-1 + \frac{ik}{mV_0}} \end{aligned}}$$

- Inciant current $\hat{j}_{in}$

$$\underline{\hat{j}_{in} = \frac{k}{m}}$$

- Reflection current $\hat{j}_R$

$$\underline{\hat{j}_R = -\frac{k}{m}|A|^2}$$

- Transmission current $\hat{j}_T$

$$\underline{\hat{j}_T = \frac{k}{m}|B|^2}$$

- Reflection probability :

$$P_R = \left| \frac{\hat{J}_R}{\hat{J}_{in}} \right| = |A|^2 = \frac{1}{1 + \left(\frac{k}{mV_0}\right)^2}$$

- Transmission probability :

$$P_T = \left| \frac{\hat{J}_T}{\hat{J}_{in}} \right| = |B|^2 = \left(\frac{k}{mV_0}\right)^2 \frac{1}{1 + \left(\frac{k}{mV_0}\right)^2}$$

- In terms of currents :

$$\boxed{\hat{J}_{in} + \hat{J}_R = \hat{J}_T}$$

$$\Downarrow$$

$$\frac{k}{m} = \frac{k}{m}\left(|A|^2 + |B|^2 \right)$$

which is indeed satisfied.