Other important 1D operators (motivation : semiconductor devices)

charge density operator : i.e. an electron in state $|\psi\rangle$

charge density $= e\,|\psi(x)|^2$. Let's check units

$$\int |\psi(x)|^2\,dx = 1 \quad , \text{or } \left[|\psi(x)|^2\right] = L^{-1} \quad ☑$$

charge density operator $\hat{\rho}(x)$: $\langle \rho(x)\rangle = e|\psi(x)|^2 = \langle\psi|\hat{\rho}|\psi\rangle$

$$\int f(x)\,\underbrace{\delta(x-a)}\,dx = f(a) \qquad \text{Dirac } \delta$$

$$\hat{\rho}(x) = e\,\delta(x-x') \qquad \langle\psi|\hat{\rho}|\psi\rangle = e\int |\psi(x')|^2\,\delta(x-x')\,dx'$$
$$= e\,|\psi(x)|^2$$

current (density) operator

$$\hat{j}(x) = \frac{1}{2m}\left(\hat{p}_x\cdot\hat{\rho}(x) + \hat{\rho}(x)\cdot\hat{p}_x\right) \quad \text{with } \hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

e.g. in 1D: $\hat{j}(x) = -\frac{ie\hbar}{2m}\left(\frac{d}{dx}\delta(x-x') + \delta(x-x')\frac{d}{dx}\right)$

$$\langle j(x)\rangle = \langle\psi|\hat{j}|\psi\rangle = -\frac{ie\hbar}{2m}\left(\int_{-\infty}^{\infty}\psi^*(x')\frac{d}{dx}\delta(x-x')\,\psi(x')\,dx' + \int_{-\infty}^{\infty}\psi^*(x')\,\delta(x-x')\frac{d}{dx}\psi(x')\,dx'\right)$$

$2^{nd}\int$: $\psi^*(x)\frac{d}{dx}\psi(x)$

$$\int u\frac{dv}{dx}dx = uv - \int v\frac{du}{dx}dx$$

$1^{st}\int$: by parts

$$|\psi(x')|^2\,\delta(x-x')\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\delta(x-x')\,\psi(x')\frac{d}{dx}\psi^*(x')\,dx' = -\psi(x)\frac{d}{dx}\psi^*(x)$$

$$\langle j_x(x)\rangle = \frac{ie\hbar}{2m}\left(\psi(x)\frac{d}{dx}\psi^*(x) - \psi^*(x)\frac{d}{dx}\psi(x)\right)$$

$[j_x] = \frac{Q}{T}$ - units of current in 1D (check)

Can show that expectation values satisfy charge conservation :

$$\frac{\partial}{\partial t}\langle\rho\rangle = -\frac{\partial}{\partial x}\langle j_x\rangle$$

HW prob : prove for $\psi = \psi(x,t)$

Note : $\psi(x,t)$ satisfies STDE

E.g. electrons tunneling thru a rectangular barrier

$\psi_L(x) = Ae^{ikx} + Be^{-ikx}$ | $\psi_B(x) = Ce^{ik_Bx} + De^{-ik_Bx}$ | $\psi_R(x) = Fe^{ikx}$

$k_B = \sqrt{\frac{2m}{\hbar^2}(E-V)}$ can be imaginary

To the right: $j_x = \frac{ie\hbar}{2m}\left(Fe^{ikx}(-ik)F^*e^{-ikx} - F^*\cancel{e^{-ikx}}\,ik\,F\cancel{e^{ikx}}\right)$

$j_x = e|F|^2\frac{\hbar k}{m}$, $\frac{\hbar k}{m} \backsim \frac{p}{m} = v$ - behaves like classical velocity

To the left: $j_x = e\frac{\hbar}{2m}i\left(\psi_L\frac{d}{dx}\psi_L^* - \psi_L^*\frac{d}{dx}\psi_L\right) = e\frac{\hbar k}{m}\left(|A|^2 - |B|^2\right)$

$e|A|^2v$ - incident current
$e|B|^2v$ - reflected current
$e|F|^2v$ - transmitted current
$|A|^2 - |B|^2 = |F|^2$ - charge conservation

transmitted fraction $\eta = \frac{|F|^2}{|A|^2} = \frac{|A|^2 - |B|^2}{|A|^2}$ more next lecture

Effective mass (detour)

semiclassical eqn. of motion

$\langle v\rangle = \frac{\langle p\rangle}{m_0}$, get rid of mass : $E = \frac{\hbar^2k^2}{2m_0}$ (free part.)

$\frac{dE}{dk} = \frac{\hbar(\hbar k)}{m_0}$

$$\begin{cases} \langle v\rangle = \frac{1}{\hbar}\frac{dE(k)}{dk} \\ F_{ext} = \hbar\frac{dk}{dt} \end{cases}$$

$$a = \frac{dv}{dt} = \frac{1}{\hbar}\frac{d}{dt}\frac{dE(k)}{dk} = \frac{1}{\hbar}\frac{d^2E(k)}{dk^2}\frac{dk}{dt} = \left[\frac{1}{\hbar^2}\frac{d^2E(k)}{dk^2}\right]F_{ext}$$

$$\boxed{m^* = m_{eff} = \hbar^2\left(\frac{d^2E(k)}{dk^2}\right)^{-1}}$$

m^* is usually given in units of m_0

- periodic potential in crystals affect $E(k) \neq \frac{\hbar^2k^2}{2m_0}$
- effective mass allows to retain much classical intuition

(more when we get to solid state)

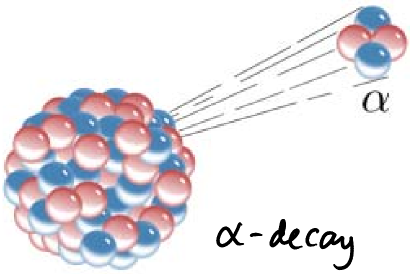
For 1D Hamiltonian $m_0 \to \underset{m_{eff}}{m^*}$ (if $m^* \neq m^*(x)$)
we postulate

$$\hat{H} = -\frac{\hbar^2}{2}\frac{d}{dx}\left(\frac{1}{m_{eff}(x)}\frac{d}{dx}\right) + V(x)$$

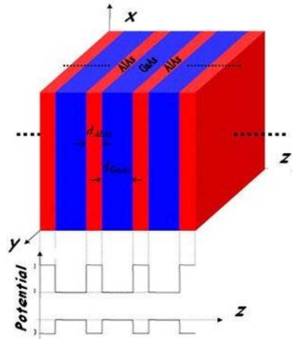
Tunneling:

many applications:

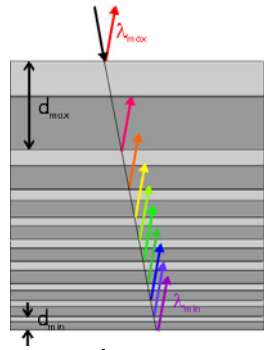
- → charge transport in semiconductors
- → field emission / photoemission } Richardson eqn.
- → α-decay



α-decay

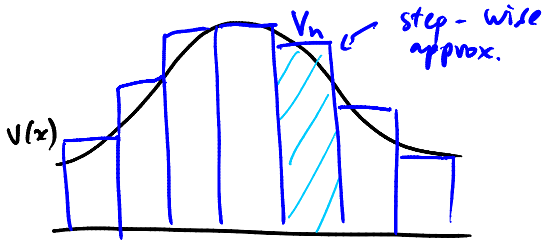


superlattice (semiconductor devices)



multilayer optics (broadband mirrors)

Trasfer matrix approach



x_n layer n $\quad\quad$ x_{n+1} layer $n+1$

$\rightarrow A_n$ $\quad\quad$ $\rightarrow A_{n+1}$

$\leftarrow B_n$ $\longleftarrow$ width d_n $\longrightarrow$ $\leftarrow B_{n+1}$

ψ cont.
$d\psi/dx$ cont.

$$\psi_n(\Delta x) = A_n e^{ik_n \Delta x} + B_n e^{-ik_n \Delta x} \qquad \Delta x = x - x_n$$

$$k_n = \sqrt{\frac{2m_{eff}}{\hbar}(E - V_n)} \quad \leftarrow \text{can be imaginary}$$

if can relate $\begin{pmatrix} A_n \\ B_n \end{pmatrix}$ to $\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix}$

$\Rightarrow$ problem solved

$$\left.\begin{aligned} \psi_n(d_n) &= A_n e^{ik_n d_n} + B_n e^{-ik_n d_n} = \psi_{n+1}(0) = A_{n+1} + B_{n+1} \\ \underbrace{\frac{d}{dx}\psi_n(d_n)} &= \frac{d}{dx}\psi_{n+1}(0) \end{aligned}\right\} \text{ wavefcn continuity}$$

$$\frac{ik_n A_n e^{ik_n d_n}}{ik_{n+1}} - \frac{ik_n B_n e^{-ik_n d_n}}{ik_{n+1}} = \frac{ik_{n+1}}{ik_{n+1}} A_{n+1} - \frac{ik_{n+1}}{ik_{n+1}} B_{n+1}$$

$$A_{n+1} = \frac{1}{2}\left[A_n e^{ik_n d_n}\left(1 + \frac{k_n}{k_{n+1}}\right) + B_n e^{-ik_n d_n}\left(1 - \frac{k_n}{k_{n+1}}\right)\right]$$

$$B_{n+1} = \frac{1}{2}\left[A_n e^{ik_n d_n}\left(1-\frac{k_n}{k_{n+1}}\right) + B_n e^{-ik_n d_n}\left(1+\frac{k_n}{k_{n+1}}\right)\right]$$

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = T_n \begin{pmatrix} A_n \\ B_n \end{pmatrix} \; ; \quad \boxed{T_n = \begin{pmatrix} \frac{1}{2}\alpha_n(1+\beta_n) & \frac{1}{2}\alpha_n^{-1}(1-\beta_n) \\ \frac{1}{2}\alpha_n(1-\beta_n) & \frac{1}{2}\alpha_n^{-1}(1+\beta_n) \end{pmatrix} \quad \alpha_n \equiv e^{ik_n d_n}, \quad \beta_n = \frac{k_n}{k_{n+1}}}$$

To compute full matrix

$$\boxed{T = T_N \ldots T_n \ldots T_2 T_1}$$

Overall, for the entire potential barrier: $\quad N$ - tot. number of slabs

$$\begin{pmatrix} A_N \\ B_N \end{pmatrix} = \begin{pmatrix} F \\ 0 \end{pmatrix} = T \begin{pmatrix} A \\ B \end{pmatrix}, \Rightarrow \quad F = T_{11} A + T_{12} B$$

$$0 = T_{21} A + T_{22} B$$

transmission:

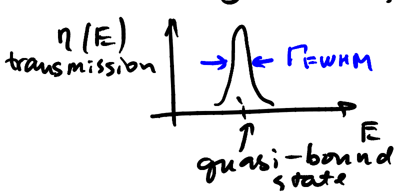
$$\boxed{\eta = 1 - \frac{|B|^2}{|A|^2} = \frac{|F|^2}{|A|^2} = 1 - \frac{|T_{21}|^2}{|T_{22}|^2}}$$

if effective mass changes $\beta_n \to \beta_n = \frac{k_n}{k_{n+1}} \frac{m_{eff,n+1}}{m_{eff,n}}$

Matlab example

Quasi-bound states

$\eta(E)$ displays peaks for finite walls @ quasi-bound



$$\Gamma_{FWHM} = \Delta E \; ;$$

$$\tau \cdot \Gamma_{FWHM} \sim \hbar \;, \Rightarrow$$

lifetime $\tau \sim \frac{\hbar}{\Gamma_{FWHM}}$