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HW#8 Phys 240a
Condensed Matter
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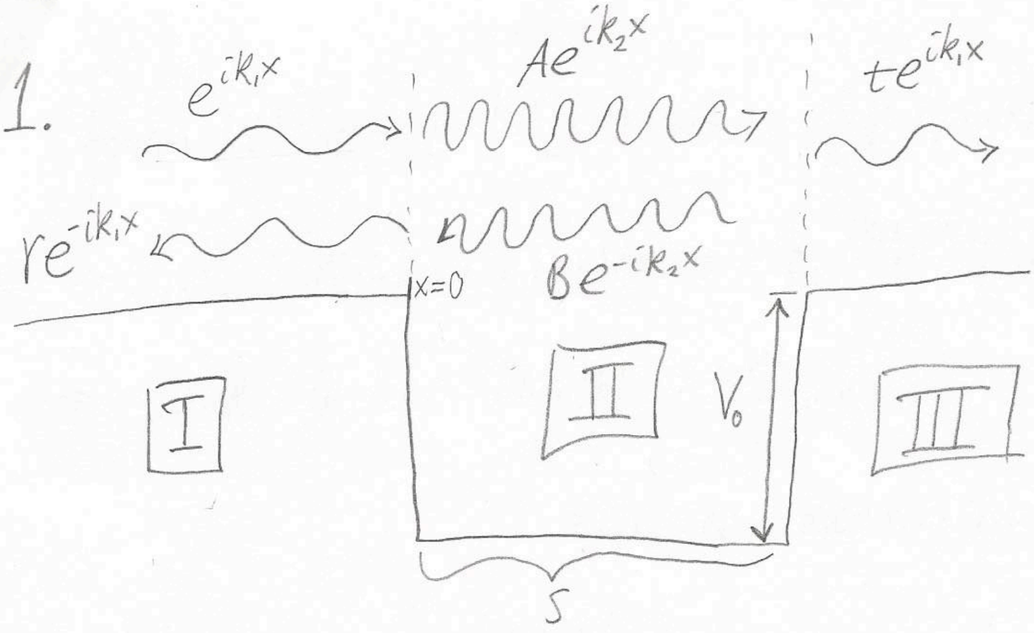
1.



a) $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = \varepsilon\psi, \ \varepsilon > 0$

I, III : $V(x) = 0 \Rightarrow \psi'' = -\frac{2m}{\hbar^2}\varepsilon\psi \Rightarrow k_1 \equiv \sqrt{\frac{2m}{\hbar^2}\varepsilon}$

II: $V(x) = -V_0 \Rightarrow \psi'' = -\frac{2m}{\hbar}(\varepsilon + V_0)\psi \Rightarrow k_2 = \sqrt{\frac{2m}{\hbar}(\varepsilon + V_0)}$

ψ continuous & smooth $\forall x$

$\psi_I(0) = \psi_{II}(0) \Rightarrow 1 + r = A + B$

$\psi_I'(0) = \psi_{II}'(0) \Rightarrow k_1(1-r) = k_2(A-B) \rightarrow A - B = \frac{k_1}{k_2}(1-r)$

$\hookrightarrow A = \frac{1}{2}\left[(1+r) + \frac{k_1}{k_2}(1-r)\right], \ B = \frac{1}{2}\left[(1+r) - \frac{k_1}{k_2}(1-r)\right]$

$\Rightarrow \psi_{II} = (1+r)\cos k_2x + i\frac{k_1}{k_2}(1-r)\sin k_2x$

(1) $\psi_{II}(s) = \psi_{III}(s) \Rightarrow (1+r)\cos k_2s + i\frac{k_1}{k_2}(1-r)\sin k_2s = te^{ik_1s}$

(2) $\psi_{II}'(s) = \psi_{III}'(s) \Rightarrow -k_2(1+r)\sin k_2s + ik_1(1-r)\cos k_2s = ik_1te^{ik_1s}$

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from (1), $t = e^{-ik_1 s}\left[(1+r)\cos k_2 s + i\frac{k_1}{k_2}(1-r)\sin k_2 s\right]$

$\hookrightarrow$ (2): $-k_2(1+r)\sin k_2 s + ik_1(1-r)\cos k_2 s = ik_1 e^{ik_1 s}e^{-ik_1 s}\left[(1+r)\cos k_2 s + i\frac{k_1}{k_2}(1-r)\sin k_2 s\right]$

$$\Rightarrow -k_2\sin k_2 s + ik_1\cos k_2 s - ik_1\cos k_2 s - i^2\frac{k_1^2}{k_2}\sin k_2 s$$

$$= r\left[k_2\sin k_2 s + ik_1\cos k_2 s + ik_1\cos k_2 s - i^2\frac{k_1^2}{k_2}\sin k_2 s\right]$$

$$\hookrightarrow \frac{k_1^2-k_2^2}{k_2}\sin k_2 s = r\left[\frac{k_1^2+k_2^2}{k_2}\sin k_2 s + 2ik_1\cos k_2 s\right]$$

$$\Rightarrow \boxed{r = \frac{(k_1^2-k_2^2)\sin k_2 s}{(k_1^2+k_2^2)\sin k_2 s + 2ik_1k_2\cos k_2 s}}$$

with $k_1 = \sqrt{\frac{2m}{\hbar^2}\varepsilon}$ & $k_2 = \sqrt{\frac{2m}{\hbar^2}(\varepsilon+V_0)}$

$$\hookrightarrow t = \frac{e^{-ik_1 s}}{(k_1^2+k_2^2)\sin\theta + 2ik_1k_2\cos\theta}\left[2k_1^2\sin\theta\cos\theta + 2ik_1k_2\cos^2\theta + i\frac{k_1}{k_2}\cdot 2k_2^2\sin^2\theta + i\frac{k_1}{k_2}(2ik_1k_2)\sin\theta\cos\theta\right]$$

with $\theta = k_2 s$

$$= \frac{e^{-ik_1 s}\cdot 2ik_1k_2}{(k_1^2+k_2^2)\sin\theta + 2ik_1k_2\cos\theta} \rightarrow \text{define } D^2 = (k_1^2+k_2^2)^2\sin^2\theta + 4k_1^2k_2^2\cos^2\theta$$

$$\hookrightarrow t = \frac{1}{D^2}\left[2k_1k_2(\sin k_1 s + i\cos k_1 s)\left((k_1^2+k_2^2)\sin\theta - 2ik_1k_2\cos\theta\right)\right], \text{ let } \alpha = k_1 s$$

$$= \frac{1}{D^2}\left[\left\{(k_1^2+k_2^2)\sin\alpha\sin\theta + 2k_1k_2\cos\theta\cos\alpha\right\} + i\left\{(k_1^2+k_2^2)\cos\alpha\sin\theta - 2k_1k_2\sin\alpha\cos\theta\right\}\right]$$

$$|r| = \sqrt{r^* r} = \left(\frac{1}{D^2}\left(k_1^2 - k_2^2\right)^2 \sin^2\theta\right)^{\frac{1}{2}}$$

$$t^2 + r^2 = 1 \Rightarrow t^2 = 1 - r^2 = \frac{1}{D^2}\left\{\left(k_1^2 + k_2^2\right)^2 \sin^2\theta + 4k_1^2 k_2^2 \cos^2\theta - \left(k_1^2 - k_2^2\right)^2 \sin^2\theta\right\}$$

$$= 4k_1^2 k_2^2\left(\sin^2\theta + \cos^2\theta\right)$$

$$\Rightarrow \boxed{|t| = \frac{2k_1 k_2}{\sqrt{\left(k_1^2 + k_2^2\right)^2 \sin^2 k_2 s + 4k_1^2 k_2^2 \cos^2 k_2 s}}}$$

$$\delta = \tan^{-1}\left(\frac{Im(t)}{RE(t)}\right) \Rightarrow \boxed{\delta = \tan^{-1}\left[\frac{\left(k_1^2 + k_2^2\right)\cos k_1 s \sin k_2 s - 2k_1 k_2 \sin k_1 s \cos k_2 s}{\left(k_1^2 + k_2^2\right)\sin k_1 s \sin k_2 s + 2k_1 k_2 \cos k_1 s \cos k_2 s}\right]}$$

$$\Rightarrow t = |t| e^{i\delta} \text{ with } k_1 = \sqrt{\frac{2m}{\hbar^2}\varepsilon} \;\&\; k_2 = \sqrt{\frac{2m}{\hbar^2}(\varepsilon + V_0)} \qquad \square$$

b) $$t = \frac{2ik_1 k_2 e^{-ik_1 s}}{\left(k_1^2 + k_2^2\right)\sin(k_2 s) + 2ik_1 k_2 \cos(k_2 s)}$$

vary $s \to s^*$ & show $t^* = t$

add $2\pi n$ to argument of sinusoidal parts to leave unchanged:

$$k_1 s \to k_1 s^* = k_1 s + 2\pi n \Rightarrow s^* = s + 2\pi \frac{n}{k_1}$$

$$k_2 s \to k_2 s^* = k_2 s + 2\pi m \Rightarrow s^* = s + 2\pi \frac{m}{k_2}$$

$\hookrightarrow \frac{n}{k_1} = \frac{m}{k_2}$ or $\frac{k_1}{k_2} = \frac{n}{m}$ — ie, ratio of wavenumbers must be rational

Then $\sqrt{\frac{\varepsilon}{\varepsilon + V_0}}$ must be rational. In this case, any s^* of the form

$s^* = s + 2\pi l$ with $l = \frac{n}{k_1} = \frac{m}{k_1}$ leaves t unchanged

2. $$\hat{H}\varphi_i^v(\vec{r}) = [-\frac{1}{2}\nabla^2 + V(\vec{r})]\varphi_i^v(\vec{r}) = \varepsilon_i \varphi_i^v(\vec{r}).$$

$$|\varphi_i^v(\vec{r})\rangle = |\tilde{\varphi}_i^v(\vec{r})\rangle + \sum_j B_{ij}|\varphi_j^c(\vec{r})\rangle$$

$$\underbrace{\langle \varphi_{j'}^c(\vec{r})|\varphi_i^v(\vec{r})\rangle}_{0} = \langle \varphi_{j'}^c(\vec{r})|\tilde{\varphi}_i^v(\vec{r})\rangle + \sum_j B_{ij}\,\delta_{jj'}$$

$$\Rightarrow B_{ij} = -\langle \varphi_j^c(\vec{r})|\tilde{\varphi}_i^v(\vec{r})\rangle$$

$$\Rightarrow [-\frac{1}{2}\nabla^2 + V(\vec{r})](\tilde{\varphi}_i^v(\vec{r}) + \sum_j B_j \varphi_j^c(\vec{r})) = \varepsilon_i^v \tilde{\varphi}_i^v(\vec{r}) + \varepsilon_i^v \sum_j B_{ij}\varphi_j^c(\vec{r}).$$

$$\Rightarrow \hat{H}\tilde{\varphi}_i^v(\vec{r}) + \sum_j (\varepsilon_j^c - \varepsilon_i^v) B_{ij}\varphi_j^c(\vec{r}) = \varepsilon_i^v \varphi_i^v(\vec{r}).$$

$$\hat{H}\tilde{\varphi}_i^v(\vec{r}) + \underbrace{\sum_j (\varepsilon_i^v - \varepsilon_j^c)\langle \varphi_j^c(\vec{r})|\varphi_i^v(\vec{r})\rangle \varphi_j^c(\vec{r})}_{V^R\tilde{\varphi}_i^v(\vec{r})} = \varepsilon_i^v \varphi_i^v(\vec{r})$$

$$(\hat{H} + V^R)\tilde{\varphi}_i^v(\vec{r}) = \varepsilon_i^v \tilde{\varphi}_i^v(\vec{r}).$$

$$H^{PKA}\tilde{\varphi}_i^v(\vec{r}) = \varepsilon_i^v \tilde{\varphi}_i^v(\vec{r})$$

3.

(a). $W(r-R) = \sum_k e^{ikR} \varphi_k(\vec{r})$

$$= \frac{a}{2\pi} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk\, e^{ikR} \left(\frac{\alpha}{2} (e^{ikr} + e^{-ikr}) + \frac{\beta}{2i} (e^{i2kr} - e^{-ikr}) \right)$$

$$= \frac{a}{2\pi} \left\{ \frac{\alpha}{2} \left[\frac{1}{i(R+r)} e^{ik(R+r)} + \frac{1}{i(R-r)} e^{ik(R-r)} \right] + \frac{\beta}{2i} \left[\frac{1}{i(R+2r)} e^{ik(R+2r)} \right.\right.$$

$$\left.\left. - \frac{1}{i(R-2r)} e^{ik(R-2r)} \right] \right\} \Big|_{-\frac{\pi}{a}}^{\frac{\pi}{a}}$$

$$= \frac{a}{2\pi} \left\{ \frac{\alpha}{2} \left[\frac{1}{i(R+r)} 2i \sin\pi \frac{R+r}{a} + \frac{1}{i(R-r)} 2i \sin\pi \frac{R-r}{a} \right] \right.$$

$$\left. + \frac{\beta}{2i} \left[\frac{1}{i(R+2r)} 2i \sin\pi \frac{R+2r}{a} - \frac{1}{i(R-2r)} 2i \sin\pi \frac{R-2r}{a} \right] \right.$$

$$= \frac{1}{2\pi} \left\{ \alpha \left[\frac{\sin\pi \frac{R+r}{a}}{(R+r)/a} + \frac{\sin\pi \frac{R-r}{a}}{(R-r)/a} \right] - i\beta \left[\frac{\sin\pi \frac{R+2r}{a}}{(R+2r)/a} - \frac{\sin\pi \frac{R-2r}{a}}{(R-2r)/a} \right] \right\} \quad *$$

$\boxed{\text{No symmetry}}$ $\quad Re\{W(r)\} = Re\{W(-r)\}$

$Im\{W(r)\} = -Im\{W(-r)\}$ *

(b)

With $R=0$, $\alpha=\beta=1$,

$W(r) = \frac{a}{\pi r} \sin\frac{\pi r}{a}$ } Plot out to few lattice constant.

$R=0,\ \alpha=0 \Rightarrow W(r)=0.$ *

$R=0,\ \beta=0 \Rightarrow W(r) = \frac{a\alpha}{\pi r} \cdot \sin\frac{\pi r}{a}$ *