Physics 460/560

Problem set # 5 Solutions

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a) $$\psi(a/2) = e^{ika}\,\psi(-a/2) \qquad (1)$$

$$\psi'(a/2) = e^{ika}\,\psi'(-a/2) \qquad (2)$$

$$\psi(x) = A\,\psi_\ell(x) + B\,\psi_r(x)$$

$\Rightarrow$ 2 homogeneous equations in 2 unknowns.

$$\psi_\ell(x) = \begin{cases} e^{iKx} + r e^{-iKx}, & x \le -\frac{a}{2} \\ t e^{iKx}, & x \ge \frac{a}{2} \end{cases}$$

$$\psi_r(x) = \begin{cases} t e^{-iKx}, & x \le -\frac{a}{2} \\ e^{-iKx} + r e^{iKx}, & x \ge \frac{a}{2} \end{cases}$$

(1) $$A\left(\psi_\ell(a/2) - e^{ika}\psi_\ell(-a/2)\right) + B\left(\psi_r(a/2) - e^{ika}\psi_r(-a/2)\right) = 0$$

(2) $$A\left(\psi_\ell'(a/2) - e^{ika}\psi_\ell'(-a/2)\right) + B\left(\psi_r'(a/2) - e^{ika}\psi_r'(-a/2)\right) = 0$$

$$\Rightarrow \quad 0 = \begin{vmatrix} \psi_\ell(a/2) - e^{ika}\psi_\ell(-a/2) & \psi_r(a/2) - e^{ika}\psi_r(-a/2) \\ \psi_\ell'(a/2) - e^{ika}\psi_\ell'(-a/2) & \psi_r'(a/2) - e^{ika}\psi_r'(-a/2) \end{vmatrix}$$

To avoid confusion, let $k \rightarrow \mathscr{k}$.

$$0 = \left(t - re^{ika} - e^{i(k-K)a}\right)\left(e^{-iKa} - r - te^{ika}\right) + \left(e^{-iKa} + r - te^{ika}\right)\left(t + re^{ika} - e^{i(k-K)a}\right)$$

$$0 = te^{-iKa} \cancel{- tr} - t^2e^{ika} \cancel{- re^{i(k-K)a}} + r^2e^{ika} \cancel{+ tre^{i2ka}} - e^{i(k-2K)a} \cancel{+ re^{i(k-K)a}} + te^{i(2k-K)a}$$
$$+ te^{-iKa} \cancel{+ tr} - t^2e^{ika} \cancel{+ re^{i(k-K)a}} + r^2e^{ika} \cancel{- tre^{2ika}} - e^{i(k-2K)a} \cancel{- re^{i(k-K)a}} + te^{i(2k-K)a}$$

$$0 = 2te^{-iKa} - 2t^2e^{ika} + 2te^{i(2k-K)a} + 2r^2e^{ika} - 2e^{i(k-2K)a}$$

- multiply by $\frac{e^{ika} e^{-ika}}{2t}$

$$e^{-ika} - te^{ika} + e^{ika}$$

$$+ \frac{r^2}{t} e^{ika} - \frac{1}{t} e^{-ika} = 0$$

- $$\cos ka = \frac{t^2 e^{ika} - r^2 e^{ika}}{2t} + \frac{1}{2t} e^{-ika}$$

$$\boxed{\cos ka = \frac{t^2 - r^2}{2t} e^{ika} + \frac{1}{2t} e^{-ika}}$$

b) $W(\phi_1, \phi_2) = \phi_1'(x)\, \phi_2(x) - \phi_1(x)\, \phi_2'(x)$

- $$-\frac{\hbar^2}{2m} \phi_i'' + V\phi_i = E\phi_i$$

- $W'(\phi_1, \phi_2) = \phi_1'' \phi_2 - \phi_1 \phi_2''$

$$\phi_i'' = (V - E)\frac{2m}{\hbar^2}\phi_i$$

$$W'(\phi_1, \phi_2) = \phi_2 (V - E)\frac{2m}{\hbar^2}\phi_1$$
$$- \phi_1 (V - E)\frac{2m}{\hbar^2}\phi_2 = 0$$

- c) $W(\psi_\ell, \psi_\ell^*) = \psi_\ell' \psi_\ell^* - \psi_\ell \psi_\ell^{*\prime}$

For $x \geq \frac{a}{2}$, $\psi_\ell(x) = t e^{iKx}$
$$\psi_\ell'(x) = iKte^{iKx}$$

$$W(\psi_\ell, \psi_\ell^*) = iKte^{iKx}(t^* e^{-iKx})$$
- $$- te^{iKx}(-iK t^* e^{-iKx})$$
$$= 2iK |t|^2$$

- For $x \leq -\frac{a}{2}$,

$$\psi_\ell(x) = e^{ikx} + re^{-ikx}$$

$$\psi_\ell'(x) = ik(e^{ikx} - re^{-ikx})$$

$$W(\psi_\ell, \psi_\ell^*) = ik(e^{ikx} - re^{-ikx})(e^{-ikx} + r^* e^{ikx})$$

$$- (e^{ikx} + re^{-ikx})(-ik)(e^{-ikx} - r^* e^{ikx})$$

- $$= ik(1 - |r|^2 - re^{-2ikx} + r^* e^{2ikx})$$

$$+ ik(1 - |r|^2 + re^{-2ik} - r^* e^{2ikx})$$

$$= 2ik(1 - |r|^2)$$

- But $W(\psi_\ell, \psi_\ell^*)$ is independent of x.

$$\Rightarrow \boxed{|t|^2 = 1 - |r|^2}$$

d) $W(\psi_\ell, \psi_r^*) = \psi_\ell' \psi_r^* - \psi_\ell \psi_r^{*\prime}$

For $x \geq \frac{a}{2}$,

$$\psi_\ell = te^{iKx}$$

$$\psi_\ell' = iKte^{iKx}$$

$$\psi_r^* = e^{iKx} + r^* e^{-iKx}$$

$$\psi_r^{*\prime} = iK(e^{iKx} - r^* e^{-iKx})$$

$$W(\psi_\ell, \psi_r^*) = iKte^{iKx}(e^{iKx} + r^* e^{-iKx}) - te^{iKx} iK(e^{iKx} - r^* e^{-iKx})$$

$$= iKte^{iKx}\left(\cancel{e^{iKx}} + r^* e^{-iKx} \cancel{- e^{iKx}} + r^* e^{-iKx}\right)$$

$$= 2iKtr^*$$

For $x \le \frac{a}{2}$, $\psi_l = e^{ikx} + re^{-ikx}$

$\psi_l' = ik(e^{ikx} - re^{-ikx})$

$\psi_r^* = t^* e^{ikx}$

$\psi_r^{*\prime} = ikt^* e^{ikx}$

$$W(\psi_l, \psi_r^*) = ik(e^{ikx} - re^{-ikx})t^* e^{ikx} - (e^{ikx} + re^{-ikx}) ikt^* e^{ikx}$$

$$= ikt^* e^{ikx} \left(\cancel{e^{ikx}} - re^{-ikx} \cancel{- e^{ikx}} - re^{-ikx} \right)$$

$$= -2ikt^* r$$

$$\Rightarrow 2ikt r^* = -2ikt^* r$$

$$t r^* = -t^* r$$

$$tr^* + t^* r = 0$$

$$tr^* + (tr^*)^* = 0$$

$\Rightarrow$ tr^* is pure imaginary.

$$t = |t| e^{i\delta} \qquad \text{Let } r = |r| e^{i\theta}$$

$$rt^* = r|t| e^{-i\delta} = |r||t| e^{i(\theta-\delta)}$$

$$0 = \mathrm{Re}\{rt^*\} = |r||t| \cos(\theta - \delta) = 0$$

$$\theta - \delta = (2n+1)\frac{\pi}{2} \qquad n \in \mathbb{Z}$$

$$e^{i\theta} = e^{i\delta} e^{i\pi n} e^{i\pi/2}$$

$$= i e^{i\delta} (-1)^n$$

$$\Longrightarrow \quad r = |r| e^{i\theta} = \pm i |r| e^{i\delta}$$

e) $$\cos ka = \frac{t^2 - r^2}{2t} e^{ika} + \frac{1}{2t} e^{-ika}$$

$$t = |t| e^{i\delta} \qquad r = \pm i |r| e^{i\delta}$$

$$\cos ka = \frac{|t|^2 + |r|^2}{2|t|} e^{i\delta} e^{ika} + \frac{1}{2|t|} e^{-ika} e^{-i\delta}$$

$$\boxed{\cos ka = \frac{\cos(ka + \delta)}{|t|}, \quad \mathcal{E} = \frac{\hbar^2 k^2}{2m}}$$

f) $|t| \approx 1$, $|r| \ll 1$

$$|t| = \sqrt{1 - |r|^2} \simeq 1 - \frac{|r|^2}{2} + \cdots$$

Also, assume
$\delta \approx 0$.

$$\cos ka = \frac{\cos Ka}{|t|} > 1 \quad \text{is forbidden}$$

Gaps lie between the points
satisfying $\dfrac{\cos Ka}{|t|} = \pm 1$

$$\cos Ka = \pm |t| \simeq \pm\left(1 - \frac{|r|^2}{2} + \cdots\right)$$

For $Ka = n\pi + \epsilon$, one has

$$\cos Ka = (-1)^n \left(1 - \frac{\epsilon^2}{2} + \cdots\right)$$

$$\Rightarrow \quad 1 - \frac{\epsilon^2}{2} \simeq 1 - \frac{|r|^2}{2}$$

$$|\epsilon| = |r|$$

- $\epsilon = ka - n\pi = \pm |r|$

$ka = n\pi \pm |r|$

$$\mathcal{E} = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a} \pm \frac{|r|}{a}\right)^2$$

$$\simeq \frac{\hbar^2 n^2 \pi^2}{2ma^2} \pm \frac{\hbar^2 n\pi |r|}{ma^2}$$

- The energy gap is thus

$$\Delta \cong \frac{2\pi n \hbar^2}{ma^2} |r|$$

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g) $\cos(ka + \delta) = |t| \cos ka$

- $|\cos(ka+\delta)| \leq |t| \ll 1$

$\Rightarrow ka + \delta = (2n+1)\frac{\pi}{2} + \epsilon, \quad \epsilon \ll 1$

- $$\cos(ka+\delta) = \cos\left[(2n+1)\frac{\pi}{2} + \epsilon\right]$$

$$\simeq -\sin\left[(2n+1)\frac{\pi}{2}\right]\epsilon = (-1)^{n+1}\epsilon$$

$$(-1)^{n+1}\epsilon \cong |t|\cos ka$$

$$\epsilon \simeq (-1)^{n+1}|t|\cos ka$$

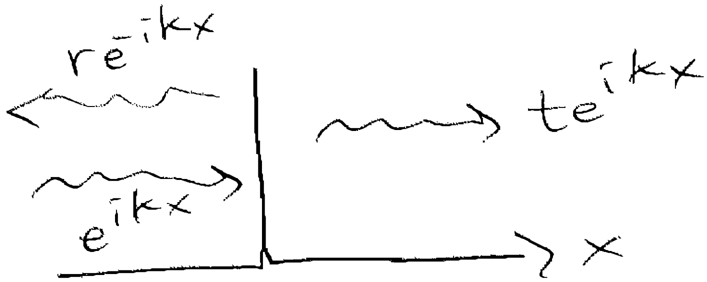
- $$\mathcal{E} = \frac{\hbar^2 K^2}{2m} = \frac{\hbar^2}{2m}\left((2n+1)\frac{\pi}{2a} \underset{-\frac{\delta}{a}}{} + \frac{\epsilon}{a}\right)^2$$

$$\cong \frac{\hbar^2\pi^2}{2ma^2}\left(n+\frac{1}{2}\right)^2 + \frac{\hbar^2\pi}{ma^2}\left(n+\frac{1}{2}\right)\epsilon$$

$$\mathcal{E} \simeq \text{Const.} + (-1)^{n+1}\frac{\hbar^2\pi}{ma^2}\left(n+\frac{1}{2}\right)|t|\cos ka$$

- $\Rightarrow$ Bandwidth $\mathcal{O}(|t|)$.

h) $V(x) = g\,\delta(x)$



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

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

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

$$\psi'(\epsilon) - \psi'(-\epsilon) = \frac{2mg}{\hbar^2}\psi(0) - \int_{-\epsilon}^{\epsilon} dx\,\frac{2m}{\hbar^2}E\,\psi(x)$$

$$\lim_{\epsilon\to 0^+}\psi'(\epsilon) - \psi'(-\epsilon) = \frac{2mg}{\hbar^2}\psi(0) - 0$$

$$\psi'(0^+) - \psi'(0^-) = \frac{2mg}{\hbar^2}\psi(0)$$

- The second condition is $\psi(0^+) = \psi(0^-)$ (wave function must be continuous).

$\Rightarrow 1 + r = t.$

- $$\psi'(0^+) - \psi'(0^-) = \frac{2mg}{\hbar^2}\psi(0^+)$$

$$ikt - ik(1-r) = \frac{2mg}{\hbar^2} t$$

$$ik(t - 1 + r) = \frac{2mg}{\hbar^2} t$$

$$2ik(t-1) = \frac{2mg}{\hbar^2} t$$

- $$t\left(ik - \frac{mg}{\hbar^2}\right) = ik$$

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$$t = \frac{ik}{ik - \frac{mg}{\hbar^2}} = |t|e^{i\delta}$$

$$t = \frac{1}{1 + i\frac{mg}{\hbar^2 k}} = |t|e^{i\delta}$$

$$\tan\delta = -\frac{mg}{\hbar^2 k} \qquad \cot\delta = -\frac{\hbar^2 k}{mg}$$

$$|t|^2 = \frac{1}{1 + \left(\frac{mg}{\hbar^2 k}\right)^2} = \frac{1}{1 + \tan^2\delta}$$

$$= \frac{\cos^2\delta}{\cos^2\delta + \sin^2\delta} = \cos^2\delta$$

$$|t| = \cos\delta$$

Q.E.D.