731 Homework #7

Due October 27th, 2006

1. A&M, problem 8.1
   a) 10 pts
   b) 5
   c) 5
   d) 5
   e) 5
   f) 5
   g) 5
   h) 5
   total 45

2. A&M, problem 8.2
   a) 5 pts
   b) 10
   c) 10
   total 25

8.1

a) $\psi(x) = A\psi_l(x) + B\psi_r(x)$ is general solution to all regions

Bloch condition

$$\begin{cases} \psi(x+a) = e^{iKa}\psi(x) \\ \psi'(x+a) = e^{iKa}\psi'(x) \end{cases} \quad \text{let } x = -a/2$$

$$\Rightarrow \begin{cases} A\psi_l(a/2) + B\psi_r(a/2) = e^{iKa}A\psi_l(-a/2) + e^{iKa}B\psi_r(-a/2) \\ A\psi_l'(a/2) + B\psi_r'(a/2) = e^{iKa}\left(A\psi_l'(-a/2) + B\psi_r'(-a/2)\right) \end{cases}$$

$\Rightarrow$ to Solve $\longrightarrow$ $\boxed{\cos Ka = \frac{t^2 - r^2}{2t} e^{iKa} + \frac{1}{2t} e^{-iKa} \qquad \varepsilon = \frac{\hbar^2 k^2}{2m}}$

$t = 1$, $r = 0$ no Barrier:

$$\cos Ka = \frac{1}{2} e^{iKa} + \frac{1}{2} e^{-iKa} = \cos Ka$$

$\rightarrow$ free electron case.

b) $W = \varphi_1'\varphi_2 - \varphi_1\varphi_2'$; $\frac{\partial W}{\partial x} = \varphi_1''\varphi_2 - \varphi_1\varphi_2''$

$$\left.\begin{aligned} -\frac{\hbar^2}{2m}\varphi_1'' + V\varphi_1 &= \frac{\hbar^2 k^2}{2m}\varphi_1 \quad * \ \varphi_2 \\ -\frac{\hbar^2}{2m}\varphi_2'' + V\varphi_2 &= \frac{\hbar^2 k^2}{2m}\varphi_2 \quad * \ (-\varphi_1) \end{aligned}\right\} \xrightarrow{+} \varphi_1''\varphi_2 = \varphi_1\varphi_2'' \quad \rightarrow \frac{\partial W}{\partial x} = 0$$

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

$W\big|_{-a/2} = W\big|_{x=-a/2} = 2ik(1-|r|^2)$

$W\big|_{a/2} = 2ik|t|^2$

$\frac{\partial W}{\partial x} = 0 \rightarrow$ W independence of x $\Rightarrow W\big|_{a/2} = W\big|_{-a/2}$

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

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

$$\left.\begin{aligned} W(\varphi_\ell, \varphi_r^*)\big|_{-a/2} &= -2ik t^* r \\ W(\varphi_\ell, \varphi_r^*)\big|_{a/2} &= 2ik t r^* \end{aligned}\right\} t^* r = -t r^* = -(t^* r)^*$$

$\Rightarrow t^* r$ is pure imaginary, $t = |t| \cdot e^{i\delta}$, $r = \pm i |r| e^{i\delta}$

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

$$= \frac{1}{2|t|}\Big[\underbrace{(|t|^2 + |r|^2)}_{1} e^{i\delta} e^{ika} + e^{-i\delta} e^{-ika}\Big]$$

$$\boxed{\cos ka = \frac{1}{|t|}\cos(ka+\delta)}$$

f) barrier is very weak $|t| \approx 1$, $|r| \approx 0$, $\delta \approx 0$

$$\frac{\cos(ka+\delta)}{|t|} \simeq \frac{\cos(ka+\delta)}{\sqrt{1-|r|^2}} \approx \cos(ka+\delta)\left[1 - \tfrac{1}{2}(-|r|^2)\right]$$

$$= \cos(ka+\delta)\left(1 + \tfrac{1}{2}|r|^2\right)$$

$\Rightarrow \exists\ ka + \delta = n\pi$ where $\left|\frac{\cos(ka+\delta)}{|t|}\right| \to$ maximum.

$$\left|\frac{\cos(ka+\delta)}{|t|}\right| \simeq 1$$

$\Rightarrow \left|\cos(n\pi + \Delta k a)\left(1 + \frac{1}{2}|r|^2\right)\right| = 1$; $\Delta k = k - \frac{n\pi}{a}$

expand $\cos(n\pi + \Delta k a)$

$\Rightarrow \left|\left(\cos n\pi + \frac{1}{2}(-\cos n\pi)\Delta k^2 a^2\right)\left(1 + \frac{1}{2}|r|^2\right)\right| = 1$

$$\Leftrightarrow \quad \left| \cos n\pi \left(1 - \frac{1}{2}\Delta k^2 a^2\right)\left(1 + \frac{1}{2}|r|^2\right) \right| = 1 \qquad (4)$$

$$\left| 1 + \frac{1}{2}|r|^2 - \frac{1}{2}\Delta k^2 a^2 \right| = 1$$

$$\Leftrightarrow \quad \frac{1}{2}|r|^2 = \frac{1}{2}\Delta k^2 a^2$$

$$\Rightarrow \quad \boxed{\Delta k \simeq \frac{|r|}{a}}$$

$$\mathcal{E}_{gap} = \mathcal{E}\left(\frac{n\pi}{a} + \frac{|r|}{a}\right) - \mathcal{E}\left(\frac{n\pi}{a} - \frac{|r|}{a}\right)$$

$$= \frac{\hbar^2}{2m}\left(\frac{n^2\pi^2}{a^2} + \left(\frac{|r|}{|a|}\right)^2 + 2\frac{n\pi}{a^2}|r|\right) - \frac{\hbar^2}{2m}\left(\frac{n^2\pi^2}{a^2} + \frac{|r|^2}{a^2} - 2\frac{n\pi|r|}{a^2}\right)$$

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

g) $|t| \approx 0$, $|r| \approx 1$

$\exists$ $ka + \delta = n\pi + \frac{\pi}{2}$ so $\frac{\cos(ka+\delta)}{|t|} = 0$

when $k \neq n\pi + \pi/2$; $\left| \frac{\cos(ka+\delta)}{|t|} \right| = 1$

$$\cos(ka+\delta) \overset{k \approx \pi/2a}{=} \cos(\bar{k}a + \delta + \Delta k . a) = \cos(n\pi + \frac{\pi}{2} + \Delta ka)$$

$$\left| \frac{\cos(ka+\delta)}{|t|} \right| = \frac{\cos(n\pi + \pi/2) + \sin(n\pi + \pi/2)\, \Delta ka + \ldots}{|t|}$$

$$= \frac{\sin(n\pi + \frac{\pi}{2})}{|t|} \Delta k . a = 1$$

$$\Rightarrow \boxed{\Delta k = \frac{|t|}{a}}$$

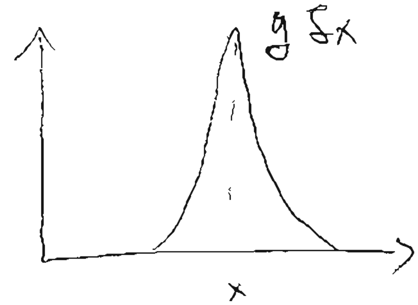
$$\varepsilon_{gap} = \frac{\hbar^2}{2m} \left[\left(k + \frac{|t|}{a}\right)^2 - \left(k - \frac{|t|}{a}\right)^2 \right]$$

$$= \frac{\hbar^2}{2m} 4k \frac{|t|}{a}$$

$$\simeq |t| \simeq O(t)$$

h)

$$\psi_e = \begin{cases} e^{ikx} + r e^{-ikx} \\ t e^{ikx} \end{cases}$$



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

$$\psi(0^+) = \psi(0^-)$$

integrate fo $-\varepsilon$ to ε. $\quad \varepsilon \ll 1 \; ; \; \varepsilon \to 0$

$$-\frac{\hbar^2}{2m}\left(\psi'(0+) - \psi'(0-)\right) = g\psi(0)$$

$$-\frac{\hbar^2}{2m}\left(ikt - ik + ikr\right) = gt \qquad (r = t-1)$$

$$\Leftrightarrow \quad \frac{i\hbar^2}{2m}k\,(t-1) = gt \Rightarrow t = \frac{1}{1 + \frac{mg}{\hbar^2 k} i}$$

$$|t| = \frac{1}{\sqrt{1 + \frac{mg^2}{\hbar^2 k^2}}} = \cos\delta \qquad (t = |t|e^{i\delta})$$

$$\cot\delta = \frac{\cos\delta}{\sin\delta} = -\frac{\hbar^2 k}{mg}$$

$-$ sign due to 4^{th} quadrant

a) $$g_n(\mathcal{E}) = \int_{S_n(\mathcal{E})} \frac{dS}{4\pi^3} \frac{1}{|\nabla \mathcal{E}_n(k)|}$$

$$g_n(\mathcal{E}_F) = \int_{S_n(\mathcal{E}_F)} \frac{dS}{4\pi^3} \frac{1}{|\nabla_k \mathcal{E}_n(k)|} \quad ; \quad \mathcal{E}_n(k) = \frac{\hbar^2 k^2}{2m}$$

$$g_n(\mathcal{E}_F) = \frac{4\pi k_F^2}{4\pi^3} \cdot \frac{1}{\frac{\hbar^2}{m} k_F} = \frac{m k_F}{\hbar^2 \pi^2}$$

b) $$g_n(\mathcal{E}) = \int \frac{d\vec{k}}{4\pi^3} \delta(\mathcal{E} - \mathcal{E}_n(k)) = \int \frac{dk}{4\pi^3} \delta(\ldots)$$

$$g_n(\mathcal{E}) = \int \frac{d\vec{k}}{4\pi^3} \delta\left(\mathcal{E} - \mathcal{E}_0 - \frac{\hbar^2}{2}\frac{k_x^2}{m_x} - \frac{\hbar^2}{2}\frac{k_y^2}{m_y} - \frac{\hbar^2}{2}\frac{k_z^2}{m_z}\right)$$

$$k_i' = \frac{\hbar}{\sqrt{2m_i}} k_i$$

$$g_n(\mathcal{E}) = \sqrt{m_x m_y m_z} \left(\frac{\sqrt{2}}{\hbar}\right)^3 \int \frac{dk_x' \, dk_y' \, dk_z'}{4\pi^3} \delta(\mathcal{E} - \mathcal{E}_0 - (k_x'^2 + k_y'^2 + k_z'^2))$$

$$= \text{Constant.} \int q\,dq \int dq_z \, \delta(q^2 + q_z^2 + \mathcal{E}_0 - \mathcal{E})$$

$$\{ q^2 = q_x^2 + q_y^2, \ q, \varphi, q_z \text{ cylindrical} \}$$

$$\int \delta(f(x))\,dx = \sum_{x_0} \frac{1}{\left(\frac{\partial f}{\partial x}\right)_{x_0}}$$

$$f(x_0) = 0.$$

$$g_n(\varepsilon) = c \int q\,dq \sum_{q_0} \frac{1}{2|q_{z0}|} \quad ; \; c \text{ is constant}$$

$$q_{z0} = \pm\sqrt{\varepsilon - \varepsilon_0 - q^2} \quad , \; f(q_z) = 0$$

$$g_n(\varepsilon) = c/2 \int_0^{\sqrt{\varepsilon-\varepsilon_0}} \frac{q}{\sqrt{\varepsilon-\varepsilon_0-q^2}}\,dq \sim \sqrt{\varepsilon-\varepsilon_0}$$

$$\Rightarrow \frac{\partial g}{\partial \varepsilon} \sim (\varepsilon-\varepsilon_0)^{-1/2} \xrightarrow{\varepsilon\to\varepsilon_0} 0$$

$$g_n(\varepsilon_F) = \frac{c}{2}\sqrt{\varepsilon_F - \varepsilon_0}$$

$$n = \int d\varepsilon\, g(\varepsilon) = \frac{c}{3}(\varepsilon_F - \varepsilon_0)^{3/2}$$

$$\Rightarrow g_n(\varepsilon_F) = \frac{3}{2}\, n/\varepsilon_F - \varepsilon_0$$

c)

$$g_n = c \int q\,dq \sum_{q_z} \frac{1}{2|q_{z0}|} \quad ; \; q_{z0} = \pm\sqrt{\varepsilon_0 - \varepsilon + q^2}$$

$$g_n(\varepsilon) = \frac{c}{4} \int \frac{dq^2}{\sqrt{\varepsilon_0-\varepsilon+q^2}}$$

if $\varepsilon < \varepsilon_0 \rightarrow \quad g_n(\varepsilon) = \frac{c}{2}\sqrt{\varepsilon_0 - \varepsilon}$

$$g_n'(\varepsilon) \approx (\varepsilon_0 - \varepsilon)^{-1/2}$$

if $\varepsilon > \varepsilon_0$

$$g_n(\varepsilon) = \frac{\cancel{c}}{2}\sqrt{\varepsilon_0 - \varepsilon + q^2}\,\Big|_{\varepsilon - \varepsilon_0}^{\varepsilon - \varepsilon_0 + \theta(\varepsilon - \varepsilon_0)}$$

$$\simeq \theta(\varepsilon - \varepsilon_0).$$

$$g_n'(\varepsilon) = \text{constant.}$$