PHYS 635 Solid State Physics
Take home exam 1

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Problem 1:Ashcroft & Mermin, Ch.10, p.189, prob.2

a) Let's prove

$$\beta_{xx} = \beta_{yy} = \beta_{zz} = \beta \tag{1}$$

$$\begin{aligned} \beta_{xx} = & -\int d\mathbf{r} \cdot \Psi_x^*(\mathbf{r}) \cdot \Psi_x(\mathbf{r}) \cdot \Delta U(\mathbf{r}) = -\int d\mathbf{r} \cdot x^2 \cdot |\phi(\mathbf{r})|^2 \cdot \Delta U(\mathbf{r}) \\ = & -\int d\mathbf{r} \cdot y^2 \cdot |\phi(\mathbf{r})|^2 \cdot \Delta U(\mathbf{r}) = -\int d\mathbf{r} \cdot \Psi_y^*(\mathbf{r}) \cdot \Psi_y(\mathbf{r}) \cdot \Delta U(\mathbf{r}) = \beta_{yy} \end{aligned} \tag{2}$$

Now

$$0 = \beta_{xx} - \beta_{yy} = -\int d\mathbf{r} \cdot (x^2 - y^2) \cdot |\phi(\mathbf{r})|^2 \cdot \Delta U(\mathbf{r}) \tag{3}$$

If we here make the change of variables: $x\prime = x - y; y\prime = x + y$, which is basically rotation in space, then we will get

$$0 = \beta_{xx} - \beta_{yy} = -\int d\mathbf{r}\prime \cdot (x\prime \cdot y\prime) \cdot |\phi(\mathbf{r}\prime)|^2 \cdot \Delta U(\mathbf{r}\prime) = \beta_{xy} = 0 \tag{4}$$

b) In the case of a simple cubic Bravais lattice with $\gamma_{ij}(\mathbf{R})$ negligible for all but the nearest-neighbor $\mathbf{R}$ let's calculate $\tilde{\gamma}_{xy}(\mathbf{k})$. We should take into account 6 neighbors:

$$\mathbf{R} = a(\pm 1, 0, 0); a(0, 0, \pm 1); a(0, \pm 1, 0) \tag{5}$$

$$\begin{aligned} \tilde{\gamma}_{xy}(\mathbf{k}) = & - e^{ik_x a} \int d\mathbf{r} \cdot xy\phi(\mathbf{r})\phi\left(\left((x-a)^2 + y^2 + z^2\right)^{\frac{1}{2}}\right) \Delta U(\mathbf{r}) \\ & - e^{-ik_x a} \int d\mathbf{r} \cdot xy\phi(\mathbf{r})\phi\left(\left((x+a)^2 + y^2 + z^2\right)^{\frac{1}{2}}\right) \Delta U(\mathbf{r}) \\ & - e^{ik_y a} \int d\mathbf{r} \cdot x(y-a)\phi(\mathbf{r})\phi\left(\left(x^2 + (y-a)^2 + z^2\right)^{\frac{1}{2}}\right) \Delta U(\mathbf{r}) \\ & - e^{-ik_y a} \int d\mathbf{r} \cdot x(y+a)\phi(\mathbf{r})\phi\left(\left(x^2 + (y+a)^2 + z^2\right)^{\frac{1}{2}}\right) \Delta U(\mathbf{r}) \\ & - e^{ik_z a} \int d\mathbf{r} \cdot xy\phi(\mathbf{r})\phi\left(\left(x^2 + y^2 + (z-a)^2\right)^{\frac{1}{2}}\right) \Delta U(\mathbf{r}) \\ & - e^{-ik_z a} \int d\mathbf{r} \cdot xy\phi(\mathbf{r})\phi\left(\left(x^2 + y^2 + (z+a)^2\right)^{\frac{1}{2}}\right) \Delta U(\mathbf{r}) = 0 \end{aligned} \tag{6}$$

, because under rotation transformation x→y, y→-x each integral changes sign.

c) The energies are found by setting to zero the determinant:

$$|(\varepsilon(\mathbf{k}) - E_p)\delta_{ij} + \beta_{ij} + \tilde{\gamma}_{ij}(\mathbf{k})| = 0 \tag{7}$$

First we will prove that

$$\varepsilon(\mathbf{k}) - E_p + \beta + \tilde{\gamma}_{xx}(\mathbf{k}) = \varepsilon(\mathbf{k}) - lon^0(\mathbf{k}) + 4\gamma_0 cos\left(\frac{1}{2}k_y a\right) cos\left(\frac{1}{2}k_z a\right) \tag{8}$$

, where $\varepsilon^0(\mathbf{k})$,$\gamma_0$,$\gamma_1$ and γ_2 are those from A & M. In nearest-neighbor approximation we will have the 12 nearest neighbors of the origin at

$$\mathbf{R} = \frac{a}{2}(\pm1, \pm1, 0); \frac{a}{2}(\pm1, 0, \pm1); \frac{a}{2}(0, \pm1, \pm1) \tag{9}$$

In order to prove (6) we should calculate $\tilde{\gamma}_{xx}(k)$ in this approximation:

$$\begin{aligned}
\tilde{\gamma}_{xx}(k) = &\sum_R e^{i\mathbf{kR}}\gamma_{xx}(\mathbf{R}) = \\
&- e^{i\frac{a}{2}(k_x+k_y)} \int d\mathbf{r}\cdot x\left(x-\frac{a}{2}\right)\phi(\mathbf{r})\phi\left(\left(\left(x-\frac{a}{2}\right)^2 + \left(y-\frac{a}{2}\right)^2 + z^2\right)^{\frac{1}{2}}\right)\Delta U(\mathbf{r}) \\
&- e^{i\frac{a}{2}(k_x-k_y)} \int d\mathbf{r}\cdot x\left(x-\frac{a}{2}\right)\phi(\mathbf{r})\phi\left(\left(\left(x-\frac{a}{2}\right)^2 + \left(y+\frac{a}{2}\right)^2 + z^2\right)^{\frac{1}{2}}\right)\Delta U(\mathbf{r}) \\
&- e^{i\frac{a}{2}(-k_x+k_y)} \int d\mathbf{r}\cdot x\left(x+\frac{a}{2}\right)\phi(\mathbf{r})\phi\left(\left(\left(x+\frac{a}{2}\right)^2 + \left(y-\frac{a}{2}\right)^2 + z^2\right)^{\frac{1}{2}}\right)\Delta U(\mathbf{r}) \\
&- e^{i\frac{a}{2}(-k_x-k_y)} \int d\mathbf{r}\cdot x\left(x+\frac{a}{2}\right)\phi(\mathbf{r})\phi\left(\left(\left(x+\frac{a}{2}\right)^2 + \left(y+\frac{a}{2}\right)^2 + z^2\right)^{\frac{1}{2}}\right)\Delta U(\mathbf{r}) \\
&- e^{i\frac{a}{2}(k_x+k_z)} \int d\mathbf{r}\cdot x\left(x-\frac{a}{2}\right)\phi(\mathbf{r})\phi\left(\left(\left(x-\frac{a}{2}\right)^2 + y^2 + \left(z-\frac{a}{2}\right)^2\right)^{\frac{1}{2}}\right)\Delta U(\mathbf{r}) \\
&- e^{i\frac{a}{2}(k_x-k_z)} \int d\mathbf{r}\cdot x\left(x-\frac{a}{2}\right)\phi(\mathbf{r})\phi\left(\left(\left(x-\frac{a}{2}\right)^2 + y^2 + \left(z+\frac{a}{2}\right)^2\right)^{\frac{1}{2}}\right)\Delta U(\mathbf{r}) \\
&- e^{i\frac{a}{2}(-k_x+k_z)} \int d\mathbf{r}\cdot x\left(x+\frac{a}{2}\right)\phi(\mathbf{r})\phi\left(\left(\left(x+\frac{a}{2}\right)^2 + y^2 + \left(z-\frac{a}{2}\right)^2\right)^{\frac{1}{2}}\right)\Delta U(\mathbf{r}) \\
&- e^{i\frac{a}{2}(-k_x-k_z)} \int d\mathbf{r}\cdot x\left(x+\frac{a}{2}\right)\phi(\mathbf{r})\phi\left(\left(\left(x+\frac{a}{2}\right)^2 + y^2 + \left(z+\frac{a}{2}\right)^2\right)^{\frac{1}{2}}\right)\Delta U(\mathbf{r}) \\
&- e^{i\frac{a}{2}(k_y+k_z)} \int d\mathbf{r}\cdot x^2\phi(\mathbf{r})\phi\left(\left(x^2 + \left(y-\frac{a}{2}\right)^2 + \left(z-\frac{a}{2}\right)^2\right)^{\frac{1}{2}}\right)\Delta U(\mathbf{r}) \\
&- e^{i\frac{a}{2}(k_y-k_z)} \int d\mathbf{r}\cdot x^2\phi(\mathbf{r})\phi\left(\left(x^2 + \left(y-\frac{a}{2}\right)^2 + \left(z+\frac{a}{2}\right)^2\right)^{\frac{1}{2}}\right)\Delta U(\mathbf{r}) \\
&- e^{i\frac{a}{2}(-k_y+k_z)} \int d\mathbf{r}\cdot x^2\phi(\mathbf{r})\phi\left(\left(x^2 + \left(y+\frac{a}{2}\right)^2 + \left(z-\frac{a}{2}\right)^2\right)^{\frac{1}{2}}\right)\Delta U(\mathbf{r}) \\
&- e^{i\frac{a}{2}(-k_y-k_z)} \int d\mathbf{r}\cdot x^2\phi(\mathbf{r})\phi\left(\left(x^2 + \left(y+\frac{a}{2}\right)^2 + \left(z+\frac{a}{2}\right)^2\right)^{\frac{1}{2}}\right)\Delta U(\mathbf{r})
\end{aligned} \tag{10}$$

Notice that

$$-\int d\mathbf{r}\cdot x\left(x-\frac{a}{2}\right)\phi(\mathbf{r})\phi\left(\left(\left(x-\frac{a}{2}\right)^2 + \left(y-\frac{a}{2}\right)^2 + z^2\right)^{\frac{1}{2}}\right)\Delta U(\mathbf{r}) = \gamma_2 \tag{11}$$

$$-\int d\mathbf{r}\cdot x^2\phi(\mathbf{r})\phi\left(\left(x^2 + \left(y+\frac{a}{2}\right)^2 + \left(z+\frac{a}{2}\right)^2\right)^{\frac{1}{2}}\right)\Delta U(\mathbf{r}) = \gamma_0 + \gamma_2 \tag{12}$$

Thus we have:

$$\begin{aligned}\tilde{\gamma}_{xx}(\mathbf{k}) =&\Big(e^{i\frac{a}{2}(k_x+k_y)} + e^{i\frac{a}{2}(k_x-k_y)} + e^{-i\frac{a}{2}(k_x+k_y)} + e^{-i\frac{a}{2}(k_x-k_y)}\\ &+ e^{i\frac{a}{2}(k_x+k_z)} + e^{i\frac{a}{2}(k_x-k_z)} + e^{-i\frac{a}{2}(k_x+k_z)} + e^{-i\frac{a}{2}(k_x-k_z)}\Big)\gamma_2\\ &+ \Big(e^{i\frac{a}{2}(k_y+k_z)} + e^{i\frac{a}{2}(k_y-k_z)} + e^{-i\frac{a}{2}(k_y+k_z)} + e^{-i\frac{a}{2}(k_y-k_z)}\Big)(\gamma_2+\gamma_0)\end{aligned} \tag{13}$$

And

$$\begin{aligned}\tilde{\gamma}_{xx}(\mathbf{k}) =&\Big(2cos\left(\frac{a}{2}(k_x+k_y)\right) + 2cos\left(\frac{a}{2}(k_x-k_y)\right)\\ &+ 2cos\left(\frac{a}{2}(k_x+k_z)\right) + 2cos\left(\frac{a}{2}(k_x-k_z)\right)\Big)\gamma_2\\ &+ \left(2cos\left(\frac{a}{2}(k_y+k_z)\right) + 2cos\left(\frac{a}{2}(k_y-k_z)\right)\right)(\gamma_2+\gamma_0) =\\ &\left(4cos\left(\frac{1}{2}k_xa\right)cos\left(\frac{1}{2}k_ya\right) + 4cos\left(\frac{1}{2}k_xa\right)cos\left(\frac{1}{2}k_za\right)\right)\gamma_2\\ &+ 4cos\left(\frac{1}{2}k_ya\right)cos\left(\frac{1}{2}k_za\right)(\gamma_2+\gamma_0)\end{aligned} \tag{14}$$

Now let's get back to (6):

$$\begin{aligned}&\varepsilon(\mathbf{k}) - E_p + \beta + \tilde{\gamma}_{xx}(\mathbf{k}) =\\ &\varepsilon(\mathbf{k}) - E_p + \beta + \left(4cos\left(\frac{1}{2}k_xa\right)cos\left(\frac{1}{2}k_ya\right) + 4cos\left(\frac{1}{2}k_xa\right)cos\left(\frac{1}{2}k_za\right)\right)\gamma_2 +\\ &4cos\left(\frac{1}{2}k_ya\right)cos\left(\frac{1}{2}k_za\right)(\gamma_2+\gamma_0) =\\ &\varepsilon(\mathbf{k}) - E_p + \beta + \Big(4cos\left(\frac{1}{2}k_xa\right)cos\left(\frac{1}{2}k_ya\right) + 4cos\left(\frac{1}{2}k_xa\right)cos\left(\frac{1}{2}k_za\right) +\\ &4cos\left(\frac{1}{2}k_ya\right)cos\left(\frac{1}{2}k_za\right)\Big)\gamma_2 + 4cos\left(\frac{1}{2}k_ya\right)cos\left(\frac{1}{2}k_za\right)\gamma_0 =\\ &\varepsilon(\mathbf{k}) - \varepsilon^0(\mathbf{k}) + 4\gamma_0 cos\left(\frac{1}{2}k_ya\right)cos\left(\frac{1}{2}k_za\right)\end{aligned} \tag{15}$$

The same way one can verify other elements of matrix (10.33) in A & M.

d) For $\mathbf{k}$=0 all three bands are degenerate and $\varepsilon_0 = E_p - \beta - 12\gamma_2 - 4\gamma_0 \Rightarrow E_p - \beta = \varepsilon_0 + 12\cdot\gamma_2 + 4\cdot\gamma_0$; ΓX - $\mathbf{k} = \left(\frac{2\pi\mu}{a}, 0, 0\right)$, where $0 \le \mu \le 1$.

$$\frac{e_1(\mu)}{e_0} = 1 + \frac{8\cdot\gamma_2}{e_0}\cdot(1 - cos(\pi\cdot\mu)) \tag{16}$$

$$\frac{e_2(\mu)}{e_0} = 1 + \frac{8\cdot\gamma_2 + 4\cdot\gamma_0}{e_0}\cdot(1 - cos(\pi\cdot\mu)) \tag{17}$$

the energy band (16) is double degenerate; ΓL - $\mathbf{k} = \frac{2\pi}{a}(\mu,\mu,\mu)$, where $0 \le \mu \le \frac{1}{2}$

$$\frac{e_1(\mu)}{e_0} = 1 + \frac{12\cdot\gamma_2 + 4\cdot\gamma_0 - 4\cdot\gamma_1}{e_0}\cdot(sin^2(\pi\cdot\mu)) \tag{18}$$

the energy band (18) is double degenerate,

$$\frac{e_2(\mu)}{e_0} = 1 + \frac{12\cdot\gamma_2 + 4\cdot\gamma_0 + 8\cdot\gamma_1}{e_0}\cdot(sin^2(\pi\cdot\mu)) \tag{19}$$

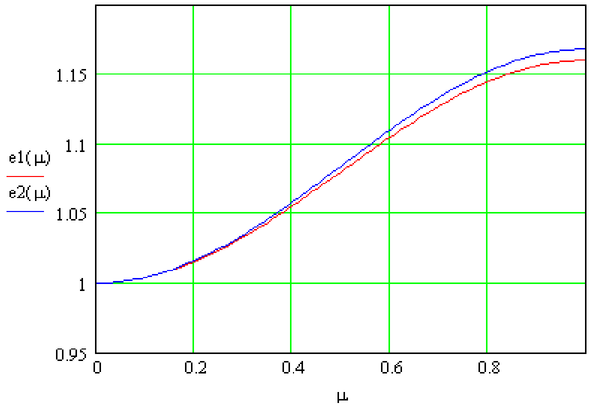

Figure 1: Energy bands along ΓX.

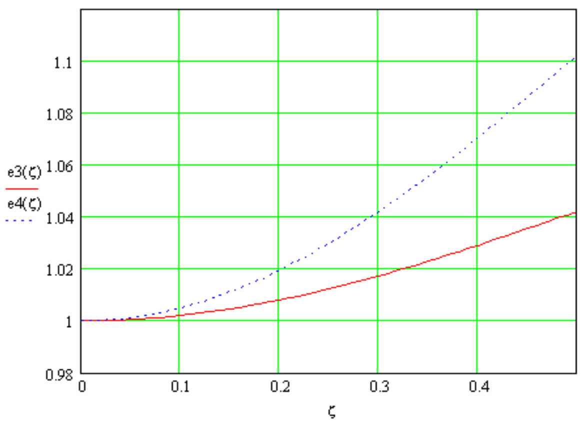

Figure 2: Energy bands along ΓL.

Problem 2 Solution was kindly provided by Professor Vinay Ambegaokar

a) Best done in scalar potential gauge:

$$H = \frac{p^2}{2m} + e\phi(\vec{x}) = \frac{p^2}{2m} - e\vec{E}\cdot\vec{x}$$
$$\dot{\vec{p}} = \frac{1}{i\hbar}[\vec{p},\vec{H}] = e\vec{E} \tag{20}$$

b) Best done in the vector potential gauge:

$$H' = e^{-\frac{i}{\hbar}\vec{E}\cdot\vec{x}t} H \exp\frac{i}{\hbar}\vec{E}\cdot\vec{x}t + e\vec{E}\cdot\vec{x} = \frac{1}{2m}(\vec{p} + \frac{e}{c}\vec{E}t)^2 \tag{21}$$

Note:Eigenvalues depend on $\vec{p}(t) = \vec{p}_0 + e\vec{E}t, \dot{\vec{p}} = e\vec{E}$
Shrödinger equation in this gauge

$$i\hbar\frac{\partial\psi'}{\partial t} = [\frac{1}{2m}(\vec{p} + \frac{e}{c}\vec{E}t)^2 + U(x)]\psi', \tag{22}$$

where U(x) is periodic potetial

$$a(t) \equiv \int d^3x \cdot e^{-i\vec{k}_0\cdot\vec{x}}\psi'(\vec{x},t)$$
$$b(t) \equiv \int d^3x \cdot e^{-i(\vec{k}_0 - \vec{K})\cdot\vec{x}}\psi'(\vec{x},t) \tag{23}$$

Assume that only two Fourier components of U are inportant

$$
\begin{aligned}
U(x) &= U_k e^{i\vec{K}\cdot\vec{x}} + U_{-k} e^{-i\vec{K}\cdot\vec{x}} \\
i\hbar\frac{da}{dt} &= \frac{\hbar^2}{2m}(\vec{k_1} + \frac{e}{c}\vec{E}t)^2 a + U_k b \\
i\hbar\frac{db}{dt} &= \frac{\hbar^2}{2m}(\vec{k_0}' + \frac{e}{c}\vec{E}t)^2 b + U_{-k} a \\
\vec{k_0'} &= \vec{k_0} - \vec{K}
\end{aligned}
\tag{24}
$$

Note:in this problem inversion symmetry $U_{-K} = U_K$ is assumed. Time-reversal invariance assures $U_{-K} = U_k^*$

c) Remove the diagonal terms by the transformation

$$
\begin{aligned}
\bar{a} &= e^{\frac{i}{\hbar}\int_0^t \epsilon(t')dt'} a \\
\bar{b} &= e^{\frac{i}{\hbar}\int_0^t \epsilon'(t')dt'} b
\end{aligned}
\tag{25}
$$

to obtain

$$
\begin{aligned}
i\hbar\frac{d\bar{a}}{dt} &= e^{\frac{i}{\hbar}\int_0^t [\epsilon(t')-\epsilon'(t')]dt'} U_k \bar{b} \\
i\hbar\frac{d\bar{b}}{dt} &= e^{-\frac{i}{\hbar}\int_0^t [\epsilon(t')-\epsilon'(t')]dt'} U_k^* \bar{a}
\end{aligned}
\tag{26}
$$

The most important time is when the levels cross $\vec{k} = -\vec{k}' = \frac{\vec{K}}{2}$. The integrand in the expression (20) is then $\frac{\hbar^2}{m}\frac{e}{\hbar}\vec{E}\cdot\vec{K}(t-t_0)$. Define $\Delta \equiv \frac{e}{m}\vec{E}\cdot\vec{K}$. Note that Δ has units of $(time)^{-2}$. For very weak U_K, $\bar{a} = const \approx 1$.

$$
\begin{aligned}
i\hbar\frac{d\bar{b}}{dt} &= e^{-i\frac{\Delta}{2}(t-t_0)^2} e^{\frac{i\Delta}{2}t_0^2} U_K^* \\
i\hbar\bar{b} &= U_K^* \int dt \cdot e^{-i\frac{\Delta}{2}(t-t_0)^2} \times phase
\end{aligned}
\tag{27}
$$

The transition from $\bar{b} = 0$ to finite $\bar{b}$ occures on the time scale $\Delta^{-\frac{1}{2}}$. In the small U_K or strong E limit, this time is much smaller than the mixing time for a and b, $\frac{\hbar}{|U_K|}$. One can then do the integral over all times

$$
\int_{-\infty}^{\infty} dt \cdot e^{-i\frac{\Delta}{2}(t-t_0)^2} = \sqrt{-i}\sqrt{\frac{2\pi}{\Delta}}
\tag{28}
$$

So finally one has

$$
|\bar{b}|^2 = |b|^2 = \frac{2\pi|U_k|^2}{\hbar^2\Delta^2}
\tag{29}
$$

which is the answer given.

d) $|b^2| \ll 1$ is the condition

$$
|U_k|^2 \ll \frac{\hbar^2 eEK}{m}
\tag{30}
$$

Since $K \sim \frac{1}{a_0}$ a_0 is an atomic length and $\frac{\hbar^2}{ma_0^2} \approx \epsilon_F$ a typical electron energy The condition is

$$
eEa_0 \gg \frac{|U_K|^2}{\epsilon_f}
\tag{31}
$$

The opposite of the condition for no electrical breakdown.