PHY 521 Solutions Set 5

1) a) 2D square lattice with lattice constant a

$\Rightarrow$ R.L. vectors are $\frac{2\pi}{a}(n,m)$

$\Rightarrow$ boundaries of 1st BZ are at $k_x = \pm\frac{\pi}{a}$, $k_y = \pm\frac{\pi}{a}$

$\Rightarrow$ area of 1st BZ $= \left(\frac{2\pi}{a}\right)^2$

Each primitive cell (such as 1st BZ) contains 2N electron states, where N is number of sites in the square Bravais lattice.

$\Rightarrow$ density of electron states in k-space is

$$\frac{2N}{(2\pi/a)^2}$$

$\Rightarrow$ a free fermi circle of radius k_F contains

$$\pi k_F^2 \cdot \frac{2N}{\left(\frac{2\pi}{a}\right)^2} \quad \text{electron states}$$

$$= \frac{(k_F a)^2 N}{2\pi}$$

So if we wish to contain mN electron states, we must have k_F such that

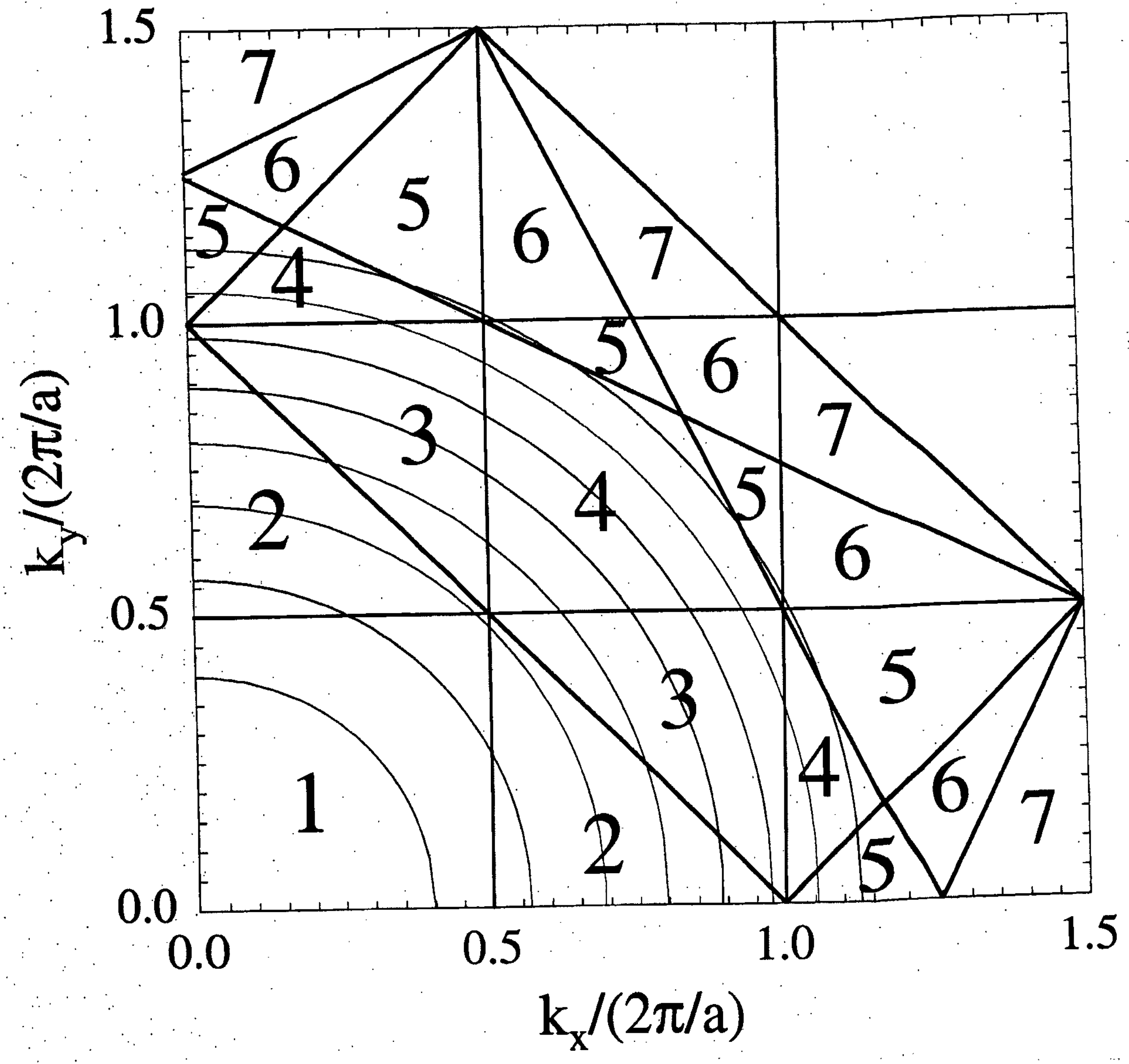
$$\frac{(k_F a)^2 N}{2\pi} = mN \Rightarrow k_F a = \sqrt{2\pi m}$$

$$\text{or} \quad \frac{k_F}{(2\pi/a)} = \sqrt{\frac{m}{2\pi}}$$

This yields the radii

n	1	2	3	4	5	6	7	8
$\frac{k_F}{(2\pi/a)}$	0.399	0.564	0.691	0.798	0.892	0.977	1.055	1.13

In the figure below we plot the free Fermi circles for the above radii in k-space. The intersection of a circle with the nth Brillouin zone indicates that there will be occupied states in that zone.

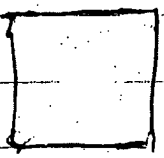


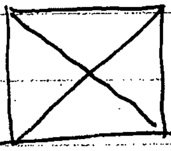
From the figure we see that the circle for $m=7$ intersects the 5^{th} BZ but no higher BZ. The circle for $m=8$ just barely intersects the 6^{th} BZ at the points ~~[illegible]~~ $\left(\frac{a}{2\pi}\right)(k_x, k_y) = \left(\frac{1}{2}, 1\right)$ ad $\left(1, \frac{1}{2}\right)$

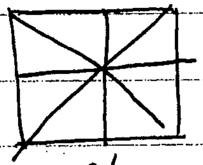
BZ \ m	1	2	3	4	5	6	7
1	○	○	●	●	●	●	●
2		○	○	○	○	○	●
3				○	○	○	○
4				○	○	○	○
5							○
6							

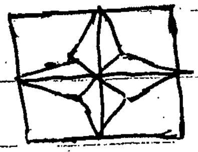
where ○ indicates a partially occupied zone and ● indicates a completely occupied zone

b) The pieces of the 1st 4 BZ's can be translated back into the 1^{st} BZ to look like

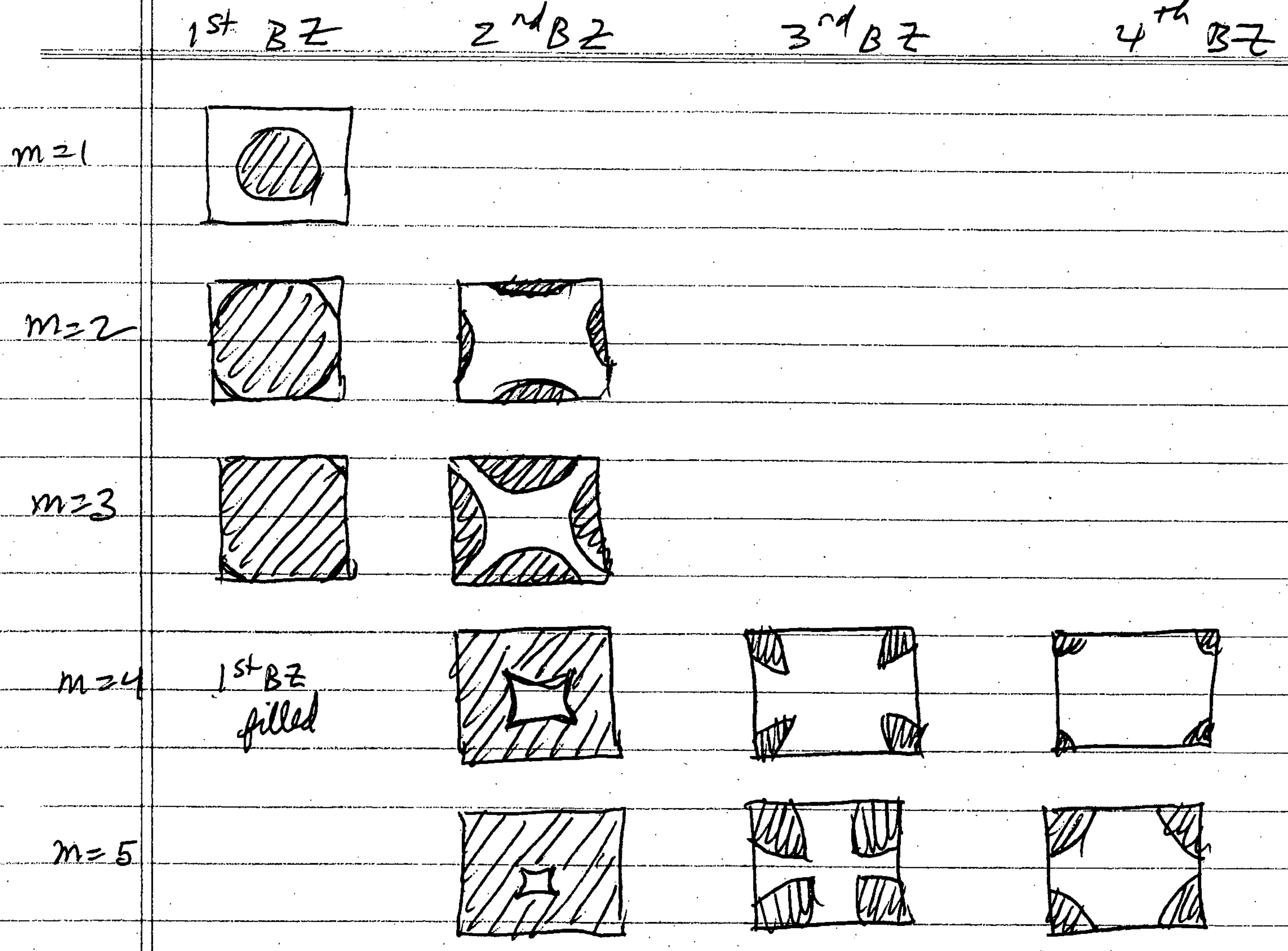

1^{st} BZ


2^{nd} BZ


3^{rd} BZ


4th BZ

Translating the section of the circles in the previous plot back into the 1^{st} BZ we get the branches of the Fermi circle in the reduced zone scheme.



shaded areas are occupied states

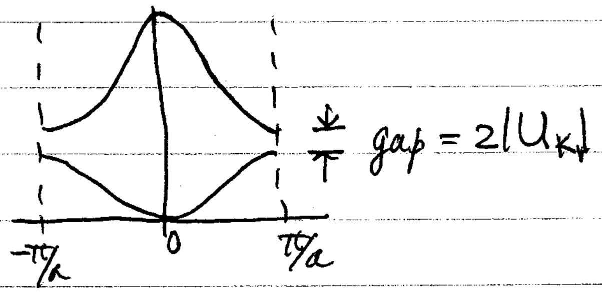
2) a) Primitive vector is $\vec{a} = a\hat{x}$

Wigner - Seitz cell is $-\frac{a}{2} < x \leq \frac{a}{2}$

Reciprocal lattice vectors are $\vec{K}_n = \left(\frac{2\pi}{a}\right) n\, \hat{x}$ with n integer

1st Brillouin Zone is $-\frac{\pi}{a} < k \leq \frac{\pi}{a}$

b) band structure in weak potential approximation looks like

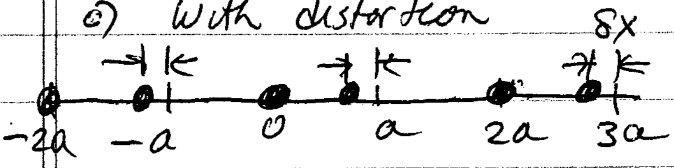


each band contains 2N electron states, where N is the number of ions. If each ion contributes m conduction electrons then,

If $m = 2l$ is even, the lowest l bands are completely full and the higher bands are completely empty $\Rightarrow$ $\boxed{m \text{ even} \Rightarrow \text{insulator}}$

If $m = 2l+1$ is odd, the lowest l bands are completely full and the $(l+1)^{st}$ band is half full $\Rightarrow$ $\boxed{m \text{ odd} \Rightarrow \text{metal}}$

c) With distortion



Now we have a Bravais lattice with a 2 point basis! Since all ions no longer equivalent.

primitive vector $\vec{a} = 2a\hat{x}$, basis vectors $\begin{cases}\vec{d}_1 = 0 \\ \vec{d}_2 = (a-\delta x)\hat{x}\end{cases}$

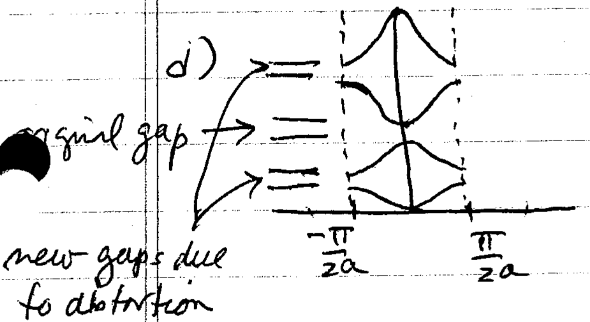
Wigner-Seitz cell $-a < x \leq a$

Reciprocal lattice vectors $\vec{K}_n = \frac{2\pi n}{2a}\hat{x} = \frac{\pi n}{a}\hat{x}$ with n integer

1st Brillouin zone $-\frac{\pi}{2a} < k \leq \frac{\pi}{2a}$

Note: the 1st BZ is half the size of the original undistorted lattice

d)



each band now holds $2\left(\frac{N}{2}\right) = N$ electrons (since the Bravais lattice now has only $\frac{N}{2}$ sites - since the primitive cell doubled due to the distortion). To have the same number of electron states as shown in part (b) we therefore need twice as many bands.

If each ion gives one electron there are N electrons. Since each band can hold N electrons $\Rightarrow$ The lowest band is now completely filled and the others are completely empty. $\Rightarrow$ crystal is now an $\boxed{\text{insulator}}$ instead of a metal as was the case before the distortion

e) $U(x) = \sum_i V(x - x_i)$

$$= \sum_{\substack{n \\ \text{even}}} V(x - na) + \sum_{\substack{n \\ \text{odd}}} V(x - (na - \delta x))$$

↑ expand for small δx

$$= \sum_{\substack{n \\ \text{even}}} V(x-na) + \sum_{\substack{n \\ \text{odd}}} \left[V(x-na) + \frac{dV}{dx}(x-na)\, \delta x \right]$$

$$= \sum_{\substack{n \\ \text{all}}} V(x-na) + \sum_{\substack{n \\ \text{odd}}} \frac{dV}{dx}(x-na)\, \delta x$$

$$= U_0(x) + \delta U(x)$$

period of $U_0(x)$ is a as $U_0(x+a) = U_0(x)$

period of $\delta U(x)$ is $2a$ as:

$$\delta U(x) = \sum_{l = \text{integer}} \frac{dV}{dx}\big(x - \overbrace{(2l+1)}^{\text{odd}} a\big)\, \delta x$$

$$\delta U(x+a) = \sum_{l} \frac{dV}{dx}\big(x + a - (2l+1)a\big)\, \delta x$$

$$= \sum_{l} \frac{dV}{dx}\big(x - \overbrace{2l}^{\text{even}} a\big)\, \delta x \neq \delta U(x)$$

since sum now over even s

But $\delta U(x+2a) = \sum_l \frac{dV}{dx}\big(x - \overbrace{(2l-1)}^{\text{odd}} a\big)\, \delta x = \delta U(x)$

since sum remains over odd sites

The potential due to the distortion is proportional to the distortion

$$\boxed{\delta U(x) \propto \delta x}$$

f) Since the potential $U_0(x)$ has period a, its Fourier transform has non vanishing coefficients only at wavevectors $K = \frac{2\pi}{a} n$, and the smallest Bragg plane from $U_0(x)$ is thus at $k = \frac{\pi}{a}$. $U_0(x)$ therefore cannot play any role in the energy gap at $k = \frac{\pi}{2a}$.

Since $\delta U(x)$ has period $2a$, its Fourier transform has non vanishing coefficients at wave vectors $K = \frac{\pi}{a} n$ (see part (c)), and the smallest Bragg plane due to $\delta U(x)$ is thus at $k = \frac{\pi}{2a}$. Thus it is the Fourier coefficient $\delta U_{K=\frac{\pi}{a}}$ that gives rise to the energy gap at $k = \frac{\pi}{2a}$.

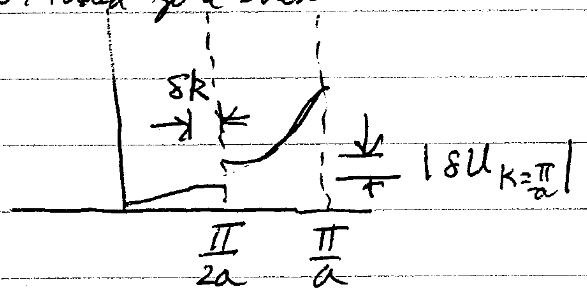
In the weak potential approximation the energy spectrum, as k approaches the Bragg plane at $k = \frac{\pi}{2a}$ ~~becomes~~ due to $K = \frac{\pi}{a}$ becomes

$$(*) \quad \varepsilon_-(k) = \frac{\varepsilon^0_k + \varepsilon_{k-K}}{2} - \sqrt{\left(\frac{\varepsilon^0_k - \varepsilon^0_{k-K}}{2}\right)^2 + |\delta U_{K=\frac{\pi}{a}}|^2}$$

we took $(-)$ sign for the lower ~~band~~ filled band (upper ~~filled~~ band is empty)

the lowering of $\varepsilon(k)$ compared to $\varepsilon^0(k)$ results in a net decrease of the total electronic energy, which we estimate as follows:

extended zone scheme



1) The electrons which have their energy lowered by being near the Bragg plane, have their energy lowered by an amount $\sim |\delta U_{K=\frac{\pi}{a}}|$

2) All the electrons within $\delta\varepsilon$ of ε_F have their energy lowered, where $\delta\varepsilon = \frac{d\varepsilon}{dk}\delta k$ with δk as shown in the figure above. To estimate $\delta\varepsilon$, note

$k_F = \frac{\pi}{2a}$
$K = \frac{\pi}{a}$

$$\varepsilon_k^0 = \frac{\hbar^2}{2m}(k_F-\delta k)^2 = \frac{\hbar^2}{2m}(k_F^2 - 2k_F\delta k) \equiv \varepsilon_F - \delta\varepsilon$$

$$\varepsilon_{k-K}^0 = \frac{\hbar^2}{2m}(k_F-\delta k-2k_F)^2 = \frac{\hbar^2}{2m}(k_F^2 + 2k_F\delta k) \equiv \varepsilon_F + \delta\varepsilon$$

where we ignored terms of $O(\delta k^2)$

So $\left|\frac{\varepsilon_k^0 - \varepsilon_{k-K}^0}{2}\right| = \delta\varepsilon$ and so from (*)

we see that the electron energies will be different from their free electron values when

$$\delta\varepsilon \gtrsim |\delta U_{K=\frac{\pi}{a}}|$$

So we take $\delta\varepsilon = |\delta U_{K=\frac{\pi}{a}}|$

3) The number of electrons per unit length that have their energy lowered is then

$$g(\varepsilon_F)\,\delta\varepsilon$$

where $g(\varepsilon_F)$ is the density of states at ε_F

In 1D

$$\underset{\text{spin}\uparrow\text{and}\downarrow}{\overset{\nearrow}{2}}\cdot\underset{+k\text{ and }-k}{\overset{\uparrow}{2}}\frac{dk}{2\pi} = g(\varepsilon)\,d\varepsilon \qquad \cancel{\Rightarrow g(\varepsilon) = \frac{\pi}{2}\left(\frac{d\varepsilon}{dk}\right)^{-1}}$$

$$\cancel{= \frac{\pi}{2}\left(\frac{\hbar^2}{m}k\right)^{-1}}$$

$$\Rightarrow g(\varepsilon_F) = \frac{2}{\pi}\frac{1}{\frac{d\varepsilon}{dk}} = \frac{2}{\pi}\frac{1}{\frac{\hbar^2}{m}k_F} = \frac{2m}{\pi\hbar^2 k_F}$$

$$= \frac{4am}{\pi^2\hbar^2} \qquad \text{using } k_F = \frac{\pi}{2a}$$

Putting it together, the total electronic energy per length <u>decreases</u> by

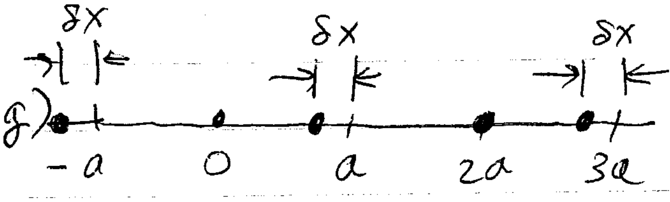
$$\frac{\Delta E}{L} \simeq |\delta U_{K=\frac{\pi}{2}}|\, g(\varepsilon_F)\,\delta\varepsilon$$

$$= |\delta U_{K=\frac{\pi}{2}}|^2 \frac{4am}{\pi^2\hbar^2}$$

Since $\delta U \propto \delta x$ we can write $|\delta U_{K=\frac{\pi}{2}}|^2 = A\,\delta x^2$ with A some constant independent of δx

$$\frac{\Delta E}{L} = \frac{4am}{\pi^2\hbar^2} A\,\delta x^2$$

g)



For each ion the cost in elastic energy is $\frac{1}{2}c(\delta x)^2$, since each ion to its right is either δx closer or δx farther away than in the undistorted case. The cost in energy per length due to the elastic distortion is thus

$$\frac{\Delta E}{L} \quad \frac{1}{2}\frac{c}{a}(\delta x)^2$$

The total change in elastic + electronic energy is therefore

$$\frac{\Delta E^{total}}{L} = \left(\underset{\underset{\text{elastic}}{\uparrow}}{\frac{c}{2a}} - \underset{\underset{\text{electronic}}{\uparrow}}{\frac{4amA}{\pi^2\hbar^2}}\right)\delta x^2$$

depending on the sign of the coefficient of the δx^2, which depends on the strength of the elastic energy c and the distortion in ionic potential A, the distortion will be favored or not.

If the coefficient < 0, then distortion occurs and the size of the distortion δx will be determined by higher order terms.
We have a metal to insulator instability.

Peierl's Instability — exact calculation of electronic energy

In fact, the estimate of the change in electronic energy in part (f) is too simplistic. We can do the calculation exactly and get an important new result.

From the weak potential approximation

$$\mathcal{E}_k = \frac{\mathcal{E}^0_k + \mathcal{E}^0_{k-K}}{2} - \sqrt{\left(\frac{\mathcal{E}^0_k - \mathcal{E}^0_{k-K}}{2}\right)^2 + \left|\delta U_{K=\frac{\pi}{a}}\right|^2}$$

let $k = k_F - \delta k$

$$k - K = k_F - \delta k - 2k_F = -(k_F + \delta k)$$

where $k_F = \frac{\pi}{2a}$, $K = \frac{\pi}{a}$

$$\mathcal{E}^0_k = \frac{\hbar^2}{2m}\left(k_F^2 - 2k_F\delta k + \delta k^2\right)$$

$$\mathcal{E}^0_{k-K} = \frac{\hbar^2}{2m}\left(k_F^2 + 2k_F\delta k + \delta k^2\right)$$

$$\mathcal{E}_k = \frac{\hbar^2}{2m}\left\{k_F^2 + \delta k^2 - \sqrt{(2k_F\delta k)^2 + \left(\frac{2m|\delta U_K|}{\hbar^2}\right)^2}\right\}$$

↑ we will use this for $\mathcal{E}_k$ for all k in 1st BZ

Total change in electronic energy is

$$\frac{\Delta E}{L} = \underset{\substack{\uparrow \\ \text{spin}\uparrow,\downarrow}}{2} \cdot \underset{\substack{\uparrow \\ +k,-k}}{2} \int_0^{k_F} \frac{dk}{2\pi}\left(\mathcal{E}_k - \mathcal{E}^0_k\right)$$

$$\frac{\Delta E}{L} = \frac{2}{\pi}\frac{\hbar^2}{2m}\int_0^{k_F} dk \left[2k_F\,\delta k - \sqrt{4k_F^2\,\delta k^2 + \left(\frac{2m}{\hbar^2}|\delta U_{k=\frac{\pi}{a}}|\right)^2} \right]$$

$$= \frac{\hbar^2}{\pi m}\int_0^{k_F} d\,\delta k \left[2k_F\,\delta k - \sqrt{4k_F^2\,\delta k^2 + \left(\frac{2m}{\hbar^2}|\delta U_{k=\frac{\pi}{a}})|\right)^2} \right]$$

To evaluate the 2nd piece use

$$\int dx\,\sqrt{x^2+a^2} = \frac{x}{2}\sqrt{x^2+a^2} + \frac{a^2}{2}\ln\left(x+\sqrt{x^2+a^2}\right)$$

$$\frac{\Delta E}{L} = \frac{\hbar^2}{\pi m}\left\{ k_F^3 - 2k_F\left[\frac{k_F}{2}\sqrt{k_F^2+\gamma^2} + \frac{\gamma^2}{2}\ln\left(\frac{k_F+\sqrt{k_F^2+\gamma^2}}{\gamma}\right)\right]\right\}$$

where $\gamma \equiv \dfrac{2m\,|\delta U_{k=\frac{\pi}{2}}|}{2\hbar^2 k_F}$

$$\equiv \frac{\hbar^2 k_F^3}{\pi m}\left\{ 1 - \sqrt{1+\lambda^2} - \lambda^2\ln\left(\frac{1+\sqrt{1+\lambda^2}}{\lambda}\right)\right\}$$

where $\lambda \equiv \dfrac{\gamma}{k_F} = \dfrac{|\delta U_{k=\pi/2}|}{2\left(\frac{\hbar^2 k_F^2}{2m}\right)} = \dfrac{1}{2}\dfrac{|\delta U_{k=\frac{\pi}{2}}}{\varepsilon_F}$

Recall $\lambda \propto |\delta U_{k=\pi/2}| \propto \delta x$, the distortion

So λ is small. Expand for small λ

$$\frac{\Delta E}{L} = \frac{\hbar^2 k_F^3}{\pi m}\left\{ -\frac{\lambda^2}{2} - \lambda^2\ln\left(\frac{2}{\lambda}\right) + O(\lambda^4)\right\}$$

$$= -\frac{\hbar^2 k_F^3}{\pi m}\frac{\lambda^2}{2}\left\{ 1 + 2\ln\left(\frac{2}{\lambda}\right)\right\}$$

↑ diverges as $\lambda \to 0$!

$$\frac{\Delta E}{L} = -\frac{\hbar^2 k_F^3}{\pi m} \frac{|\delta U_{k=\frac{\pi}{2}}|^2}{4\, \varepsilon_F^2 \; 2} \left\{ 1 + 2 \ln\left(\frac{2}{\lambda}\right) \right\}$$

$$= -\frac{\hbar^2 k_F^3}{\pi m} \frac{|\delta U_{k=\frac{\pi}{2}}|^2}{8 \; \frac{\hbar^4 k_F^4}{4 m^2}} \left\{ 1 + 2 \ln \frac{2}{\lambda} \right\}$$

$$= -\frac{m}{2\pi} \frac{|\delta U_{k=\frac{\pi}{2}}|^2}{\hbar^2 k_F} \left\{ 1 + 2 \ln \frac{2}{\lambda} \right\}$$

use $|\delta U_{k=\frac{\pi}{2}}|^2 = A\, \delta x^2$, $k_F = \frac{\pi}{2a}$

$$\frac{\Delta E}{L} = -\frac{m a}{\pi^2 \hbar^2} A\, \delta x^2 \left\{ 1 + 2 \ln \frac{2}{\lambda} \right\}$$

except for a factor 4, the 1st term is the same as we got from the crude esitimate.

Add elastic energy

$$\frac{\Delta E^{\text{total}}}{L} = \left[\frac{C}{2a} - \frac{m a}{\pi^2 \hbar^2} \left(1 + 2 \ln \frac{2}{\lambda} \right) \right] \delta x^2$$

But since $\lambda \propto \delta x$, for small δx $\ln(2/\lambda)$ diverges. $\Rightarrow$ coefficient of δx^2 is *always* negative for small enough δx

$\Rightarrow$ Peierl's instability *always* takes place!

3) 2D square B.L. $\vec{a}_1 = a\hat{x}$, $a_2 = a\hat{y}$

R.L. $\vec{b}_1 = \frac{2\pi}{a}\hat{x}$, $\vec{b}_2 = \frac{2\pi}{a}\hat{y}$, $\vec{K} = \frac{2\pi}{a}(n, m)$

$\uparrow$ integers

Potential is $-4U\cos(\frac{2\pi x}{a})(\frac{2\pi y}{a})$

a) $$U_K = \frac{1}{a^2}\int d^2r\, e^{-i\vec{K}\cdot\vec{r}}\, U(\vec{r})$$

primitive cell of B.L.

$$U_K = -\frac{4U}{a^2}\int_0^a dx\, e^{-iK_x x}\cos(\frac{2\pi x}{a})\int_0^a dy\, e^{-iK_y y}\cos(\frac{2\pi y}{a})$$

do one of the integrals

$$\int_0^a dx\, e^{iK_x x}\cos(\frac{2\pi x}{a}) = \int dx\, e^{-iK_x x}\,\frac{1}{2}\left(e^{i\frac{2\pi x}{a}}\quad e^{-i\frac{2\pi x}{a}}\right)$$

$$= \int_0^a dx\,\frac{1}{2}\left(e^{-i(K_x-\frac{2\pi}{a})x} + e^{-i(K_x+\frac{2\pi}{a})x}\right)$$

$$= \frac{1}{2}\left\{\frac{e^{-i(K_x-\frac{2\pi}{a})x}}{-i(K_x-\frac{2\pi}{a})} + \frac{e^{-i(K_x+\frac{2\pi}{a})x}}{-i(K_x+\frac{2\pi}{a})}\right\}_0^a$$

use $K_x = \frac{2\pi}{a}n$

$$= \frac{1}{2}\left\{\frac{e^{-i\frac{2\pi}{a}(n-1)x}}{-i\frac{2\pi}{a}(n-1)} + \frac{e^{-i\frac{2\pi}{a}(n+1)x}}{-i\frac{2\pi}{a}(n+1)}\right\}_0^a$$

$= 0$ unless $n = 1$ or $n = -1$

$= \frac{a}{2}$ $n = 1$ or $n = -1$

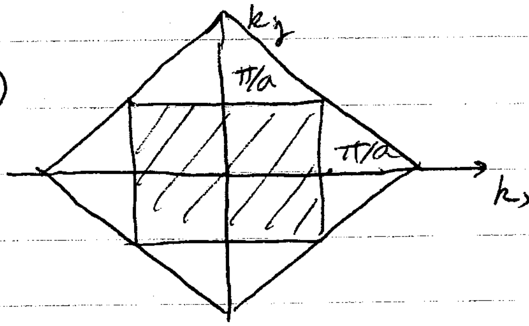
Similarly for the y-integration $\Rightarrow$ $m = 1$ or $m = -1$

So $U_K = 0$ except for $K = \frac{2\pi}{a}(n, m)$
with $n = \pm 1$ and $m = \pm 1$

ie the four RL vectors $K = \frac{2\pi}{a}(1,1)$, $\frac{2\pi}{a}(-1,-1)$,
$\frac{2\pi}{a}(1,-1)$, $\frac{2\pi}{a}(-1,1)$

For these 4 K's, $U_K = -U$.

b)



As k crosses the boundary of the 1st BZ, it crosses the Bragg plane bisecting the R-L. vector $\vec{K}_0 = \frac{2\pi}{a}(1,0)$.

However, U_{K_0} for $\vec{K}_0 = \frac{2\pi}{a}(1,0)$ vanishes! Hence there is NO jump in electron energy $\mathcal{E}(\vec{k})$ as ~~crosses~~ $\vec{k} = (k,0)$ crosses the boundary of the 1st BZ. - similarly for crossing the boundary of the 1st BZ in another direction (except along the diagonal - see part (c)).

c) For $\vec{k} = (k,k)$ along the diagonal, when $\vec{k}$ crosses the boundary of the first BZ at $(\frac{\pi}{a}, \frac{\pi}{a})$ it also crosses the boundary of the 2nd BZ. ie it crosses 3 Bragg planes that bisect the three R.L. vectors $\vec{K}_0 = \frac{2\pi}{a}(1,0)$, $\vec{K}_1 = \frac{2\pi}{a}(0,1)$, and $\vec{K}_2 = \frac{2\pi}{a}(1,1)$. But $U_{K_0} = U_{K_1} = 0$. only $U_{K_2} = -U \neq 0$. So this is the same as behavior crossing only a single Bragg plane and the energy $\mathcal{E}(\vec{k})$ will jump by an amount $2U$ as $\vec{k} = (k,k)$ crosses $(\frac{\pi}{a}, \frac{\pi}{a})$.

Why is there no jump in $\mathcal{E}(\vec{k})$ crossing the boundary of the 1st BZ? If one looks more closely at $U(x,y)$, one sees that it has a greater periodicity than just $U(x+a, y) = U(x,y)$ and $U(x, y+a) = U(x,y)$. It is also true that $U(x \pm \frac{a}{2}, y \pm \frac{a}{2}) = U(x,y)$!

So in fact $U(x,y)$ has the periodicity of a square B.L. with primitive vectors

$$\vec{a}_1 = \frac{a}{2}\hat{x} + \frac{a}{2}\hat{y} \,, \quad \vec{a}_2 = \frac{a}{2}\hat{x} - \frac{a}{2}\hat{y}$$

This has R.L. with primitive basis vectors

$$\vec{b}_1 = \frac{4\pi}{a}(\hat{x} + \hat{y}) \,, \quad \vec{b}_2 = \frac{4\pi}{a}(\hat{x} - \hat{y})$$

and R.L. vectors $\vec{K} = n\vec{b}_1 + m\vec{b}_2$.

In this way of looking at things, the vectors

$$\frac{2\pi}{a}(1,0) \,, \ \frac{2\pi}{a}(-1,0) \,, \ \frac{2\pi}{a}(0,1) \,, \ \frac{2\pi}{a}(0,-1)$$

are <u>NOT</u> in the R.L. at all! ⇒ no gaps in energy as cross planes at $x = \pm\frac{\pi}{a}$, $y = \pm\frac{\pi}{a}$.

The boundary of the 2nd BZ as drawn in part (b) is now the boundary of the 1st BZ for the square BL with $\vec{a}_1$ and $\vec{a}_2$ as above!