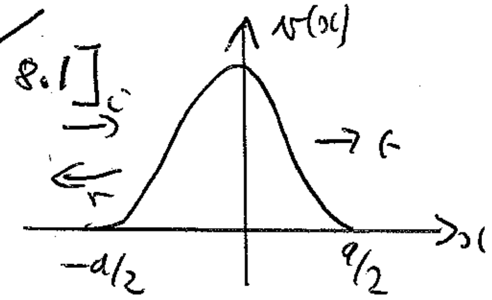
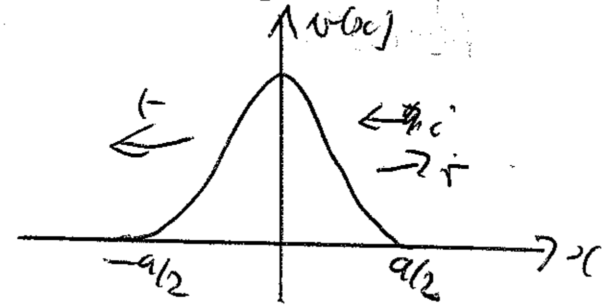
Total (28)

Physics 231 Homework 4 (Solutions)

1/ [AM 8.1]



left incidence



right incidence

(use q not K)

$$q = \left(\frac{2m\varepsilon}{\hbar^2}\right)^{1/2}$$

$$\psi_l = \begin{cases} e^{iqx} + r e^{-iqx} & x \le -a/2 \\ t e^{iqx} & x \geq a/2 \end{cases}$$

$$\psi_r = \begin{cases} t e^{-iqx} & x \le -a/2 \\ e^{-iqx} + r e^{iqx} & x \geq a/2 \end{cases}$$

$$\psi(x) = A\psi_l(x) + B\psi_r(x) = \begin{cases} A\left[e^{iqx} + r e^{-iqx}\right] + Bt e^{-iqx}, & x \le -a/2 \\ At e^{iqx} + B\left[e^{-iqx} + r e^{iqx}\right], & x \geq a/2. \end{cases}$$

$$\psi'(x) = \begin{cases} iq\left\{A\left[e^{iqx} - r e^{-iqx}\right] - Bt e^{-iqx}\right\} & x \le -a/2 \\ iq\left\{At e^{iqx} + B\left[-e^{-iqx} + r e^{iqx}\right]\right\} & x \geq a/2 \end{cases}$$

(a) The boundary conditions are $\psi(a/2) = e^{ika}\psi(-a/2)$

so $At e^{iqa/2} + B\left[e^{-iqa/2} + r e^{iqa/2}\right] = e^{ika}\left\{A\left[e^{-iqa/2} + r e^{iqa/2}\right] + Bt e^{iqa/2}\right\}$ (1)

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

$At e^{iqa/2} + B\left[-e^{-iqa/2} + r e^{iqa/2}\right] = e^{ika}\left\{A\left[e^{-iqa/2} - r e^{-iqa/2}\right] - Bt e^{-iqa/2}\right\}$ (2)

From (1)

$\frac{A}{B} = \frac{u+v}{s+h}$ (3) where $u = r e^{iqa/2}$, $v = t e^{i(\frac{q}{2}+k)a} + e^{-iqa/2}$

$s = -t e^{iqa/2} + e^{i(k-\frac{q}{2})a}$, $h = r e^{i(k+\frac{q}{2})a}$

From (2)

$\frac{A}{B} = \frac{u-v}{s-h}$ (4)

From (3) and (4) $\frac{u+v}{s+h} = \frac{u-v}{s-h}$

or $(u+v)(s-h) = (u-v)(s+h)$ or $\underline{uh = vs}$

~~$uh - vs = 0$~~

~~or $r^2 e^{ika/2} e^{iqa} = t^2 e^{iqa} e^{ika/2} + e^{ika/2} + t e^{i(q+k)a} - t$~~

$$\Rightarrow r^2 e^{ika} e^{iqa} = t^2 e^{iqa} e^{ika} + e^{ika} e^{-iqa}$$
$$-t e^{2ika} \quad -t$$

Divide by e^{ika}

$$2t \cos ka = (t^2 - r^2) e^{iqa} + e^{-iqa}$$

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

if $\underline{v = 0}$, $r = 0$, $t = 1$

$$\Rightarrow \cos ka = \tfrac{1}{2} e^{iqa} + \tfrac{1}{2} e^{-iqa} \quad \text{so } k = q = \sqrt{\frac{2m\mathcal{E}}{\hbar^2}}$$

so $\mathcal{E} = \dfrac{\hbar^2 k^2}{2m}$, as required

let $t = |t| e^{i\delta}$

let ϕ_1 and ϕ_2 be 2 solutions of Schrödinger's equation

$$-\frac{\hbar^2}{2m} \phi_i'' + v\phi_i = \frac{\hbar^2 q^2}{2m} \phi_i, \quad i = 1, 2$$

Let the Wronskian be

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

(b) $$w' = \phi_1'' \phi_2 - \phi_1 \phi_2'' = \left(-q^2 + \frac{2m}{\hbar^2} V\right) \phi_1 \phi_2 - \left(-q^2 + \frac{2mV}{\hbar^2}\right) \phi_2 \phi_1$$
$$= 0$$

Hence w is independent of x.

(c) For $x \leq -a/2$, $\cancel{\phi_1 = e^{iqx} + r e^{-iqx}}$

$$\text{Let } \phi_1 = \psi_l(x) = \cancel{A}\left[e^{iqx} + r e^{-iqx}\right] \cancel{+ Bt e^{-iqx}}$$
$$\text{let } \phi_2 = \psi_l^*(x) = \cancel{A^*}\left[e^{-iqx} + r^* e^{iqx}\right] \cancel{+ B^* t^* e^{iqx}}$$

~~Hence~~ $\cancel{w = iq \left\{ A\left[e^{iqx} + r e^{-iqx}\right] + Bt e^{-iqx} \right\}\left\{ A^*\left[-e^{-iqx} + r^* e^{iqx}\right] + B^* t^* e^{iqx} \right\} - c.c.}$

Hence $W = \phi_1' \phi_2 - \phi_2' \phi_1 = 2(1 - |r|^2) iq$ (5)

For $x \geq a/2$.

$$\phi_1 = t e^{iqx}$$
$$\phi_2 = t e^{-iqx} \quad \text{so} \quad W = 2|t|^2 iq \qquad (4)$$

Equating (3) and (4), $\Rightarrow$ $|r|^2 + |t|^2 = 1$

(d) For $x \leq -a/2$. $\quad \phi_1 = \psi_\ell = e^{iqx} + r e^{-iqx}$

$$\phi_2 = \psi_r^* = t^* e^{iqx}.$$

Hence $W = \phi_1' \phi_2 - \phi_1 \phi_2' = -2iq\, r t^*$ (5)

For $x \geq a/2$ $\quad \phi_1 = \psi_\ell = t e^{iqx}$

$$\phi_2 = \psi_r^* = e^{iqx} + r^* e^{-iqx}.$$

Hence $W = 2iq\, r^* t$ (6)

Equating (5) and (6) implies $r t^*$ is pure imaginary.

i.e. $r = \pm i t c = \pm i |t| e^{i\delta} c$ where c is real.

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

(e) Since $t = |t| e^{i\delta}$

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

then, from the answer to part (a),

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

$$= \left(\frac{|t|^2 + |r|^2}{2|t|}\right) e^{i(\delta + qa)} + \frac{1}{2|t|} e^{-i(\delta + qa)}$$

i.e. $\cos ka = \dfrac{\cos(qa + \delta)}{2|t|}$

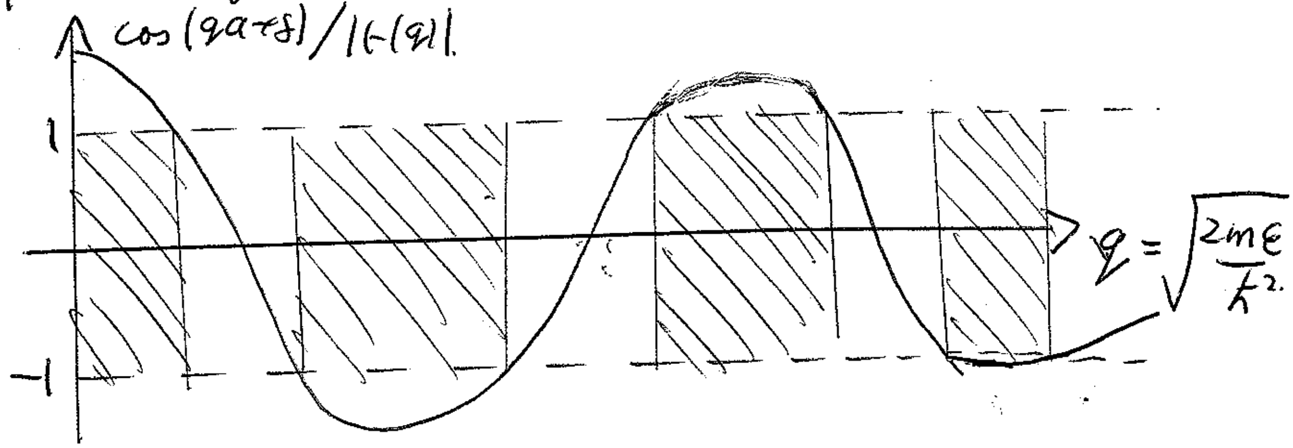
since $|t|^2 + |r|^2 = 1$.

Remember q is related to the energy by

$$q = \sqrt{\frac{2m\varepsilon}{\hbar^2}}$$

Note $|t|$ and δ depend on the energy (i.e. on q).

$|t| < 1$ but $|t| \to 1$ as $\varepsilon \to \infty$, hence we have.



Now $\dfrac{\cos(qa+\delta)}{|t(q)|} = \cos ka$ and so $\left|\dfrac{\cos(qa+\delta)}{|t(q)|}\right| < 1$

to have a solution for real k.

Hence solutions in the shaded regions are <u>forbidden</u>.

There <u>are solutions</u> in the <u>unshaded regions</u>.

Hence there are <u>energy bands</u>.

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

Now the gaps are near where $qa + \delta = n\pi$.

let $qa + \delta - n\pi = \underline{\varepsilon}$ then $|\cos(qa+\delta)| = 1 - \dfrac{\varepsilon^2}{2}$.

We need $\dfrac{1 - \varepsilon^2/2}{|t|} > 1$ for no solutions

i.e. $\dfrac{1 - \varepsilon^2/2}{\sqrt{1-|r|^2}} > 1$ or $1 - \varepsilon^2 > 1 - |r|^2$

i.e. $|\varepsilon| < |r|$

Hence gap in q is ~~$\delta q = 2a r$~~ $\delta q = \dfrac{2|r|}{a}$

Hence gap in ε is $\delta\varepsilon = \frac{\hbar^2 q}{m}\,\delta q = \frac{\hbar^2}{m}\,\frac{n\pi}{a}\,\frac{2|r|}{a}$

$$\delta\varepsilon \approx 2\pi n\,\frac{\hbar^2}{m a^2}\,|r| \qquad (=\varepsilon_{gap})$$

(g) Suppose the barrier is very strong so $|t| \approx 0$, $|r| \approx 1$

The center of the band is at $q_0 a + \delta = (n+\frac{1}{2})\pi$

and in this region

$$\frac{\cos(qa+\delta)}{|t|} \approx (-1)^{n+1}\frac{(q-q_0)\,a}{|t|}$$

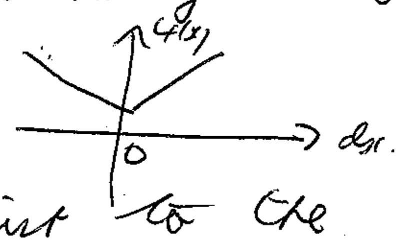
we need this to be less than 1 in magnitude so the width of the band in q is of order $|t|$.

Similarly, as a function of energy,

$$\varepsilon_{max} - \varepsilon_{min} = O(|t|)$$

(h) $v(x) = g\,\delta(x)$, The "Kronig–Penney" model.

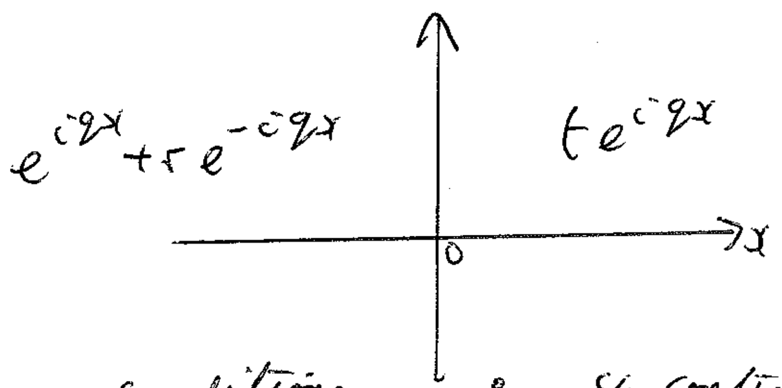
$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + v(x)\,\psi = \varepsilon\,\psi$$



Integrate from just to the left to just to the right of $x = 0$

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

$$\text{i.e. } \underbrace{\psi'(0^+) - \psi'(0^-)}_{\text{discontinuity in slope.}} = \frac{2mg}{\hbar^2}\,\psi(0)$$



Boundary conditions : • ψ continuous
• ψ' has discontinuity of $\frac{2mg}{\hbar^2}\psi(0)$

$$\Rightarrow \quad 1 + r = t$$

$$iq\left[t - (1-r)\right] = \frac{2mg}{\hbar^2} t \quad \Rightarrow \quad t - 1 = -\frac{mg}{q\hbar^2} t \cdot i$$

$$t = \frac{1}{1 + \frac{mg}{q\hbar^2} i}.$$

$$\frac{1}{t} = \frac{e^{-i\delta}}{|t|} = 1 + \frac{mg\, i}{q\hbar^2} \Rightarrow \underline{\underline{\cot\delta = -\frac{q\hbar^2}{mg}}}$$

also $|t| = \frac{1}{\sqrt{1 + \tan^2\delta}} = \frac{1}{\sec\delta} = \cos\delta$

i.e. $\underline{\underline{|t| = \cos\delta}}$ (Phew!)

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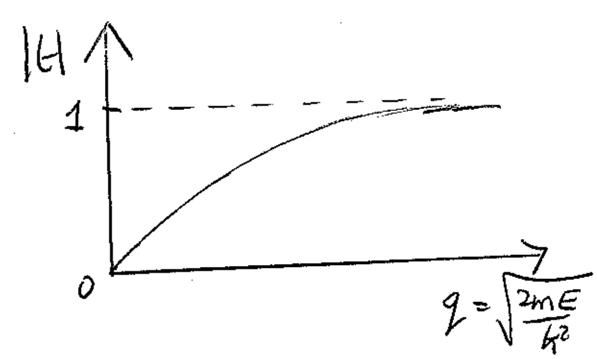
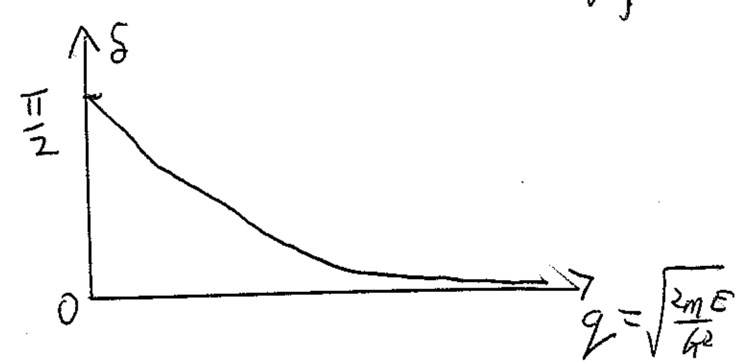


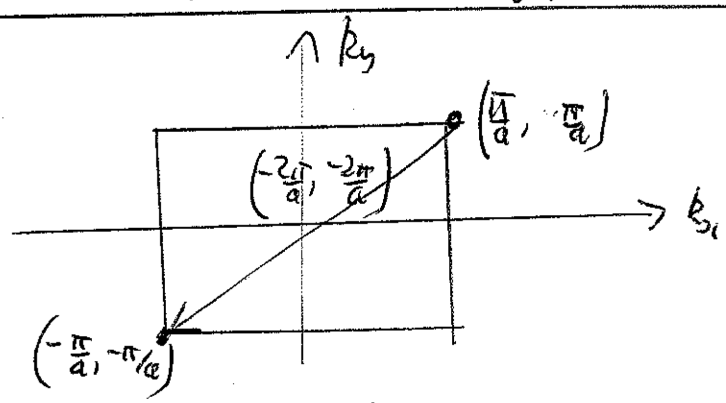


2 (a)
$$U(x,y) = -4U\cos\left(\frac{2\pi x}{a}\right)\cos\left(\frac{2\pi y}{a}\right)$$
$$= -U\left[e^{\frac{2\pi i}{a}(x+y)} + e^{-\frac{2\pi i}{a}(x+y)} + e^{\frac{2\pi i}{a}(x-y)} + e^{-\frac{2\pi i}{a}(x-y)}\right]$$

Hence $U_{11} = U_{-1,-1} = U_{1,-1} = U_{-1,1} = -U$.

All other Fourier coefficients are zero

(b)



The state at $\left(\frac{\pi}{a}, \frac{\pi}{a}\right)$ is connected to the degenerate state at $\left(-\frac{\pi}{a}, -\frac{\pi}{a}\right)$ by the ~~the~~ Fourier component of the potential $U_{-1,-1}$ $(= U)$

To leading order in the potential we just consider mixing of degenerate levels, i.e.

let $\psi = c_1\psi_1 + c_2\psi_2$ where $\begin{cases}\psi_1 = \psi(\frac{\pi}{a}, \pi/a) \\ \psi_2 = \psi(-\frac{\pi}{a}, -\pi/a)\end{cases}$

Then Schrödinger's eq. is

$$\begin{vmatrix} \varepsilon_0 & -U \\ -U & \varepsilon_0 \end{vmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \lambda \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

where $\varepsilon_0 = \varepsilon_{\left(\frac{\pi}{a}, \frac{\pi}{a}\right)} = \varepsilon_{\left(-\frac{\pi}{a}, -\frac{\pi}{a}\right)}$

The eigenvalues are given by

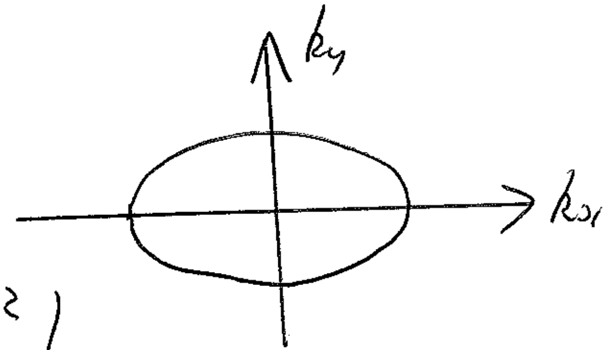
$$\begin{vmatrix} \varepsilon_0 - \lambda & -U \\ -U & \varepsilon_0 - \lambda \end{vmatrix} = 0$$

so $\lambda = \varepsilon_0 \pm |U|$

Hence the energy gap is $2|U|$

3

3/ The surface of constant energy is an ellipsoid



(a) $\varepsilon(k) = \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} + \frac{k_z^2}{m_z}\right)$

i.e $\frac{k_x^2}{a^2} + \frac{k_y^2}{b^2} + \frac{k_z^2}{c^2} = 1$ where $a^2 = \frac{2 m_x \varepsilon}{\hbar^2}$ etc.

The volume is $\frac{4\pi}{3} abc = \frac{4\pi}{3}\left(\frac{2\varepsilon}{\hbar^2}\right)^{3/2}(m_x m_y m_z)^{1/2}$

Hence Number of states less than ε is

$$\frac{2}{(2\pi)^3}\,\frac{4\pi}{3}\left(\frac{2\varepsilon}{\hbar^2}\right)^{3/2}(m_x m_y m_z)^{1/2}$$

The density of states is the derivative of this with respect to ε

$$\text{i.e. } g(\varepsilon) = \frac{\cancel{2}}{(2\pi)^3}\,\cancel{\frac{3}{2}}\,\frac{4\pi}{\cancel{3}}\left(\frac{2}{\hbar^2}\right)^{3/2}(m_x m_y m_z)^{1/2}\varepsilon^{1/2}$$

$$= \frac{1}{\hbar^2\pi^2}\left(\frac{2 m_x m_y m_z\,\varepsilon}{\hbar^2}\right)^{1/2} \qquad (1)$$

Same as for free electrons but with m replaced by $(m_x m_y m_z)^{1/3}$

(b) Specific heat

$$\frac{C_V}{k_B} = \frac{\pi^2}{3} k_B T\, g(\varepsilon_F)$$

Need ε_F

Now $n = \int_0^{\varepsilon_F} g(\varepsilon_F)\, d\varepsilon_F = \frac{1}{\hbar^2\pi^2}\left(\frac{2 m_x m_y m_z}{\hbar^2}\right)^{1/2}\frac{2}{3}\varepsilon_F^{3/2}$

Hence $\varepsilon_F^{1/2} = (n\,\hbar^2\pi^2)^{1/3}\left(\frac{\hbar^2}{2 m_x m_y m_z}\right)^{1/6}\left(\frac{3}{2}\right)^{1/3}$

i.e. $q_F^{1/2} \propto n^{1/3} (m_x m_y m_z)^{-1/6}$

so

$$C_V \propto k_B T\, n^{1/3} (m_x m_y m_z)^{1/3}$$ (from Eq. (1) on previous page)

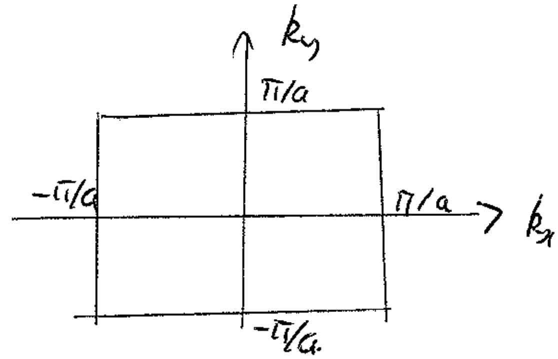
The free electron results would have have m rather than $(m_x m_y m_z)^{1/3}$

3 Hence the linear specific heat of an anisotropic band corresponds to an effective mass $m^* = (m_x m_y m_z)^{1/3}$

i.e. the geometric mean of the eigenvalues of the effective mass tensor.

4/ For Qu 4, See Separate typed solution

5 (a)



Area of 1st BZ is $\left(\frac{2\pi}{a}\right)^2$.

This can accomodate 2 electrons per cell. Consider a circle of radius $R = \frac{\pi}{a} r$.

Area $A = \pi\left[\frac{\pi}{a} r\right]^2$.

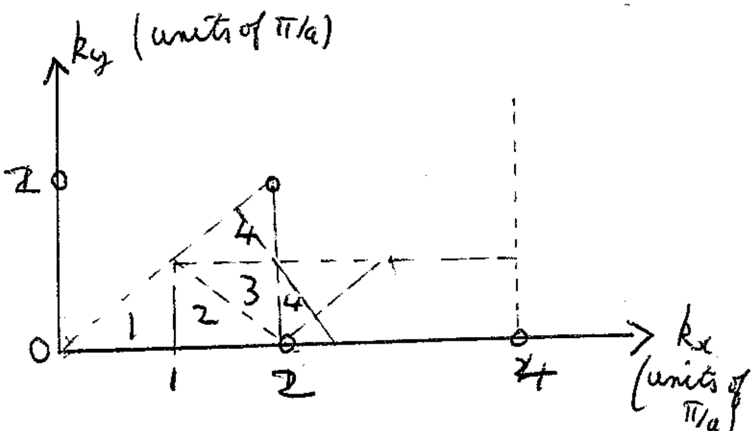
Number of electrons / cell which can be accommodated is

$$m = \frac{2\,\pi\left[\frac{\pi}{a} r\right]^2}{\left(\frac{2\pi}{a}\right)^2} = \frac{2}{4}\pi r^2 = \frac{\pi}{2} r^2.$$

Hence $\underline{\underline{r = \left(\frac{2}{\pi} m\right)^{1/2}}}$.

(b)

m	r
1	0.80
2	1.13
3	1.38
4	1.60
5	1.78
6	1.95



Furthest distance of a point in 1st BZ from origin is $\sqrt{2} \simeq 1.41$
Closest - - - - - - - - - - - - - - - - 0
Furthest - - - - - - - - 2nd - - - - - - - - 2.
Closest - - - - - - - - - - - - - - - - 1.
Furthest - - - - - - - - 3rd - - - - - - - - $\sqrt{5} \simeq 2.24$
Closest - - - - - - - - 3rd - - - - - - - - $\sqrt{2} \simeq 1.41$
Furthest - - - - - - - - 4th - - - - - - - - ~~clearly~~ > 2.
Closest - - - - - - - - 4th - - - - - - - - $\sqrt{2} \simeq 1.41$

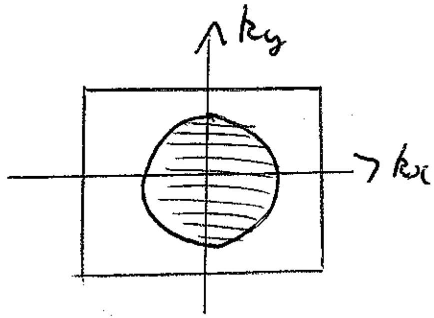
Hence the filling of the zones is as follows:

{ E = empty
P = partially full
F = full

m	1st BZ	2nd BZ	3rd BZ	4th BZ
1	P	E	E	E
2	P	P	E	E
3	P	P	E	E
4	F	P	P	P
5	F	P	P	P
6	F	P	P	P

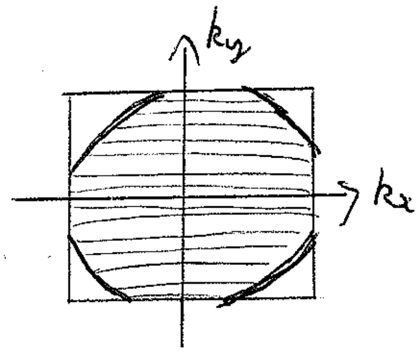
(c)

m=1

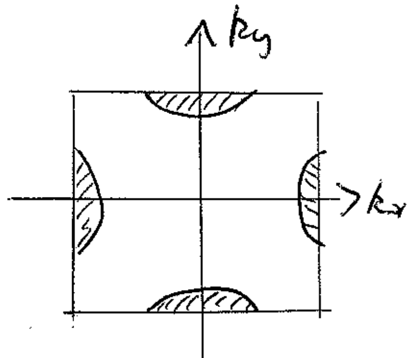


1st BZ, other BZ empty

m=2.

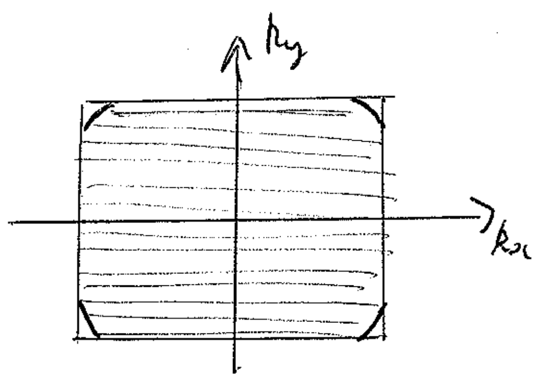


1st BZ

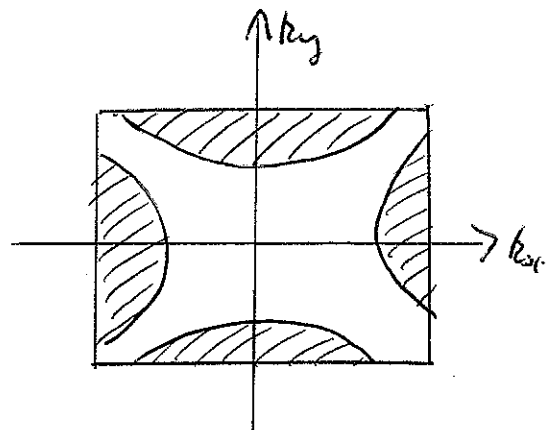


2nd BZ

m=3



1st BZ



2nd BZ

4