Physics 211A — HW3 Solutions — Fall 2014

Ch6, prob 1

Eq. (6.2) is

$$H\Psi = \sum_{\ell=1}^{N} \left[\frac{-\hbar^2}{2m} \nabla_\ell^2 + U(r_\ell) \right] \Psi(r_1 \ldots r_N) = \mathcal{E}\, \Psi(r_1 \ldots r_N)$$

Fn $\Psi(r_1 \ldots r_N) = \psi_1(r_1)\, \psi_2(r_2) \ldots \psi_N(r_N)$

with $-\frac{\hbar^2}{2m} \nabla_\ell^2 \psi_\ell(r_\ell) + U(r_\ell)\, \psi_\ell(r_\ell) = \varepsilon_\ell\, \psi_\ell(r_\ell)$

since $\nabla_\ell^2 \Psi = \psi_1(r_1) \ldots \psi_{\ell-1}(r_{\ell-1})\, \psi_{\ell+1}(r_{\ell+1}) \ldots \psi_N(r_N)\, \nabla_\ell^2 \psi_\ell(r_\ell)$

we get $\sum_{\ell=1}^{N} \psi_1(r_1) \ldots \psi_{\ell-1}(r_{\ell-1})\, \psi_{\ell+1}(r_{\ell+1}) \ldots \psi_N(r_N) \underbrace{\left[\frac{-\hbar^2}{2m} \nabla_\ell^2 + U(r_\ell) \right] \psi_\ell(r_\ell)}_{= \varepsilon_\ell \psi_\ell(r_\ell)} = \mathcal{E}\, \psi_1(r_1) \ldots \psi_N(r_N)$

so the product of ψ's cancels from both sides since it is the same for all terms in the sum

$\Rightarrow$ we are left with $\sum_{\ell=1}^{N} \varepsilon_\ell = \mathcal{E}$

(b) The correct form of a wavefunction is

$$\Psi = \frac{1}{N!} \sum_S (-1)^S \prod_{\ell=1}^{N} \psi_{S\ell}(r_\ell)$$

Now we have a double sum on the left, $\sum_{\ell,S} = \sum_S \sum_\ell$ and $\sum_S$ on the right.

For each term in the ℓ sum we do the same as before, and end up with the same $\sum_S$ on both sides, which cancels out, leading again to

$$\sum_{\ell=1}^{N} \varepsilon_\ell = \mathcal{E}$$

Ch 6, prob 2

Free Fermi gas with N electrons. Find energy of ground state as N varies from 1 to 15. We can put 2 electrons in each $\vec{k}$ state.

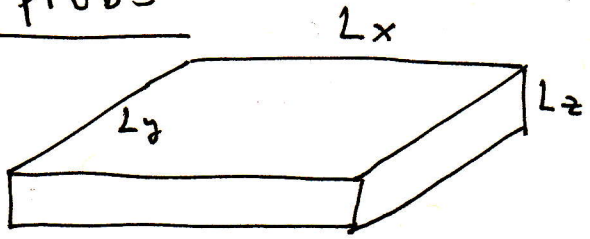
$$\vec{k} = \frac{2\pi}{L}(k_x, k_y, k_z) \quad ; \quad \varepsilon_k = \frac{\hbar^2 k^2}{2m} \quad . \quad E = \sum \varepsilon_\alpha$$

$k = |\vec{k}|$

$\vec{k} = \frac{2\pi}{L}(0,0,0)$	0	1 k	0-2 electrons
$\vec{k} = \frac{2\pi}{L}(\pm 1, 0, 0)$	$\frac{2\pi}{L}$	6 k's	3-14 electrons
$\vec{k} = \frac{2\pi}{L}(1, 1, 0)$	$\frac{2\pi}{L}\sqrt{2}$		15- electrons

# of electrons	E
0, 1, 2	0
$3 \le n \le 14$	$E = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 (n-2)$
15	$E = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 [12 + 1\cdot(\sqrt{2})^2]$

Ch.6, prob 5



$L_x = L_y = 10^6 \text{Å}$, $L_z = 4.1 \text{Å}$

wavefunction should vanish at the boundaries along z direction

$$\Rightarrow \quad \psi(x,y,z) = e^{i(k_x x + k_y y)} \sin(k_z z)$$

$$\psi(x,y,z=0) = \psi(x,y,z=L_z) = 0 \Rightarrow k_z L_z = \pi l \Rightarrow$$

$$\Rightarrow k_z = \frac{\pi}{L_z} l \quad \text{with } l = 1, 2, 3 \ldots \quad (l=0 \text{ is } \underline{\text{not}} \text{ allowed since } \psi = 0)$$

energies are

$$\varepsilon = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2) = \frac{\hbar^2}{2m}\left(\left(\frac{2\pi l_x}{L_x}\right)^2 + \left(\frac{2\pi l_y}{L_y}\right)^2 + \left(\frac{\pi}{L_z} l\right)^2\right) \Rightarrow$$

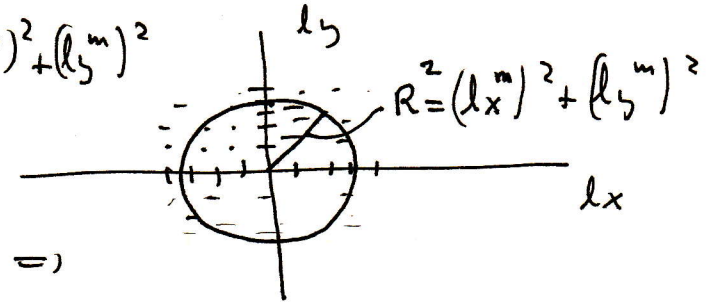
$$\varepsilon = \frac{\hbar^2 \pi^2}{2m}\left(\frac{4(l_x^2 + l_y^2)}{L_x^2} + \frac{l^2}{L_z^2}\right)$$

We set $l = 1$ and start occupying the (l_x, l_y) states. At some point it becomes advantageous to set $l = 2$ and start again with $l_x, l_y = 0, 0$ on

That point is when $\frac{4(l_x^{m2} + l_y^{m2})}{L_x^2} = \frac{3}{L_z^2}$ (diff between $l=1$ and $l=2$

$$\Rightarrow \quad l_x^{m2} + l_y^{m2} = \frac{3}{4}\frac{L_x^2}{L_z^2}$$

The number of electrons in states up to that (l_x^m, l_y^m) is the area of the circle of radius $R^2=(l_x^m)^2+(l_y^m)^2$ x 2 for spin $= 2\cdot\pi\times R^2$



$$= N = 2\times\pi\left((l_x^m)^2+(l_y^m)^2\right) \Rightarrow$$

$$\Rightarrow N = 2\pi\times\frac{3}{4}\frac{L_x^2}{L_z^2}$$. Now how many electrons are in the particle?

Ag has fcc structure, $a = 4.09\,\text{Å} \Rightarrow n = \frac{4}{(4.09\,\text{Å})^3} = 0.0585\,\frac{el}{\text{Å}^3}$ and 1 electron/atom

Our slab has $N_{el} = L_x^2 L_z n$ electrons. So they will occupy all the $l_z=1$ states provided $N_{el} < N \Rightarrow$

$$L_x^2 L_z n < 2\pi\times\frac{3}{4}\frac{L_x^2}{L_z^2} \Rightarrow L_z^3 < \frac{3\pi}{2n} \Rightarrow$$

$$\Rightarrow L_z < \left(\frac{3\pi}{2n}\right)^{1/3} = 7.31\,\text{Å}$$; since $L_z = 4.1\,\text{Å}$, all electrons occupy the $l_z=1$ states.

The highest occupied state has $l_x^{m2}+l_y^{m2} = \frac{N_{el}}{2\pi} = \frac{L_x^2 L_z n}{2\pi} \Rightarrow$ highest energy $\Rightarrow$

$$\varepsilon_H = \frac{\hbar^2\pi^2}{2m}\left(\frac{4\cdot L_z n}{2\pi}+\frac{1}{L_z^2}\right) = 7.98\,eV$$

In contrast, the Fermi energy for the bulk system is

$$\varepsilon_F = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3} = 5.50\,eV$$

The lowest energy state in the pancake has energy

$$\varepsilon_l = \frac{\hbar^2\pi^2}{2m}\frac{1}{L_z^2} \Rightarrow \text{the difference in energies is}$$

$$\varepsilon_h - \varepsilon_l = \frac{\hbar^2\pi^2}{2m}\frac{4 L_z n}{2\pi} = \frac{\hbar^2\pi}{m} L_z n = 5.74\,eV$$

somewhat larger than the kth Fermi energy.

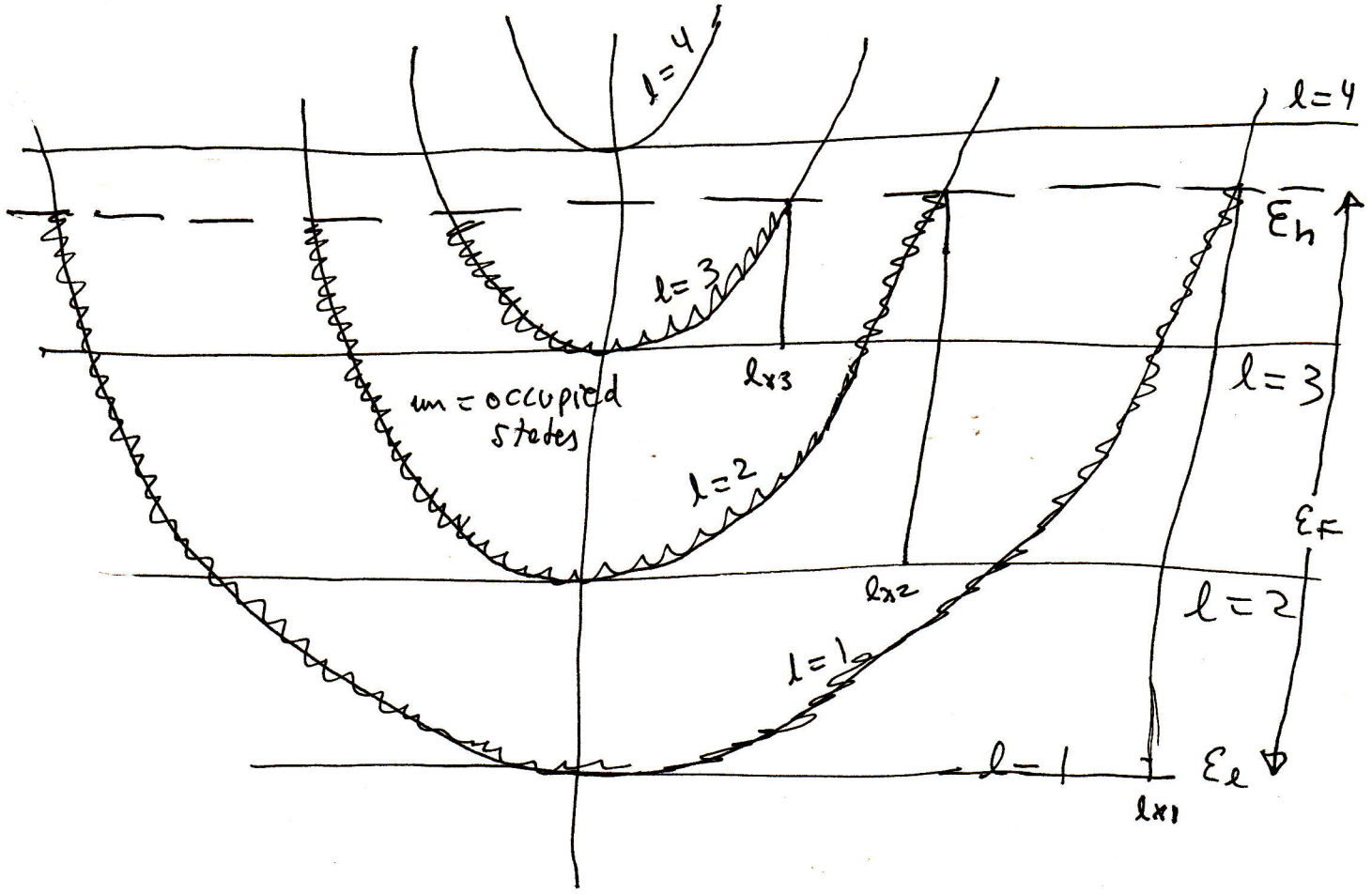
(b) For a layer of thickness $L_z = 8.2\,\text{Å}$:

$$N_{el} = L_x^2 L_z n$$

If only the $l=1$ state is occupied, the # of electrons is $N_1 = \frac{3\pi}{2}\frac{L_x^2}{L_z^2} \Rightarrow$

$$\frac{N_1}{N_{el}} = \frac{3\pi}{2n}\frac{1}{L_z^3} = 0.146\,;$$ so at least some $l=2$ states are occupied..

Let's look at the energy spectrum:



Suppose the occupied states involve $l=1$ and $l=2$ but not $l=3,4,\ldots$

Find the maximum number of electrons we can have:

For $l=2$, $4\,\dfrac{l_{x2}^2+l_{y2}^2}{L_x^2}+\dfrac{4}{L_z^2}=\dfrac{9}{L_z^2}$ gives maximum $l_{x2}^2+l_{y2}^2$

$$\Rightarrow\quad l_{x2}^2+l_{y2}^2=\frac{5}{4}\frac{L_x^2}{L_z^2}\quad,$$ number of electrons in $l=2$ states is

$N_2=2\pi\cdot\dfrac{5}{4}\dfrac{L_x^2}{L_z^2}$. Number of electrons with $l=1$ is then determined by:

$$4\,\frac{l_{x1}^2+l_{y1}^2}{L_x^2}+\frac{1}{L_z^2}=\frac{9}{L_z^2}\Rightarrow l_{x1}^2+l_{y2}^2=\frac{8}{4}\frac{L_x^2}{L_z^2}=\frac{2L_x^2}{L_z^2}\Rightarrow$$

$$N_1=2\pi\cdot\frac{2L_x^2}{L_z^2}\Rightarrow\quad N_1+N_2=2\pi\cdot\frac{13}{4}\frac{L_x^2}{L_z^2}\Rightarrow$$

$$\Rightarrow\quad\frac{N_1+N_2}{N_{el}}=2\pi\cdot\frac{13}{4}\,n\,\frac{1}{L_z^3}=0.63<1\Rightarrow l=3 \text{ states are also occupied.}$$

Assume states up to $l_{x3}^2+l_{y3}^2$ are occupied, # of electrons in $l=3$ states is $N_3=2\pi\left(l_{x3}^2+l_{y3}^2\right)$. In $l=2$,

$$4\,\frac{l_{x2}^2+l_{y2}^2}{L_x^2}+\frac{4}{L_z^2}=4\,\frac{l_{x3}^2+l_{y3}^2}{L_x^2}+\frac{9}{L_z^2}\Rightarrow l_{x2}^2+l_{y2}^2=l_{x3}^2+l_{y3}^2+\frac{5}{4}\frac{L_x^2}{L_z^2}$$

$$\Rightarrow\quad N_2=2\pi\left(l_{x2}^2+l_{y2}^2\right)=2\pi\left(l_{x3}^2+l_{y3}^2\right)+2\pi\cdot\frac{5}{4}\,\frac{L_x^2}{L_z^2}\,.$$

Similarly in $l=1$, $l_{x1}^2+l_{y1}^2=l_{x3}^2+l_{y3}^2+\dfrac{8}{4}\dfrac{L_x^2}{L_z^2}\Rightarrow$

$$\Rightarrow N_1=2\pi\left(l_{x3}^2+l_{y3}^2\right)+2\pi\cdot\frac{8}{4}\,\frac{L_x^2}{L_z^2}\Rightarrow$$

$$\Rightarrow N_1+N_2+N_3 = 6\pi\left(l_{x3}^2+l_{y3}^2\right) + 2\pi\cdot\frac{13}{4}\frac{L_x^2}{L_z^2} = L_x^2 L_z n = N_{el} \Rightarrow$$

$$\Rightarrow \frac{l_{x3}^2+l_{y3}^2}{L_x^2} = \frac{1}{6\pi}\left(-2\pi\cdot\frac{13}{4}\frac{1}{L_z^2} + L_z n\right) = 0.00934$$

The highest energy state occupied has energy

$$\varepsilon_h = \frac{\hbar^2\pi^2}{2m}\left(4\,\frac{l_{x3}^2+l_{y3}^2}{L_x^2} + \frac{3^2}{L_z^2}\right) = 6.44\,eV$$

the lowest energy state is $\varepsilon_l = \frac{\hbar^2\pi^2}{2m}\frac{1}{L_z^2} = 0.56\,eV$

and the difference is $\varepsilon_h - \varepsilon_l = 5.88\,eV$, not too far from the bulk Fermi energy $\varepsilon_F = 5.50\,eV$.

We need to verify that no $l=4$ states are occupied. The lowest $l=4$ state has energy $\varepsilon = \frac{\hbar^2\pi^2}{2m}\frac{4^2}{L_z^2} = 8.95\,eV > 6.44\,eV$,

so only states up to $l=3$ are occupied.

The fraction occupied in each of the levels $l=1$, $l=2$, $l=3$ is:

$$\frac{N_3}{N_{el}} = \frac{2\pi\left(l_{x3}^2+l_{y3}^2\right)}{L_x^2 L_z n} = \frac{l_{x3}^2+l_{y3}^2}{L_x^2}\cdot\frac{2\pi}{L_z n} = 0.00934\cdot\frac{2\pi}{L_z n} = \boxed{0.122}$$

$$\frac{N_2}{N_{el}} = \frac{2\pi\left(l_{x3}^2+l_{y3}^2\right)}{L_x^2 L_z n} + 2\pi\frac{5}{4}\frac{L_x^2}{L_x^2 L_z^3 n} = \frac{N_3}{N_{el}} + \frac{2\pi\,5}{4\,L_z^3 n} = \boxed{0.365}$$

$$\frac{N_1}{N_{el}} = \frac{2\pi\left(l_{x3}^2+l_{y3}^2\right)}{L_x^2 L_z n} + 2\pi\frac{8}{4}\frac{L_x^2}{L_x^2 L_z^3 n} = \frac{N_3}{N_{el}} + 2\pi\frac{8}{4 L_z^3 n} = \boxed{0.512}$$

sum = 1

Problem on 2D electron gas

Density of states is $D(\varepsilon) = \frac{m}{\pi\hbar^2}$; $f(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)}+1} = \frac{e^{-\beta(\varepsilon-\mu)}}{e^{-\beta(\varepsilon-\mu)}+1}$

So density of electrons at finite T is

$$n = \frac{m}{\pi\hbar^2}\int_0^\infty d\varepsilon\, f(\varepsilon) = \frac{m}{\pi\hbar^2}\int_0^\infty d\varepsilon \frac{e^{-\beta(\varepsilon-\mu)}}{e^{-\beta(\varepsilon-\mu)}+1} = \frac{m}{\pi\hbar^2} k_B T \ln\left(e^{\beta\mu}+1\right)$$

For $T=0$, $n = \frac{m}{\pi\hbar^2}\varepsilon_F \Rightarrow \varepsilon_F = k_B T \ln\left(e^{\beta\mu}+1\right)$, or

$$\mu = \varepsilon_F - \ln\left(1+e^{-\beta\mu}\right) k_B T$$

For $T = 500K$, $T_F = 10{,}000K$, $\varepsilon_F/k_B T = 20$

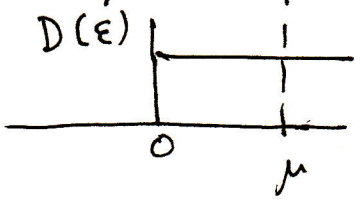
$$\frac{\mu-\varepsilon_F}{k_B T} = -\ln\left(1+e^{-\beta\mu}\right) \simeq -\ln\left(1+e^{-\beta\varepsilon_F}\right) = -\ln\left(1+e^{-20}\right) \Rightarrow$$

$$\Rightarrow \frac{\mu-\varepsilon_F}{k_B T} \simeq -e^{-20} = -2\times10^{-9}$$, or $\mu-\varepsilon_F = -8.9\times10^{-11}\,eV$

The Sommerfeld expansion gives $\mu-\varepsilon_F = -\frac{\pi^2}{6}(k_B T)^2 \frac{D'(\varepsilon_F)}{D(\varepsilon_F)} = 0$

since $D'(\varepsilon_F) = 0$ for $D(\varepsilon) =$ constant.

Sommerfeld expansion fails because $D(\varepsilon)$ is discontinuous at $\varepsilon = 0$



it uses a Taylor expansion around $\varepsilon = \mu$ which obviously can't take into account the discontinuity in $D(\varepsilon)$.