Intermediate written exam I

Exercise 1

① $t(n) = \frac{3}{5}\epsilon_F(n)$ $\qquad k_F = (3\pi^2 n)^{\frac{1}{3}}$

$$t(n) = \frac{3}{5}\frac{\hbar^2}{2m}(3\pi^2 n)^{2/3} \equiv C\, n^{2/3} \; ; \; C = \frac{3\hbar^2}{10m}(3\pi^2)^{2/3}$$

② $$E[n] = C\int d\bar{r}\, n(\bar{r})\, n^{2/3}(r) + \int d\bar{r}\, n(\bar{r})\, v(\bar{r})$$
$$= C\int d\bar{r}\, n^{5/3}(\bar{r}) + \int d\bar{r}\, n(\bar{r})\, v(\bar{r})$$

③ $$\frac{\delta E[n]}{\delta n(\bar{r})} = \frac{5}{3} C\, n^{2/3}(r) + v(\bar{r}) = \mu \,,$$

μ, Lagrange multiplier to enforce $\int d\bar{r}\, n(r) = N$

$\Rightarrow n(\bar{r}) = \left[\frac{3}{5C}(\mu - v(r))\right]^{3/2}$, all $\bar{r}$ for which $\mu - v(\bar{r}) \geq 0$!

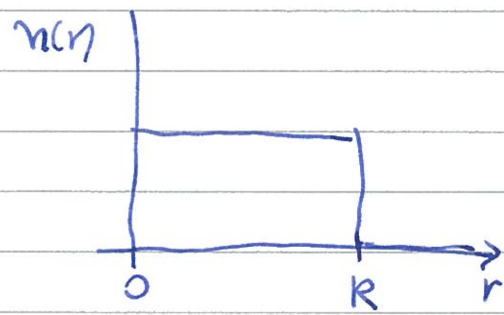
④ $v(\bar{r}) = -V_0$, $r \leq R \Rightarrow \mu - v(\bar{r}) = \mu + V_0 > 0$, $r \leq R$

$\quad = 0$, $r > R \Rightarrow \mu - v(\bar{r}) = \mu < 0$, $r > R$

(remember that $-V_0 < \mu < 0 \Rightarrow 0 < \mu + V_0$, $\mu < 0$)

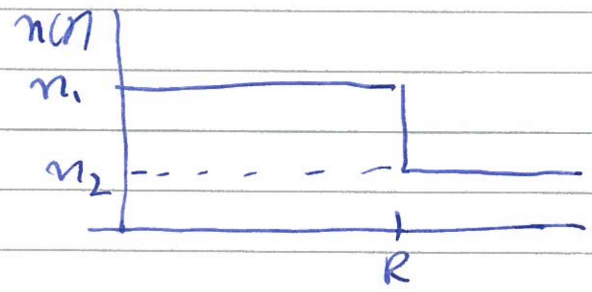
$n(r) =$ cost $\quad r \leq R$,

$\quad\;\; = 0 \quad r > R$



(5) for $\mu > 0$ $\quad \mu - v(r) = \mu + V_0 > 0 \quad , r \leq R$

$\quad = \mu > 0 \quad , r > R$



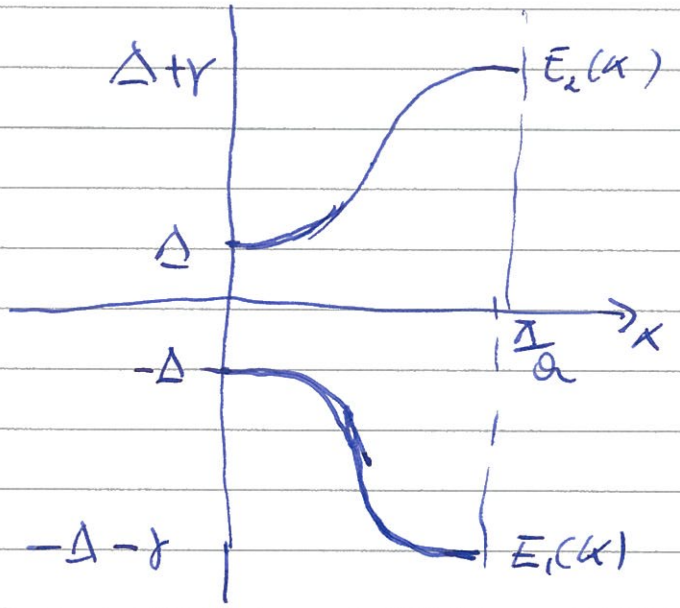
$$n_1 = \left[\frac{3}{5G}(\mu + V_0)\right]^{3/2} , \quad n_2 = \left(\frac{3}{5G}\mu\right)^{3/2} < n_1$$

(6) $n(\vec{r})$ integrates to a finite N for $-V_0 < \mu < 0$, since $n(\vec{r})$ it is finite on a finite domain (the sphere of radius R centered at the origin) and 0 elsewhere.

For $\mu > 0$ the density is finite on an infinite domain and it integrates to an "infinite" value!

Exercise 2

1



symmetric in k

2 An insulator. The lowest band accomodates exactly $2N$ electrons (N k points in the FBZ, 2 spin projection) if there are N atoms on the line L.

It is likely that $-\Delta < \mu < \Delta$, as the lower band is full and the upper one is empty

3 $$g_1(E) = \frac{2}{L} \int_{-\frac{\pi}{a}}^{\pi/a} \frac{dk}{\frac{2\pi}{L}} \delta(E - E_1(k)) = \frac{2}{L} \cdot \frac{L}{\pi} \int_0^{\pi/a} dk\, \delta(E - E_1(k))$$

as $E_1(-k) = E_1(k)$, since $E_1(k)$ is monotonous

$E - E_1(k)$ vanishes only once for $-\Delta-\gamma < E < -\Delta$ at $k^*(E)$: $E_1(k^*) = E$

Therefore

$$g_1(E) = \frac{2}{\pi} \frac{1}{|E_1'(\kappa^*(E))|}$$

$$E_1(\kappa^*) = E = -\Delta + \frac{\gamma}{2}(-1 + \cos(\kappa^* a))$$

$$\Rightarrow \cos(\kappa^* a) = \left(E + \Delta + \frac{\gamma}{2}\right)\frac{2}{\gamma} = \frac{2(E+\Delta)}{\gamma} + 1$$

$$|E_1'(\kappa^*)| = \left|-\frac{\gamma a}{2}\sin\kappa^* a\right| = \frac{\gamma a}{2}\sqrt{1-\cos^2(\kappa^* a)}$$

$$= \frac{\gamma a}{2}\sqrt{1-\left(1+2\frac{E+\Delta}{\gamma}\right)^2} = \frac{\gamma a}{2}\sqrt{4\left[-\left(\frac{E+\Delta}{\gamma}\right)^2 - \frac{E+\Delta}{\gamma}\right]}$$

$$= \gamma a\sqrt{\frac{-E-\Delta}{\gamma}\left(1+\frac{E+\Delta}{\gamma}\right)} = a\sqrt{(-E-\Delta)(\gamma+\Delta+E)}$$

$$\boxed{g_1(E) = \frac{2}{\pi a}\frac{1}{\sqrt{(-E-\Delta)(\gamma+\Delta+E)}} \qquad -\gamma-\Delta < E < -\Delta}$$

Note $-\gamma-\Delta < E < -\Delta$ implies

$$E+\Delta+\gamma > 0 \quad , \quad -E-\Delta > 0 \qquad !$$

The maximum of $E_1(\kappa)$ is at $\kappa = 0$ where $E_1 = -\Delta$. Near $\kappa = 0$ is convenient the put $\epsilon = -\Delta - E$, as this is a small quantity. To leading order

$$\boxed{g_1(E) \simeq \frac{2}{\pi a}\frac{1}{\sqrt{\epsilon\gamma}} = \frac{2}{\pi a\sqrt{\gamma}\sqrt{-E-\Delta}} \quad \text{valid for } \epsilon \ll \gamma}$$

(4) On account of the previous point and the fact that $E_2(\kappa) = -E_1(\kappa)$

$$0 = E - E_2(\kappa^*) = E + E_1(\kappa^*) \Rightarrow E = \Delta - \frac{\gamma}{2}\left(-1 + \cos(\kappa^* a)\right),$$

hence
$$\cos(\kappa^* a) = \frac{2(\Delta - E)}{\gamma} + 1,$$

$$\Delta < E < \Delta + \gamma$$

So

$$g_2(E) = \frac{2}{\pi} \frac{1}{|E_2'(\kappa^*)|} = \frac{2}{\pi} \frac{1}{|E_1'(\kappa^*)|},$$

but κ^* is now different

$$E_1'(\kappa^*) = \frac{\gamma a}{2} |\sin \kappa^* a| = \frac{\gamma a}{2} \sqrt{1 - \left(1 + \frac{2(\Delta - E)}{\gamma}\right)^2}$$
$$= a\sqrt{(E-\Delta)(\gamma + \Delta - E)}$$

$$\boxed{g_2(E) = \frac{2}{\pi a} \frac{1}{\sqrt{(E-\Delta)(\gamma+\Delta-E)}} \qquad \Delta < E < \Delta + \gamma}$$

Near the minimum $\epsilon = E - \Delta$ is small and for $\epsilon \ll \gamma$

$$\boxed{g_2(E) = \frac{2}{\pi a} \frac{1}{\sqrt{\epsilon \gamma}} = \frac{2}{\sqrt{\gamma}\, \pi a \sqrt{E - \Delta}}, \qquad \epsilon \ll \gamma}$$

5 Clearly $E_1(k)$ is the valence band and $E_2(k)$ the conduction band. Therefore:

$$N_c(T) \simeq \int_0^\infty dx\, g_c(x) e^{-\beta x} \qquad x = E - \epsilon_c,$$

here $\epsilon_c = \Delta$, $g_c(x) = \frac{2}{\pi a\sqrt{\gamma}\sqrt{E-\Delta}} = \frac{2}{\pi a\sqrt{\gamma x}}$:

$$N_c(T) = \frac{2}{\pi a\sqrt{\gamma}}\sqrt{k_B T}\int_0^\infty dy\, \frac{e^{-y}}{\sqrt{y}} {}^{*} = \frac{2}{\pi a}\sqrt{\frac{\pi k_B T}{\gamma}};$$

$$P_v(T) \simeq \int_{-\infty}^0 dx\, g_v(x)\, e^{\beta x} \qquad x = \epsilon_v - E$$

here $\epsilon_v = -\Delta$, $g_v(x) = \frac{2}{\pi a\sqrt{\gamma}\sqrt{-E-\Delta}} = \frac{2}{\pi a\sqrt{\gamma x}}$

$$P_v(T) = \frac{2}{\pi a}\int_{-\infty}^0 d\cancel{x}\, \frac{e^{y}}{\sqrt{\gamma}\sqrt{y}} = \frac{2}{\pi a}\sqrt{\frac{\pi k_B T}{\gamma}}$$

$$\boxed{\begin{aligned} n_c(T) &= \frac{2}{\pi a}\sqrt{\frac{\pi k_B T}{\gamma}}\cdot e^{\beta(\mu-\Delta)} \\ p_v(T) &= \frac{2}{\pi a}\sqrt{\frac{\pi k_B T}{\gamma}}\, e^{-\beta(\mu+\Delta)} \end{aligned}}$$

$$* \int_0^\infty dy\, \frac{e^{-y}}{\sqrt{y}} = \int_0^\infty dt\, 2t\, \frac{e^{-t^2}}{t} = \int_{-\infty}^\infty dt\, e^{-t^2} = \sqrt{\pi}$$

6

$$n_c = p_v \Rightarrow e^{\beta\mu} = e^{-\beta\mu} \Rightarrow \boxed{\mu = 0}$$