Exercise 1 — APRIL 30, 2015

① 2D e-gas, unpolarized

$$2 \cdot \frac{\pi k_F^2}{\frac{(2\pi)^2}{A}} = \frac{A k_F^2}{2\pi} = N \Rightarrow k_F^2 = 2\pi\rho$$

$$\epsilon(\rho) = \frac{1}{4} 2\pi\rho - \frac{4}{3\pi}\sqrt{2\pi\rho} = \frac{\pi}{2}\rho - \frac{4}{3}\sqrt{\frac{2}{\pi}}\rho^{\frac{1}{2}}$$

$$\boxed{\epsilon(\rho) = \frac{\pi}{2}\rho - \frac{4}{3}\sqrt{\frac{2}{\pi}}\rho^{\frac{1}{2}}}$$

② $$E_I^{LDA}[\rho] = \int d\bar{r}\, \rho(\bar{r})\, \epsilon(\rho(\bar{r}))$$

$$E_I^{LDA}[\rho] = c_1 \int d\bar{r}\, \rho^2(\bar{r}) - c_2 \int d\bar{r}\, \rho(\bar{r})^{3/2}$$

$$c_1 = \frac{\pi}{2} \qquad c_2 = \frac{4}{3}\sqrt{\frac{2}{\pi}}$$

③ $$E[\rho] = E_I^{LDA}[\rho] + \int d\bar{r}\, \rho(\bar{r})\, v(\bar{r})$$

$$\begin{cases} \dfrac{\delta E[\rho]}{\delta \rho(r)} = \mu = 2c_1\rho(\bar{r}) - \dfrac{3}{2}c_2\,\rho(\bar{r})^{\frac{1}{2}} + v(\bar{r}) \\ \text{or} \\ \rho(\bar{r}) = 0 \end{cases}$$

(4)

$$\alpha^2\left(\frac{2}{\pi^2}\right) = \pi\rho(\bar{r}) - 2\sqrt{\frac{2}{\pi}}\,\rho(\bar{r})^{\frac{1}{2}} + \frac{2}{\pi^2}r^2$$

(5) $$\Rightarrow \quad \rho(r) - 2\sqrt{\frac{2}{\pi^3}}\,\rho^{\frac{1}{2}}(r) + \frac{2}{\pi^3}(r^2-\alpha^2) = 0$$

$$\rho^{\frac{1}{2}}(\bar{r}) = \sqrt{\rho_0} \pm \sqrt{\rho_0 - \rho_0(r^2-\alpha^2)}$$

$$\sqrt{\frac{\rho(\bar{r})}{\rho_0}} = 1 \pm \sqrt{1+\alpha^2-r^2}$$

$$\frac{\rho(\bar{r})}{\rho_0} = \left[\sqrt{1+\alpha^2-r^2} \pm 1\right]^2 \equiv \tilde{\rho}_\pm(r)$$

- Both $\rho_+(r)$ and $\rho_-(r)$ grow as $r^2$ at large $r$
- At large $r$ the only acceptable solution is $\rho(r) = 0$
- However $\rho_+(r)$ never vanishes, while $\rho_-(r)$ vanishes at $r=\alpha$.

The solution, therefore is

$$\begin{cases} 0 \leq r \leq \alpha & \rho_-(r) = \left[\sqrt{1+\alpha^2-r^2} - 1\right]^2 \\ \alpha < r & \rho(r) = 0 \end{cases}$$

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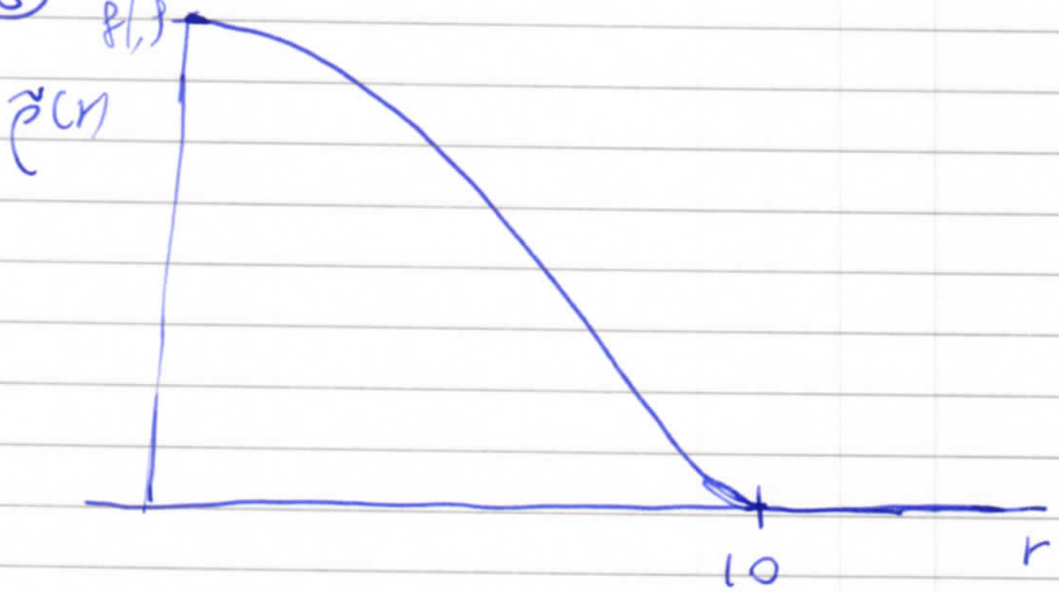

# EXERCISE 1 16-07-13

① $\omega_c = \dfrac{eB}{mc} = \dfrac{eB}{m_e c} \dfrac{1}{m/m_e}$

$\dfrac{m_c}{m_e} = \dfrac{eB}{m_e c} \dfrac{1}{\omega_c^{(c)}} = \dfrac{4.8032\times10^{-10} \times 10^3}{9.1094\times10^{-28} \times 2.9979\times10^{10}}$

$\times \dfrac{1}{5.18\times10^{10}} = 3.3954\times10^{-2} \times 10 = 0.33954$

$\dfrac{m_v}{m_e} = \dfrac{m_c}{m_e} \times \dfrac{\omega_c^{(c)}}{\omega_c^{(v)}} = 0.33954 \times \dfrac{5.18}{3.59}$

$= 0.48992$

②

$E_d^b = 13.606 \times \dfrac{m_c}{m_e} \dfrac{1}{\epsilon^2} = 0.0338$ eV

③ $\epsilon^{-1} = \sqrt{\dfrac{0.0338}{13.606 \times 0.33954}} = 0.085536$

$\epsilon = 11.691$

④ $a_B^{(d)} = a_B \dfrac{\epsilon}{m_c/m_e} = 0.52918 \times \dfrac{11.691}{0.33954}$

$= 18.221$ Å $= 34.432$

⑤ Si ( $a_B^{d} >> a_B$ ! )

$E_a^b = E_d^b \dfrac{m_v}{m_e} \dfrac{1}{m_c/m_e} = 0.0338 \times \dfrac{0.48992}{0.33954}$

$= 0.048770$

(6)

(i) $E_{th} = 0.048770\,eV$

(ii) As there are no holes and $N_d - N_a$ electrons on the donors

$$E_{th} = 0.0338 \ eV$$