COMPITO I, 10.05.19

ESERCIZIO 1

① $\epsilon(\rho) = \frac{3}{10}(3\pi^2)^{2/3}\rho^{2/3} - \frac{3}{4\pi}(3\pi^2)^{\frac{1}{3}}\rho^{\frac{1}{3}} \equiv A\rho^{2/3} - B\rho^{\frac{1}{3}}$; $A = \frac{3(3\pi^2)^{2/3}}{10}$, $B = \frac{3(3\pi^2)^{1/3}}{4\pi}$

② $E_I[\rho] = A\int d\bar{r}\, \rho(\bar{r})^{5/3} - B\int d\bar{r}\, \rho(\bar{r})^{4/3}$

③ $E[\rho] = A\int d\bar{r}\, \rho(\bar{r})^{5/3} - B\int d\bar{r}\, \rho(\bar{r})^{4/3} + \int d\bar{r}\, \rho(\bar{r})\, v(\bar{r})$

$$\frac{\delta E[\rho]}{\delta\rho(\bar{r})} = \frac{5}{3}A\rho(\bar{r})^{2/3} - \frac{4}{3}B\rho(\bar{r})^{1/3} + v(\bar{r}) = \mu$$

④ $\rho(r)^{2/3} - \frac{4}{5}\frac{B}{A}\rho(\bar{r})^{\frac{1}{3}} - \frac{3}{5A}(\mu - v(\bar{r})) = 0 \Rightarrow \rho(r)^{\frac{1}{3}} = \frac{2}{5}\frac{B}{A} \pm \sqrt{\left(\frac{2B}{5A}\right)^2 + \frac{3}{5A}(\mu - v(\bar{r}))}$

$$\rho(\bar{r})^{\frac{1}{3}} = \frac{2B}{5A}\left[1 \pm \sqrt{1 + \frac{15A}{4B^2}(\mu - v(\bar{r}))}\right.$$

⑤ $\Delta_2 E = \frac{1}{2}\int d\bar{r}\int d\bar{r}'\, g(\rho(\bar{r}))\,\delta(\bar{r}-\bar{r}')\,\delta\rho(\bar{r})\,\delta\rho(\bar{r}') = \frac{1}{2}\int d\bar{r}\, g(\rho(\bar{r}))(\delta\rho(\bar{r}))^2 \Rightarrow \Delta_2 > 0\ \forall\, \delta\rho(\bar{r})$

if $g(\rho(\bar{r})) > 0\ \forall\, \rho(\bar{r})$

⑥ $\Delta_2 E[\rho] = \int d\bar{r}\, \frac{1}{2}\left\{\frac{10}{9}A\frac{\delta\rho(\bar{r})^2}{\rho(\bar{r})^{1/3}} - \frac{4}{9}B\frac{\delta\rho(\bar{r})^2}{\rho(\bar{r})^{2/3}}\right\} =$

$$= \frac{1}{2}\int d\bar{r}\int d\bar{r}'\left[\frac{10A}{9}\frac{1}{\rho(\bar{r})^{1/3}} - \frac{4B}{9}\frac{1}{\rho(\bar{r})^{2/3}}\right]\delta(\bar{r}-\bar{r}')\,\delta\rho(\bar{r})\,\delta\rho(\bar{r}')$$

$$\frac{\delta^2 E[\rho]}{\delta\rho(\bar{r})\delta\rho(\bar{r}')} = \left[\frac{10A}{9\rho(\bar{r})^{1/3}} - \frac{4B}{9\rho(\bar{r})^{2/3}}\right]\delta(\bar{r}-\bar{r}')$$

for $\rho(\bar{r})^{\frac{1}{3}} \neq 0 \Rightarrow \rho(\bar{r})^{\frac{1}{3}} > \frac{2B}{5A} \Rightarrow \rho(\bar{r})^{\frac{1}{3}} = \frac{2B}{5A}\left[1 + \sqrt{1 + \frac{15A}{4B^2}(\mu - v(\bar{r}))}\right]$

⑦ $\mu < -\frac{4B^2}{15A}$, so that, for $r > R$, $\rho(r) = 0$ since the argument of the square root becomes negative.

The density in fact is piecewise constant and must be vanishing in the infinite range $r > R$, to deliver a finite number of particles, i.e., must be integrable!

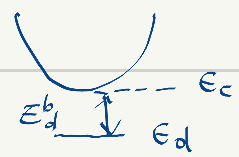
ESERCIZIO 2

① $\omega_c = \frac{eB}{mc} = \frac{eB}{m_e c}\frac{m_e}{m} \Rightarrow \frac{m}{m_e} = \frac{eB}{m_e c}\frac{1}{\omega_c}$

for $B = 1$ tesla $= 10^4$ gauss , $\frac{eB}{m_e c} = \frac{4.80\times10^{-10}\cdot10^4}{0.911\times10^{-27}\cdot3.00\times10^{10}} = 1.76\times10^{11}$

$$\frac{m_c}{m_e} = \frac{1.76\times10^{11}}{2.67\times10^{12}} = 0.0659$$

$$\frac{m_v}{m_e} = \frac{1.76\times10^{11}}{3.52\times10^{11}} = 0.500$$



② $E_d^b = 5.07\cdot10^{-3}$ eV

With donors only the photoabsorption threshold equals E_d^b, hence

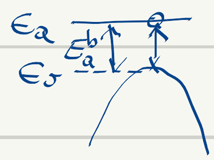
③ $E_d^b = \frac{m_c}{m_e}\frac{1}{\epsilon^2}\times13.6\text{ eV} = 5.07\times10^{-3}\text{ eV} \Rightarrow \epsilon = \sqrt{\frac{(m_c/m_e)\cdot13.6}{5.07\times10^{-3}}} = 13.3$

④ $a^*_{B,d} = \frac{\epsilon}{(m_c/m_e)}\cdot a_B = \frac{13.3}{0.0659}\times0.529\ \text{Å} = 107\ \text{Å}$

⑤ YES , $a^*_{B,d} \gg a_L \simeq \text{Å}$, where a_L is a measure of the WS cell.

⑥ We need $E_a^b = \frac{m_v}{m_e}\frac{1}{\epsilon^2}\times13.6\text{ eV} = \frac{0.500}{(13.3)^2}\times13.6 = 3.84\times10^{-2}$ eV

We restrict to very low temperatures



(2) the photoabsorption threshold is due to the promotion of an electron from the top of valence to the acceptor level : it is, therefore $3.84\cdot10^{-2}$ eV

(ii) There are no holes, while we have $N_d - N_a$ electrons on donors.

Therefore the threshold is $E_d^b = 5.07 \times 10^{-3}$ eV