① *
$$\frac{\delta E_{LDA}}{\delta \rho(\vec r)} = \lambda = \frac{d}{d\rho}\rho\epsilon(\rho)\Big|_{\rho(r)} + e^2\int d\vec r' \frac{\rho_Q(\vec r')}{|\vec r-\vec r'|} + \Phi_{ext}(\vec r)$$

②

Note: $E = N\epsilon(\rho) = V\rho\epsilon(\rho)$

$$\mu = \frac{\partial E}{\partial N}\Big|_V = V\frac{\partial \rho\epsilon(\rho)}{\partial N}\Big|_V = \frac{d\,\rho\epsilon(\rho)}{d\rho}$$

$$\lambda = \mu(\rho(\vec r)) + e^2\int d\vec r' \frac{\rho_Q(\vec r')}{|\vec r-\vec r'|} + \Phi_{ext}(\vec r)$$

$$= \mu(\rho(\vec r)) + \Phi(r)$$

③ For $\Phi_{ext} = 0$ we expect $\rho_Q(r) = 0$ which implies $\rho(r) = \rho_b$.

Thus $\lambda = \mu(\rho_b)$

④ For $\Phi_{ext}(\vec r)$ small we expect $\rho_Q(\vec r) \ll \rho_b$

Hence

$$\lambda = \mu(\rho_b) + \frac{d\mu}{d\rho}\Big|_{\rho_b}\rho_Q(\vec r) + \Phi(\vec r)$$

⑤ $\Rightarrow \rho_Q(\vec{r}) = -\dfrac{\Phi(\vec{r})}{\left.\dfrac{d\mu}{d\rho}\right|_{\rho_b}}$

$\Rightarrow \rho_Q(q) = -\dfrac{\Phi(q)}{\left.\dfrac{d\mu}{d\rho}\right|_{\rho_b}}$

$\tilde{\chi}(q) = \dfrac{\rho_Q(q)}{\Phi(q)} = -\dfrac{1}{\left.\dfrac{d\mu}{d\rho}\right|_{\rho_b}}$

⑥ $\epsilon(q) = 1 - \tilde{\chi}(q)\, v(q) = 1 + \dfrac{v(q)}{\left.\dfrac{d\mu}{d\rho}\right|_{\rho_b}}$

$\epsilon(q) = 1 + \dfrac{2\pi e^2}{\left.\dfrac{d\mu}{d\rho}\right|_{\rho_b}} \dfrac{1}{q} = 1 + \dfrac{\varkappa}{q}$

$\varkappa = \dfrac{2\pi e^2}{\left.\dfrac{d\mu}{d\rho}\right|_{\rho_b}}$

*

Derivata funzionale prima di

$$I[\rho] = \frac{e^2}{2}\int d\bar{r}\int d\bar{r}'\, \rho_a(\bar{r})\rho_a(\bar{r}')\frac{1}{|\bar{r}-\bar{r}'|}$$

$$= \frac{e^2}{2}\int d\bar{r}\int d\bar{r}'\,\frac{1}{|\bar{r}-\bar{r}'|}\left\{(\rho(\bar{r})-\rho_b)(\rho(\bar{r}')-\rho_b)\right\}$$

Consideriamo la variazione indotta da

$$\rho(\bar{r}) \to \rho(\bar{r}) + \delta\rho(\bar{r}), \quad \rho(\bar{r}') \to \rho(\bar{r}') + \delta\rho(\bar{r}')$$

Intanto

$$\rho_a \to \rho_a + \delta\rho$$

e quindi

$$I[\rho] \to I[\rho+\delta\rho] =$$

$$= \frac{e^2}{2}\int d\bar{r}\int d\bar{r}'\,\frac{1}{|\bar{r}-\bar{r}'|}\left[\rho_a(\bar{r})+\delta\rho(\bar{r})\right]\left[\rho_a(\bar{r}')+\delta\rho(\bar{r}')\right]$$

$$= I[\rho] + \boxed{\frac{e^2}{2}\int d\bar{r}\int d\bar{r}'\,\frac{1}{|\bar{r}-\bar{r}'|}\left\{\rho_a(\bar{r}')\,\delta\rho(\bar{r}) + \rho_a(\bar{r})\,\delta\rho(\bar{r}')\right\}}$$

$$+ O(\delta\rho^2) \equiv I[\rho] + \Delta_1 I[\rho] + O(\delta\rho^2)$$

$$\Delta_1 I[\rho] = \frac{e^2}{2}\int d\bar{r} \int d\bar{r}' \frac{1}{|\bar{r}-\bar{r}'|} \, 2\rho_a(\bar{r}') \, \delta\rho(\bar{r})$$

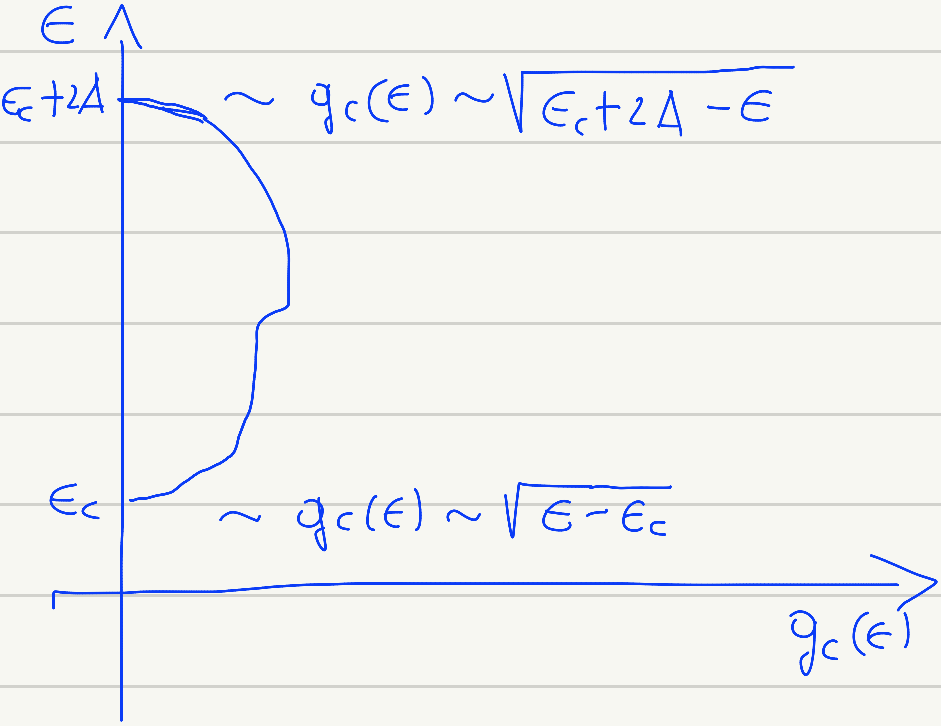
ove abbiamo scambiato gli indici muti di uno dei 2 termini presenti in $\Delta_1 I[\rho]$.

Ne consegue che

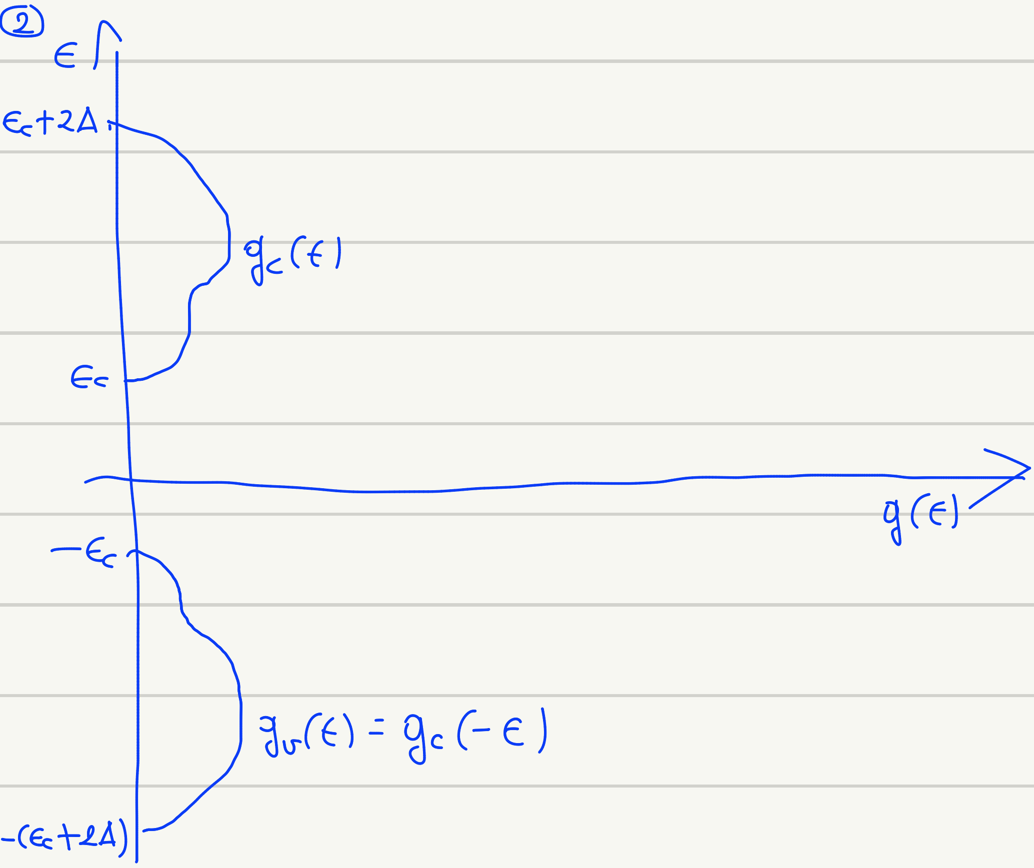
$$\boxed{\frac{\delta I[\rho]}{\delta\rho(\bar{r})} = e^2 \int d\bar{r}' \frac{\rho_a(\bar{r}')}{|\bar{r}-\bar{r}'|}}$$

ESERCIZIO 2

① Let's follow the suggestion and set $\epsilon^* = 0$, hence $g_v(-\epsilon) = g_c(\epsilon)$.



②



③ $$n_c(T) = \int_{\epsilon_c}^{\epsilon_c+2\Delta} d\epsilon \, \frac{g_c(\epsilon)}{e^{\beta(\epsilon-\mu)}+1} = p_v(T) = \int_{-\epsilon_c-2\Delta}^{-\epsilon_c} d\epsilon \, \frac{g_v(\epsilon)}{e^{\beta(\mu-\epsilon)}+1} =$$

$$\int_{-\epsilon_c-2\Delta}^{-\epsilon_c} d\epsilon \, \frac{g_c(-\epsilon)}{e^{\beta(\mu-\epsilon)}+1} = \int_{\epsilon_c}^{\epsilon_c+2\Delta} d\epsilon \, \frac{g_c(\epsilon)}{e^{\beta(\mu+\epsilon)}+1} .$$

We thus get

$$n_c(T) - p_v(T) = 0 = \int_{\epsilon_c}^{\epsilon_c+2\Delta} d\epsilon \; g_c(\epsilon) \left[\frac{1}{e^{\beta(\epsilon-\mu)}+1} - \frac{1}{e^{\beta(\epsilon+\mu)}+1} \right] \equiv X(\mu)$$

$$= \sinh\beta\mu \int_{\epsilon_c}^{\epsilon_c+2\Delta} d\epsilon \; g_c(\epsilon) \frac{2e^{\beta\epsilon}}{e^{2\beta\epsilon} + 2e^{\beta\epsilon}\cosh\beta\mu + 1} \equiv \sinh\beta\mu \cdot I(\mu)$$

Since $I(\mu) > 0$ $\forall$ $|\mu| < \infty$, $X(\mu) = 0$ implies $\sinh\beta\mu = 0$, i.e., $\mu = 0$

$$\boxed{③ \quad \mu = 0}$$

④ If the "piece" of the Bravais we are considering has N_c sites we have in P.B.C.*

$$\int_{\epsilon_c}^{\epsilon_c+2\Delta} d\epsilon \, g_c(\epsilon) = g_s N_c / V = g_s \rho_L$$

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* $g_c(\epsilon) = (g_s/V) \sum'_{\bar{k}} \delta(\epsilon - \epsilon_c(\bar{k})) \Rightarrow \int d\bar{\epsilon} \, g_c(\bar{\epsilon}) = g_s N_c / V$

So, we need to calculate

$$\int_{\epsilon_c}^{\epsilon_c+2\Delta} d\epsilon \sqrt{(\epsilon-\epsilon_c)(\epsilon_c+2\Delta-\epsilon)} = \int_{-\Delta}^{\Delta} dy \sqrt{\Delta^2-y^2} \quad ; \quad y = \epsilon-\epsilon_c-\Delta$$

Let's set $x = y/\Delta$. We get

$$\int_{-\Delta}^{\Delta} dy \sqrt{\Delta^2-y^2} = \Delta^2 \int_{-1}^{1} dx \sqrt{1-x^2} = 2\Delta^2 \int_{0}^{1} dx \sqrt{1-x^2}$$

Now we set $x = \sin t$, $0 < t \leq \pi/2$, which yields

$$\int_0^1 dx \sqrt{1-x^2} = \int_0^{\pi/2} dt \cos^2 t = \int_0^{\pi/2} dt \, \frac{1+\cos 2t}{2} = \frac{\pi}{4}.$$

Therefore

$$A\int_{\epsilon_c}^{\epsilon_c+2\Delta} d\epsilon \sqrt{(\epsilon-\epsilon_c)(\epsilon_c+2\Delta-\epsilon)} = A \cdot 2\Delta^2 \frac{\pi}{4} = g_s \rho_L,$$

$$\boxed{A = \frac{2}{\pi\Delta^2} \rho_L g_s}$$

5) $\epsilon-\epsilon_c = x \ll \Delta$

$$g_c(\epsilon) \simeq A\sqrt{x(2\Delta-x)} \simeq A\sqrt{2\Delta x} = \left(\frac{2}{\Delta}\right)^{3/2} \frac{\rho_L}{\pi} \sqrt{\epsilon-\epsilon_c} \; g_s$$

Knowing that near the minimum

$$g_c(\epsilon) = \frac{m_c^{3/2}}{\hbar^3 \pi^2} \sqrt{2(\epsilon - \epsilon_c)} \, ,$$

we have

$$m_c^{3/2} = \frac{\hbar^3 \pi^2}{\sqrt{2}} \frac{g_c(\epsilon)}{\sqrt{\epsilon - \epsilon_c}} = \frac{\hbar^3 \pi^2}{\sqrt{2}} \left(\frac{2}{\Delta}\right)^{3/2} \frac{g_s \rho_L}{\pi} = \frac{2\hbar^3 \pi \, g_s \rho_L}{\Delta^{3/2}}$$

$$\boxed{⑤ \quad m_c = \frac{\hbar^2}{\Delta} (g_s 2\pi \rho_L)^{2/3}}$$

⑥ $$m_c = \frac{\hbar^2}{\Delta} (g_s 2\pi \rho_L)^{2/3} = \frac{(1.05 \times 10^{-27})^2}{27.7 \times 1.6 \times 10^{-12}} \left(2 \times 3.14 \times 5 \times 10^{22}\right)^{2/3} g_s^{2/3}$$

$$= \frac{(1.05)^2 (314)^{2/3} \, 10^{-40}}{4.43 \times 10^{-11}} g_s^{2/3} = 11.5 \times 10^{-29} g_s^{2/3} \text{ grams}$$

$$m_c / m_e = \frac{11.5 \times 10^{-29}}{9.11 \times 10^{-28}} g_s^{2/3} = 0.126 \, g_s^{2/3}$$

$\rightarrow 0.200 \quad g_s = 2$

$\rightarrow 0.126 \quad g_s = 1$