Esercizio 1

① The HF equations are [HF notes, eq. (1.15)] for the present case

$$\left[-\frac{\hbar^2}{2m}\nabla^2+v_b(x)\right]\psi_\gamma(y)+\int dy'\sum_\beta|\psi_\beta(y')|^2 v(x'-x)\,\psi_\gamma(y)$$

$$-\int dy'\sum_{\beta'}\psi^*_\beta(y')\psi_\gamma(y')\,v(x-x')\psi_\beta(y)=\epsilon_\gamma\psi_\gamma(y)$$

where x is the cartesian coordinate of the 1D system and $y=(x,s)$ with s the spin variable.

Also

$$\psi_\gamma(y)=\frac{1}{\sqrt{L}}e^{ik_\sigma\cdot x}\delta_{\sigma s} \qquad \gamma=(\sigma,k_\sigma)$$

$$\psi_\beta(y')=\frac{1}{\sqrt{L}}e^{iq_{\sigma'}\cdot x'}\delta_{\sigma' s'}. \qquad \beta=(\sigma',q_{\sigma'})$$

Let consider the Hartree potential:

$$v_H(y)=\int dy'\sum_\beta|\psi_\beta(y')|^2 v(x'-x)$$

$$=\int dx'\sum_{s'}\sum_{\sigma' q_{\sigma'}}\frac{1}{L}\delta^2_{\sigma' s'}\,v(x'-x)=$$

$$=\int dx'\sum_{\sigma'}\sum_{q_{\sigma'}}\frac{1}{L}v(x'-x)=\int dx'\sum_{\sigma'}\frac{N_{\sigma'}}{L}v(x'-x)$$

$$=\int dx'\,\frac{N}{L}v(x'-x)=\int dx'\,e_b\,v(x-x')=-v_b(x)$$

Clearly, the Hartree potential cancels the background potential. So we are left with the exchange term

$$- \sum_{\beta} \int dy' \, \psi_\beta^*(y') \psi_\gamma(y') \, v(x'-x) \, \psi_\beta(y) =$$

$$- \int dx' \sum_{s'} \sum_{\sigma' q_{\sigma'}} \frac{1}{L^{3/2}} \delta_{\sigma' s'} \delta_{\sigma s'} \delta_{\sigma' s} \, e^{i[-q_{\sigma'} x' + k_\sigma x' + q_{\sigma'} x]} \, v(x'-x) =$$

$$- \int dx' \sum_{\sigma' q_{\sigma'}} \frac{1}{L^{3/2}} \delta_{\sigma\sigma'} \delta_{\sigma s} \, e^{i[(k_\sigma - q_\sigma) x' + (q_\sigma - k_\sigma) x]} \times v(x'-x) \, e^{i k_\sigma x} =$$

$$- \int dx' \sum_{q_\sigma} \frac{1}{L} e^{i(k_\sigma - q_\sigma)(x'-x)} \, v(x'-x) \frac{1}{\sqrt{L}} e^{i k_\sigma x} \delta_{\sigma s} =$$

$$- \frac{1}{L} \sum_{q_\sigma} \tilde{v}(k_\sigma - q_\sigma) \psi_\gamma(y) \equiv \epsilon_x(k_\sigma) \psi_\gamma(y)$$

Sfruttando i risultati precedenti otteniamo

$$\left[\frac{\hbar^2}{2m} \nabla^2 + \epsilon_x(k_\sigma) \right] \psi_\gamma(y)$$

$$\boxed{= \left[\frac{\hbar^2 k_\sigma^2}{2m} + \epsilon_x(k_\sigma) \right] \psi_\gamma(y) = \epsilon_\gamma \psi_\gamma(y)}$$

$$\boxed{\epsilon_x(k) = - \frac{1}{L} \sum_{q} \tilde{v}(k-q)}$$

- Il determinante di onde piane é soluzione HF!

(2) $$\epsilon_x(k) = -\frac{1}{L}\sum_q{}' \tilde{v}(k-q)$$

(3) $$\tilde{v}(q) = \int dx\, v(x) e^{iqx} = \int_{-\infty}^{+\infty} dx\, v_0 e^{-q_0|x| + iqx}$$

$$= v_0\left[\int_0^{\infty} dx\, e^{(-q_0+iq)x} + \int_{-\infty}^{0} dx\, e^{(q_0+iq)x}\right]$$

$$= v_0\left[\frac{1}{q_0 - iq} + \frac{1}{q_0+iq}\right] = v_0\frac{2q_0}{q_0^2+q^2}$$

(4)
$$\epsilon_x(k) = -\frac{1}{L}\sum_q{}' \tilde{v}(k-q) = -\int_{-k_F}^{k_F}\frac{dq}{2\pi}\tilde{v}(k-q)$$

$$= -\frac{v_0}{\pi} q_0 \int_{-k_F}^{k_F} dq \frac{1}{q_0^2 + (k-q)^2}$$

- k_F

$$2\times\frac{2k_F}{\frac{2\pi}{L}} = N \Rightarrow k_F = \frac{\pi}{2}\frac{N}{L} = \frac{\pi}{2}n$$

$$\boxed{t = \frac{q}{q_0}}$$

$$\epsilon_x(k) = -\frac{v_0}{\pi}\int_{-k_F/q_0}^{k_F/q_0} dt\, \frac{1}{1+\left(t-\frac{k}{q_0}\right)^2}$$

$$= -\frac{v_0}{\pi} \arctan\left(t - \frac{k}{q_0}\right)\Bigg|_{-k_F/q_0}^{k_F/q_0}$$

$$\epsilon_x(k) = -\frac{v_0}{\pi}\left[\operatorname{atan}\left(\frac{k_F-k}{q_0}\right) - \operatorname{atan}\left(\frac{-k_F-k}{q_0}\right)\right]$$

$$\epsilon_x(k) = -\frac{v_0}{\pi}\left[\operatorname{atan}\frac{k_F-k}{q_0} + \operatorname{atan}\frac{k_F+k}{q_0}\right]$$

$$\boxed{\epsilon_x(k) = \epsilon_x(-k)}$$

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$$\frac{d}{dt}\operatorname{atan}(t) = \frac{1}{1+t^2}$$

$$\frac{d^2}{dt^2}\operatorname{atan}(t) = -\frac{2t}{(1+t^2)^2}$$

$$\epsilon_x(k) \simeq -\frac{v_0}{\pi}\left[2\operatorname{atan}\frac{k_F}{q_0} + 0 + \right.$$

$$\left. + \frac{1}{2}2\left(-\frac{2t}{(1+t^2)^2}\right|_{t=\frac{k_F}{q_0}}\left(\frac{k}{q_0}\right)^2\right]$$

$$\epsilon_x(k) \simeq -\frac{2v_0}{\pi}\operatorname{atan}\frac{k_F}{q_0} + \frac{2v_0}{\pi}\frac{k_F/q_0}{[1+(k_F/q_0)^2]^2}\left(\frac{k}{q_0}\right)^2$$

$$\epsilon_x(k) \simeq \epsilon_x(0) + \epsilon_{x,2}k^2$$

$$\epsilon_{x2} = \frac{2v_0}{\pi}\frac{q_0 k_F}{(q_0^2+k_F^2)^2}$$

6 vicino al minimo

$$\epsilon(k) = \epsilon_x(0) + \left[\frac{2v_0}{\pi}\frac{q_0 k_F}{(q_0^2+k_F^2)^2} + \frac{\hbar^2}{2m_e}\right]k^2$$

$$= E_x(0) + \frac{\hbar^2}{2m^*}\kappa^2$$

$$\boxed{\frac{1}{m^*} = \frac{1}{m_e} + \frac{4J_0}{\hbar^2}\frac{}{\pi}\frac{q_0 k_F}{(q_0^2 + k_F^2)^2}}$$

ESERCIZIO 2

① $$\chi_0(q) = -\frac{2}{L}\int_{-k_F}^{k_F}\frac{dk}{\frac{2\pi}{L}}\left[\frac{1}{\frac{\hbar^2}{2m}(q^2+2qk)}+\frac{1}{\frac{\hbar^2}{2m}(q^2-2qk)}\right]$$

* vedi nota in fondo!

(1) $$\chi_0(q) = -\frac{1}{\pi}\frac{m}{\hbar^2}\frac{1}{q}\int_{-k_F}^{k_F}dk\left[\frac{1}{k+\frac{q}{2}}+\frac{1}{-k+\frac{q}{2}}\right]$$

$$= -\frac{m}{\pi\hbar^2 q}\ln\left|\frac{k+q/2}{-k+q/2}\right|\Bigg|_{-k_F}^{k_F}$$

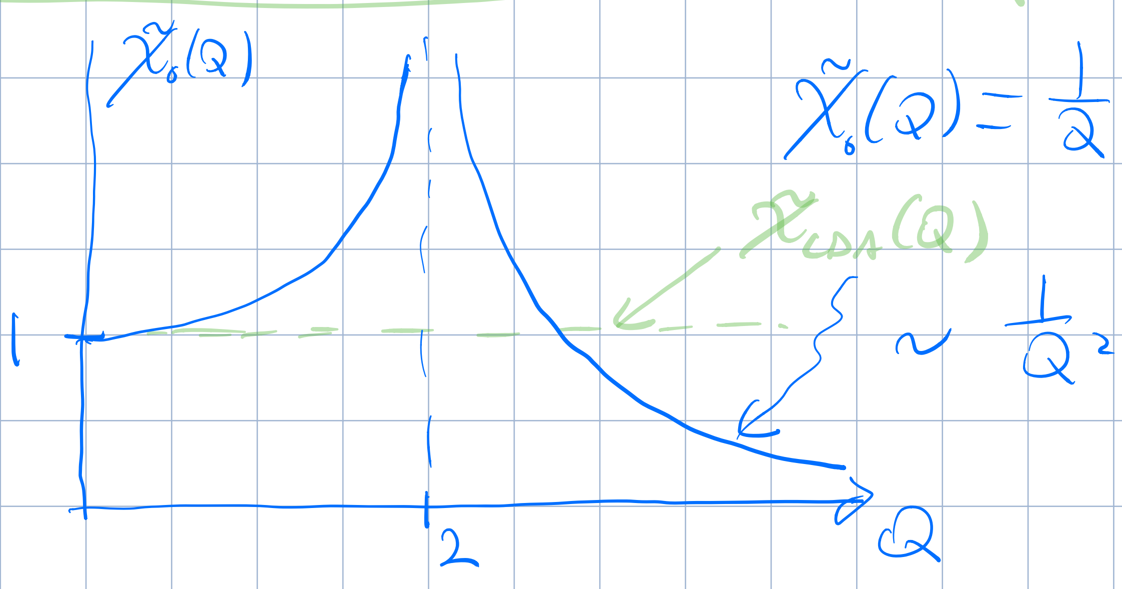
$$\chi_0(q) = -\frac{m}{\pi\hbar^2 q}\left\{\ln\left|\frac{2k_F+q}{-2k_F+q}\right|-\ln\left|\frac{-2k_F+q}{2k_F+q}\right|\right\}$$

$$\chi_0(q) = -\frac{2m}{\pi\hbar^2}\frac{1}{q}\ln\left|\frac{q+2k_F}{q-2k_F}\right|$$

$$\boxed{\chi_0(q) = -\frac{2m}{\pi\hbar^2 k_F}\frac{1}{Q}\ln\left|\frac{Q+2}{Q-2}\right|}$$

②

$$\tilde{\chi}_0(Q) = \frac{1}{Q}\ln\left|\frac{Q+2}{Q-2}\right|$$



③

$$2\frac{2k_F}{\frac{2\pi}{L}} = N \Rightarrow k_F = \frac{\pi}{2}\frac{N}{L} = \frac{\pi}{2} n$$

$$E = 2\sum_{|k|<k_F} \frac{\hbar^2 k^2}{2m} = 2\int_{-k_F}^{k_F} \frac{dk}{\frac{2\pi}{L}} \frac{\hbar^2 k^2}{2m}$$

$$= L\frac{\hbar^2}{\pi\, 2m}\int_{-k_F}^{k_F} dk\; k^2 = \frac{L\hbar^2}{2m\pi}\cdot 2\cdot\frac{k_F^3}{3}$$

$$= L\frac{\hbar^2}{\cancel{2m\pi}}\frac{2k_F^2}{3}\cdot\frac{\pi}{2} n = \frac{1}{3} N \frac{\hbar^2 k_F^2}{2m}$$

$$\frac{E}{N} = t(n) = \frac{1}{3}\frac{\hbar^2}{2m}k_F^2 = \frac{1}{3}\frac{\hbar^2}{2m}\frac{\pi^2 n^2}{4}$$

$$t_n = \frac{\hbar^2\pi^2}{24m} n^2 = C n^2 \qquad C = \frac{\hbar^2\pi^2}{24m}$$

$$T_{LDA}[n] = \int dx\; C\, n(x)^3$$

④ $$E[n] = \int dx\; C\, n(x)^3 + \int dx\; n(x)\, v(x)$$

$$\frac{\delta E}{\delta n} = \mu = 3C\, n(x)^2 + v(x)$$

$$n(x) = \left[\frac{1}{3c}\left(\mu - v(x)\right)\right]^{\frac{1}{2}} \quad \mu - v(x) > 0$$

(5) $$\chi_{LDA}(x-y) = \left.\frac{\delta n(x)}{\delta v(y)}\right|_{v=0}$$

$$n(x) = \int dy\ \delta(x-y)\left[\frac{1}{3c}\left(\mu - v(y)\right)\right]^{\frac{1}{2}}$$

$$= \int dy\ \delta(x-y)\left[\frac{\mu}{3c}\right]^{\frac{1}{2}}\left[1 - \frac{v(y)}{\mu}\right]^{\frac{1}{2}}$$

$$\simeq \int dy\ \delta(x-y)\left\{\left[\frac{\mu}{3c}\right]^{\frac{1}{2}}\left(1 - \frac{v(y)}{2\mu}\right)\right.$$

$$= n + \delta n(x)$$

$$n = \sqrt{\frac{\mu}{3c}} \qquad \delta n(x) = -\int dy\ \delta(x-y)\frac{v(y)}{2\sqrt{3c\mu}}$$

$$\Rightarrow \mu = (3cn)^2, \quad \frac{\delta n(x)}{\delta v(y)} = -\frac{\delta(x-y}{2\sqrt{3c\mu}} = \chi_{LDA}(x-y)$$

$$\chi_{LDA}(q) = -\frac{1}{2\sqrt{3c\mu}} = -\frac{1}{2\sqrt{3c\,3cn^2}}$$

$$= -\frac{1}{6cn} = -\frac{1}{\frac{\hbar^2\pi^2}{4m}n}$$

(6) $$\boxed{\chi_{LDA}(q) = -\frac{1}{\frac{\hbar^2\pi}{2m}\frac{\pi}{2}n} = -\frac{2m}{\hbar^2\pi k_F}}$$

$\chi_{LDA}(q)$ reproduces the exact result for $q \ll k_F$.

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* $$I_\pm = \int_{-k_F}^{k_F} dk \, \frac{1}{\pm k + \frac{q}{2}}$$

- per $|q| < 2k_F$ l'integrale è improprio con una divergenza a $k = \mp q/2$ nell'intervallo di integrazione; però esiste come parte principale

$$I_\pm = \lim_{\epsilon\to 0}\left[\int_{-k_F}^{\mp\frac{q}{2}-\epsilon} \frac{dk}{\pm k + \frac{q}{2}} + \int_{\mp\frac{q}{2}+\epsilon}^{k_F} \frac{dk}{\pm k + \frac{q}{2}}\right]$$

$$= \lim_{\epsilon\to 0}\left[\pm \ln\left|\frac{-\epsilon}{\mp k_F + \frac{q}{2}}\right| \pm \ln\left|\frac{\pm k_F + q/2}{\epsilon}\right|\right]$$

$$= \lim_{\epsilon\to 0}\left[\pm \ln\left|\frac{\pm k_F + q/2}{\mp k_F + \frac{q}{2}}\right|\right] = \pm \ln\left|\frac{\pm 2k_F + q}{\mp 2k_F + q}\right|$$

$$I = I_+ + I_- = \ln\left|\frac{q+2u_F}{q-2u_F}\right| - \ln\left|\frac{q-2u_F}{q+2u_F}\right|$$

$$I = 2\ln\left|\frac{q+2u_F}{q-2u_F}\right|$$