Lista 2 de FI-193

1. Mostre que, para o gás uniforme de elétrons,

$$< \hat{V} >_0 = -\frac{3}{2\pi}\left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{r_s}\ \text{Ryd.}$$

2. *Exchange Direto:* Considere o seguinte termo que foi desprezado no modelo de Hubbard

$$H_{DE} = \sum_{ij;\sigma_1\sigma_2} < ij|\hat{V}|ji > a^\dagger_{i\sigma_1} a^\dagger_{j\sigma_2} a_{i\sigma_2} a_{j\sigma_1},$$

onde

$$< ij|\hat{V}|ji > = \int d^3r_1 d^3r_2 \varphi^*_i(\vec{r}_1)\varphi_j(\vec{r}_1)\frac{e^2}{|\vec{r}_1-\vec{r}_2|}\varphi^*_j(\vec{r}_2)\varphi_i(\vec{r}_2) \equiv J^{DE}_{ij} > 0$$

é a integral coulombiana de "exchange" entre os orbitais $\varphi_i(\vec{r})$ e $\varphi_j(\vec{r})$, que é sempre positiva. Restringindo-se ao sub-espaço de ocupação simples ($\sum_\sigma a^\dagger_{i\sigma}a_{i\sigma} = 1$), prove que esse termo dá origem a um Hamiltoniano de Heisenberg ferromagnético (FM).

3. Problemas 1.3, 1.4, 1.6 do Fetter & Walecka. Os problemas são reproduzidos abaixo para sua conveniência. O problema 1.2 é reproduzido lá porque o 1.3 pede algo do seu enunciado.

1.2. Given a homogeneous system of spin-$\frac{1}{2}$ particles interacting through a potential V
(*a*) show that the expectation value of the hamiltonian in the noninteracting ground state is

$$E^{(0)} + E^{(1)} = 2\sum_{\mathbf{k}}^{k_F}\frac{\hbar^2\mathbf{k}^2}{2m} + \tfrac{1}{2}\sum_{\mathbf{k}\lambda}^{k_F}\sum_{\mathbf{k}'\lambda'}^{k_F}\{\langle\mathbf{k}\lambda\mathbf{k}'\lambda'|V|\mathbf{k}\lambda\mathbf{k}'\lambda'\rangle - \langle\mathbf{k}\lambda\mathbf{k}'\lambda'|V|\mathbf{k}'\lambda'\mathbf{k}\lambda\rangle\}$$

where λ is the z component of the spin.
(*b*) Assume V is central and spin independent. If $V(|\mathbf{x}_1-\mathbf{x}_2|)<0$ for all $|\mathbf{x}_1-\mathbf{x}_2|$ and $\int|V(x)|d^3x<\infty$, prove that the system will collapse (*Hint*: start from $(E^{(0)}+E^{(1)})/N$ as a function of density).

1.3. Given a homogeneous system of spin-zero particles interacting through a potential V
(*a*) show that the expectation value of the hamiltonian in the noninteracting ground state is $E^{(1)}/N = (N-1)V(0)/2V \approx \frac{1}{2}nV(0)$, where

$$V(\mathbf{q}) = \int d^3x\, V(\mathbf{x})\, e^{-i\mathbf{q}\cdot\mathbf{x}} \quad \text{and} \quad V(0) \text{ means } V(\mathbf{q}=0)$$

(*b*) Repeat Prob. 1.2*b*.
(*c*)‡ Show that the second-order contribution to the ground-state energy is

$$\frac{E^{(2)}}{N} = -\frac{N-1}{2V}\int\frac{d^3q}{(2\pi)^3}\frac{|V(\mathbf{q})|^2}{\hbar^2\mathbf{q}^2/m} \approx -\frac{n}{2}\int\frac{d^3q}{(2\pi)^3}\frac{|V(\mathbf{q})|^2}{\hbar^2\mathbf{q}^2/m}$$

‡ Use standard second-order perturbation theory: If $H = H_0 + H_1$ and the unperturbed eigenvectors $|j\rangle$ satisfy $H_0|j\rangle = E_j|j\rangle$, then

$$E^{(2)} = \sum_{j\neq 0}\frac{|\langle 0|H_1|j\rangle|^2}{E_0-E_j} = \langle 0|H_1\frac{P}{E_0-H_0}H_1|0\rangle$$

where $|0\rangle$ is the ground-state eigenvector of H_0 with energy E_0, and $P = 1-|0\rangle\langle 0|$ is a projection operator on the excited states.

1.4.‡ Show that the second-order contribution to the ground-state energy of an electron gas is given by $E^{(2)} = (Ne^2/2a_0)(\epsilon^r_2 + \epsilon^b_2)$, where

$$\epsilon^r_2 = -\frac{3}{8\pi^5}\int\frac{d^3q}{q^4}\int_{|\mathbf{k}+\mathbf{q}|>1}d^3k\int_{|\mathbf{p}+\mathbf{q}|>1}d^3p\,\frac{\theta(1-k)\,\theta(1-p)}{\mathbf{q}^2+\mathbf{q}\cdot(\mathbf{k}+\mathbf{p})}$$

$$\epsilon^b_2 = \frac{3}{16\pi^5}\int\frac{d^3q}{q^2}\int_{|\mathbf{k}+\mathbf{q}|>1}d^3k\int_{|\mathbf{p}+\mathbf{q}|>1}d^3p\,\frac{\theta(1-k)\,\theta(1-p)}{(\mathbf{q}+\mathbf{k}+\mathbf{p})^2\,[\mathbf{q}^2+\mathbf{q}\cdot(\mathbf{k}+\mathbf{p})]}$$

1.6. Consider a polarized electron gas in which $N_{\pm}$ denotes the number of electrons with spin-up (-down).[1]

(*a*) Find the ground-state energy to first order in the interaction potential as a function of $N = N_+ + N_-$ and the polarization $\zeta = (N_+ - N_-)/N$.

(*b*) Prove that the ferromagnetic state ($\zeta = 1$) represents a lower energy than the unmagnetized state ($\zeta = 0$) if $r_s > (2\pi/5)(9\pi/4)^{\frac{1}{3}}(2^{\frac{1}{3}} + 1) = 5.45$. Explain why this is so.

(*c*) Show that $\partial^2(E/N)/\partial\zeta^2|_{\zeta=0}$ becomes negative for $r_s > (3\pi^2/2)^{\frac{2}{3}} = 6.03$.

(*d*) Discuss the physical significance of the two critical densities. What happens for $5.45 < r_s < 6.03$?