EXCERCIZES IV PHYS 825

Consider the anti symetrized pair wave function

$$\Psi(1,2) = \frac{1}{\sqrt{2}}\left[\psi_a(1)\,\psi_b(2) - \psi_b(1)\,\psi_b(2)\right]$$

where $\psi_a(1) = \phi_a(r_1)\,\chi_{s_a}(1)$ is a product of a space and spin function.

(1) Show

$$\langle \Psi(1,2) \,|\, \Psi(1,2) \rangle = \langle \psi_a(1)\psi_b(2) \,|\, [\psi_a(1)\psi_b(2) - \psi_b(1)\psi_a(2)] \rangle$$

(2) Show

$$\langle \Psi(1,2) \,|\, \sum_{i=1}^{2} h(r_i) \,|\, \Psi(1,2) \rangle = \sum_{a,s_a} \langle \psi_a(1) \,|\, h(r_1) \,|\, \psi_a(1) \rangle$$

(3) Show

$$\langle \Psi(1,2) \,|\, v(r_{12}) \,|\, \Psi(1,2) \rangle$$

$$= \langle \phi_a(1)\,\phi_b(2)\, v(r_{12})\, \phi_a(1)\,\phi_b(2) \rangle - \delta_{s_a s_b} \langle \phi_a(1)\,\phi_b(2)\, v(r_{12})\, \phi_b(1)\,\phi_a(2) \rangle$$

(4) For a uniform electron gas, the exchange energy

$$E_{ex} = -\frac{1}{2}\sum_{i,j}{}' \langle \psi_i(1)\,\psi_j(2)\,\frac{e^2}{r - r'}\,\psi_j(1)\,\psi_i(2) \rangle$$

where $\psi_i(1) = \frac{1}{\sqrt{V}} e^{i k_i \cdot r_1}\, \chi_i(1)$

The exchange energy reduces to

$$E_{ex} = -\sum_k \frac{1}{V} \sum_q \frac{4\pi e^2}{(k-q)^2} \equiv -I(k)$$

See p. 334 A & M
p. 136 M

Show that

$$I(k) = \frac{1}{V}\sum_q \frac{4\pi e^2}{(k-q)^2} = \frac{2e^2}{k_F}\, F\!\left(\frac{k}{k_F}\right)$$

where

$$F(x) = \frac{1}{2} + \frac{(1-x^2)}{4x}\ln\frac{1+x}{1-x}$$

and

$$\int_0^1 dx\, x^2\, F(x) = \frac{1}{4}$$