Roma la Sapienza
Solid State Physics

Laurea Magistrale

Esercitazione °2

Exercise I : Density matrix and pair correlation function in Jellium

Let's consider a 3D jellium model with electronic density ρ_I. We define the adimensional parameter

$$r_s = \frac{1}{a_0}\left(\frac{3}{4\pi}\frac{1}{\rho_I}\right)^{\frac{1}{3}},$$

where $a_0 = \hbar^2/(m_e^2)$ is the Bohr radius. We consider this system within the HF theory in the colinear case. In the following, we consider the *unpolarized case* in which the number of up electrons is equal to the number of down electrons, and the *ferromagnetic case* in which all the electrons are in the spin up state. Given a generic N-electron wavefunction $|A\rangle$ we define the spin-resolved one body density matrix as

$$\rho(\mathbf{r}s, \mathbf{r}'s') = \langle A|\sum_{i=1}^{N}|\mathbf{r}'s'\rangle_{ii}\langle \mathbf{r}s|A\rangle.$$

We recall that, within the HF approximation, such matrix can be written as: $\rho(\mathbf{r}s, \mathbf{r}'s') = \langle \mathbf{r}s|P|\mathbf{r}'s'\rangle$, where P is the projector in the HF occupied subspace. For the generic wavefunction $|A\rangle$, we define the spin-resolved two body probability density as

$$\rho^{(2)}(\mathbf{r}s, \mathbf{r}'s') = \langle A|\sum_{i,j=1;i\neq j}^{N}|\mathbf{r}s\rangle_{ii}\langle \mathbf{r}s||\mathbf{r}'s'\rangle_{jj}\langle \mathbf{r}'s'|A\rangle.$$

We define the spin-resolved pair correlation as

$$g(\mathbf{r}s, \mathbf{r}'s') = \frac{\rho^{(2)}(\mathbf{r}s, \mathbf{r}'s')}{\rho(\mathbf{r}s, \mathbf{r}s)\rho(\mathbf{r}'s', \mathbf{r}'s')}.$$

We recall that the 2-electron energy can be computed from the knowledge of $\rho^{(2)}(\mathbf{r}, \mathbf{r}') = \sum_{s,s'}\rho^{(2)}(\mathbf{r}s, \mathbf{r}'s')$ as:

$$\int d^3r d^3r' \rho^{(2)}(\mathbf{r}, \mathbf{r}')\frac{e^2}{2|\mathbf{r}-\mathbf{r}'|}$$

1. Compute the Fermi momentum k_F, in both the unpolarized and ferromagnetic case within HF as a function of r_s and a_0.

2. Compute $\rho(\mathbf{r}\uparrow, \mathbf{r}'\uparrow)$ and $\rho(\mathbf{r}\uparrow, \mathbf{r}'\downarrow)$ in both the unpolarized and ferromagnetic case with the HF approximation as a function of r_s and a_0. Plot the resulting expression as a function of $k_F|\mathbf{r}-\mathbf{r}'|$.

3. Compute $g(\mathbf{r}\uparrow, \mathbf{r}'\uparrow)$ and $g(\mathbf{r}\uparrow, \mathbf{r}'\downarrow)$ in both the unpolarized and ferromagnetic case with the HF approximation. Plot the resulting expression as a function of $|\mathbf{r}-\mathbf{r}'|/(r_s a_0)$.

Ortiz, Ballone PRB 50, 1391 (1994)

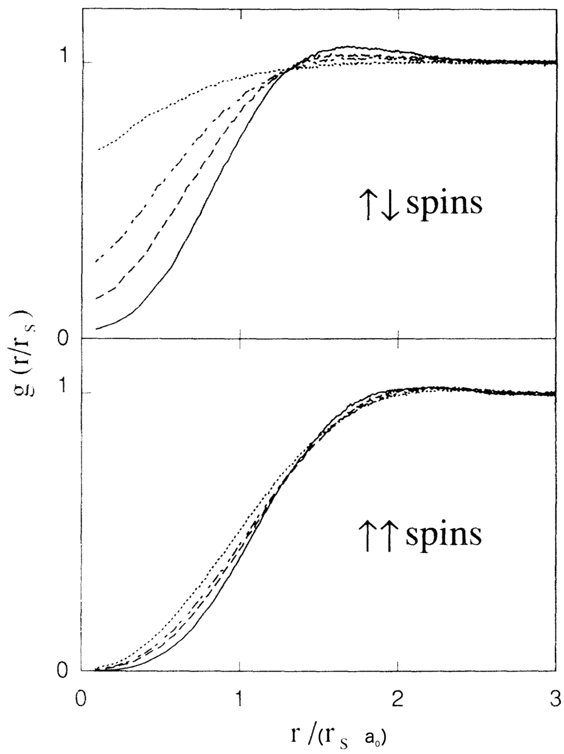

FIG. 6. Radial distribution functions $g_{\mu,\nu}(r)$ ($\zeta = 0$) computed by the DMC method (mixed estimator): $r_s = 1$ (dotted line), $r_s = 3$ (dash-dotted line), $r_s = 5$ (dashed line), and $r_s = 10$ (full line).

4. Compare and discuss the results of the HF approximation with the numerically exact (for the unpolarized case) one obtained by the Monte-Carlo calculation of Ortiz and Ballone for $r_s = 1, 3, 5, 10$, that is reported in the figure.