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ELECTRONIC DENSITY OF STATES IN THE DEFORMABLE JELLIUM MODEL

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ABSTRACT

We evaluate the one electron energy spectrum E(k) and the electronic density of states N(k) for different values of the interparticle distance r_s, for the electron gas in the jellium. We are particularly interested in the region near the Fermi level, because it determines the behavior of transport properties (such as thermal an electrical conductivities). The state functions used in these calculations are expansions of periodic functions with self-consistenly determined coefficients. Our calculations are compared with the usual plane wave results.

RESUMEN

Se calculan para el gas de electrones en el modelo de jalea, el espectro de energías de un electón E(k) y la densidad electrónica de estados N(k), para distintos valores de la distancia entre partículas caracterizada por el parámetro r_s. A fin de determinar el comportamiento de las propiedades de transporte (conductividades térmica y eléctrica, por ejemplo), se estudia especialmente la región cercana al nivel de Fermi. Como función de estado se propone un desarrollo en funciones periódicas cuyos coeficientes han sido determinados autoconsistentemente. Los resultados obtenidos se comparan con los conocidos de onda plana.

INTRODUCTION

The electron gas in the deformable jellium model is a useful model to obtain electronic properties for metallic systems$^{(1)}$, particularly for the alkalines in which a crystalline structure is not always the best model$^{(2)}$. For the electron gas in the jellium, one assumes that the conduction electrons have experienced a charge density wave (CDW) instability$^{(3)}$.

Calculations of one electron density of states N(k) are very interesting in order to predict many physical properties. Of paramount interest in N(k) near and at the Fermi level, because it is directly connected with transport properties such as thermal and electrical conductivities, and with the characteristic optical absortion of the system$^{(4)}$.

In this work, we evaluate the one electron density of states N(k). For that purpose and in order to have a better description of the system we also calculate the energy spectrum E(k). Taking into account previous results to obtain the state function for a fermion gas in the jellium model$^{(5)}$, we use as state functions for the calculations CDW type functions that are expansions in terms of periodic functions (PF), whose coefficients are self-consistenly determined. We have shown that these state functions give a better ground state energy as compared with other variational calculations$^{(6)}$. These functions also produce a natural change in the electronic and background density (deformable jellium) as a function of the interparticle distance r_s, given periodic density distribution. In the low density limit, this behaviour resembles the Wigner crystallization$^{(6)}$. The results obtained for N(k) and E(k) with these suitable functions are compared with those obtained using plane waves (PW) as state function.

THEORY

The self-consistent wave function for the calculations in the independent particle model is given by the Slater's determinant of the orthonormalized spin-orbitals:

$$\psi = \frac{1}{\sqrt{N!}} \det [\varphi_{\underline{n}_i,\ \lambda_i}(\underline{r}_i)] \quad , \tag{1}$$

where $\varphi_{\underline{n}_i,\lambda_i}(\underline{r}_i) = \varphi_{\underline{n}_i}(\underline{r}_i)\ \chi_{\lambda_i}$ and χ_{λ_i} are the spin functions

The general expression for the orbitals we propose is

$$\psi_{\underline{n},\lambda}(r) \equiv |\underline{n},\underline{k},\lambda\rangle = \chi_\lambda f_{\underline{k}}(\underline{r}) \sum_{n_x=N_1}^{N_2} \sum_{n_y=N_1}^{N_2} \sum_{n_2=N_1}^{N_2} C_{n_x n_y n_z} |\underline{n}\rangle \quad , \tag{2}$$

in this equation $|\underline{n}\rangle$ is a basis with an expansion in terms of a discrete index. The function $f_{\underline{k}}(\underline{r})$ is a plane wave because we know that PW are adequate solutions for small r_s, and in this case, the basis is selected as

$$|\underline{n}\rangle \equiv |n_x,\ n_y,\ n_z\rangle = \exp(-i\ q_o\ \underline{n}\cdot\underline{r}) \quad , \tag{3}$$

where $\underline{n} = \hat{\imath}\ n_x + \hat{\jmath}\ n_y + \hat{k} n_z$.

This state function guarantees the periodic character in three independent directions. As a particular case we can describe some interesting systems which present periodic behaviour in only one or two directions$^{(7)}$.

The Hamiltonian for an electron gas in a positive background of density $\eta\ (\underline{R})$ is

$$\hat{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i,j}^{N} V(\underline{r}_i - \underline{r}_j) \tag{4}$$

$$+ \frac{1}{2} \int \int \eta(\underline{R})\ \ \eta(\underline{R}')\ V(\underline{R}-\underline{R}')\ d^3R\ d^3R'$$

$$- \sum_{i=1}^{N} \int \eta(\underline{R})\ V(\underline{r}_i - \underline{R})\ d^3R \quad ,$$

The first two terms belong to the electronic Hamiltonian and and the third and fourth are the background-background and the electron-background interactions. Capital arguments are used for the background variables.

In order to get the coefficients C_n in Eq.(2) we have to solve self-consistenly the following equations$^{(8)}$:

$$\sum_{n_{3x},n_{3y},n_{3z}} \left\{ <\underline{n}_1\underline{k}_1|T|\underline{n}_3\underline{k}_1> - \sum_{\substack{n_{2x},n_{2y},n_{2z}\\ n_{4x},n_{4y},n_{4z}}} <\underline{n}_1\underline{k}_1,\underline{n}_2\underline{k}_2|V|\underline{n}_4\underline{k}_2,\underline{n}_3\underline{k}_1> \cdot \; C^*_{n_{2x}n_{2y}n_{2z}} C^*_{n_{4x}n_{4y}n_{4z}} \right\} C_{n_{3x}n_{3y}n_{3x}} = \varepsilon_{n_{1x}n_{1y}n_{1z}} \; C_{n_{1x}n_{1y}n_{1z}} \quad . \qquad (5)$$

Once we have determined the coefficients, *i.e.*, the state function, we can use this function to evaluate properties of the electron gas.

It is interesting to observe that the self-consistent solution is a plane wave for r_s up to 32, when $-N_1 = N_2$, and for r_s up to 65 when $N_1 = 0$ and $N_2 > 0$. The solutions deviate from PW starting with these values for r_s. The periodic character gives a localization of the electrons, and this becomes more pronounced as r_s increases. The transition point in the case of symmetric functions is at $r_s = 32$ and it is the same for periodicity in one, two or three directions. The equivalent transition for non-symmetrical functions is at $r_s = 65$ and this is also the same for periodicity in one, two or three directions. This result indicates that for the Coulombic interaction the transition depends strongly on general characteristics of the basis.

With these state functions, we evaluate first the one electron energy spectrum E(k). This is given by

$$E(\underline{k}) = \frac{\hbar^2 k_f^2}{2m} \sum_{n_{1x}n_{1y}n_{1z}} |C_{n_{1x}n_{1y}n_{1z}}|^2 \left(\frac{\underline{k}}{k_f} - 2\underline{n}_1\right)^2$$

$$- \frac{e^2 k_f}{2\pi} \sum_{\underline{n}_1\underline{n}_2} \sum_{\underline{n}_3\underline{n}_4} C^*_{n_{1x}n_{1y}n_{1z}} C^*_{n_{2x}n_{2y}n_{2z}} C_{n_{3x}n_{3y}n_{3z}} \qquad (6)$$

$$C_{n_{4x}n_{4y}n_{4z}} \; \delta_{\underline{n}_1+\underline{n}_2,\underline{n}_3+\underline{n}_4} \left\{ \frac{k_f^2 - Q^2}{k_f Q} \ln\left|\frac{k_f + Q}{Q - k_f}\right| + 2 \right\} ,$$

where $Q = |\underline{k} + 2N\underline{k}_f|$ and $N = |\underline{n}_1 - \underline{n}_4|$.

As it is known$^{(1)}$ the electronic density of states is given by a term which depends in the inverse derivative of $E(k)$, *i.e.*, $[\frac{dE(k)}{dk}]^{-1}$. In order to have explicit calculations for the behaviour of $N(k)$ in terms of the wave number and of the density parameter r_s, and because of its simplicity we will take the particular case in which the electron gas has periodicity in only one direction and homogeneity in the other two. Without any further loss of generality we can take $n_x = n_y = 0$ and $0 \leqslant n_z \leqslant n$. This conditions in Eq.(2) lead to Wigner crystallization in only one axis. Then

$$\frac{dE(k)}{dk} = \frac{\hbar^2 k_f}{m} \sum_{n_1=0}^{n} |Cn_1|^2 \left(\frac{k}{k_f} - 2n, \cos\theta\right)$$

$$- \frac{e^2 k_f}{2\pi} \sum_{n_1=0}^{n} \sum_{n_2=0}^{n} \sum_{n_3=0}^{n} \sum_{n_4=0}^{n} \delta_{n_1+n_2, n_3+n_4} C^*_{n_1} C^*_{n_2} C_{n_3} C_{n_4}$$

$$\left\{ - \frac{(k+2Nk_f \cos\theta)(k_f^2+k^2+4N^2k_f^2+4Nk_f\, k\cos\theta)}{k_f\,[k^2+4N^2k_f^2 + 4Nk_f\, k\cos\theta]^{3/2}} \right.$$

$$\left. \ln \left| \frac{\sqrt{k^2+4N^2k_f^2+4Nk_f k\cos\theta} + k_f}{\sqrt{k^2+4N^2k_f^2+4Nk_f\, k\cos\theta} - k_f} \right| + \frac{2(k+2Nk_f\cos\theta)}{k^2+4N^2k_f^2+4Nk+k\cos\theta} \right\} . \qquad (7)$$

Taking into account that we have gotten very good convergence in previous calculations for the ground state energy$^{(6)}$ when the upped limit is n=3, we have taken this value in Eqs.(6) and (7). The difference between the energy results for n=3 and n=4 or greated is less than 1%.

RESULTS AND DISCUSSION

The results obtained with periodic functions are compared with the corresponding for the plane wave. We show in the figures the one electron energy spectrum E(k) and the electronic density N(k). In Fig.1 we see the one electron energy spectrum in terms of the wave number k. The full lines belong to calculations with periodic functions and the dashed line is obtained using the plane wave solution. As it can be seen E(k) is lower for the periodic function that for plane wave at r_s = 100. The slope becomes infinite with respect to the wave vector at the Fermi level for the three cases shown in the figure.

In Figs. 2 to 4, we show the electronic density. The convention will be as in Fig. 1, full lines for results with periodic functions and dashed lines for results using plane wave state function. In Fig. 2, we show the electronic density of one electron states near and at the Fermi level, for different values of the parameter r_s. The self-consistent periodic solutions begin with r_s = 65, so we have drawn results at this value of the parameter and for r_s = 100. As it can be seen, the electronic density goes to zero at the Fermi level. Figure 3 is an enlarged view of the region near the Fermi level in Fig. 2. Here we can see that the electronic densities with plane waves go to zero faster than those obtained with periodic functions. In Fig. 4, we have results for periodic and plane waves at r_s = 100, in order to compare results for the same value of the parameter. As can be seen in the Figs. (2-4) the electronic density N(k) goes to zero at the Fermi level. This is a consequence of the fact that the Coulomb interaction is singular for zero momentum transfer. It is interesting to notice that the electronic density with periodic functions is considerably greater than the PW electronic density in the neighborhood of the Fermi level as can be seen in Figs. 3 and 4. We conclude that this fact affects some properties of the system which are strongly dependent in the values of the densities near the Fermi level, such as transport properties and optical absorption$^{(9)}$.

APPENDIX

We outline here the main results of Ref. 8 on the derivation of Eq. (5). Starting with Eq.(4), the ground state energy for the electron

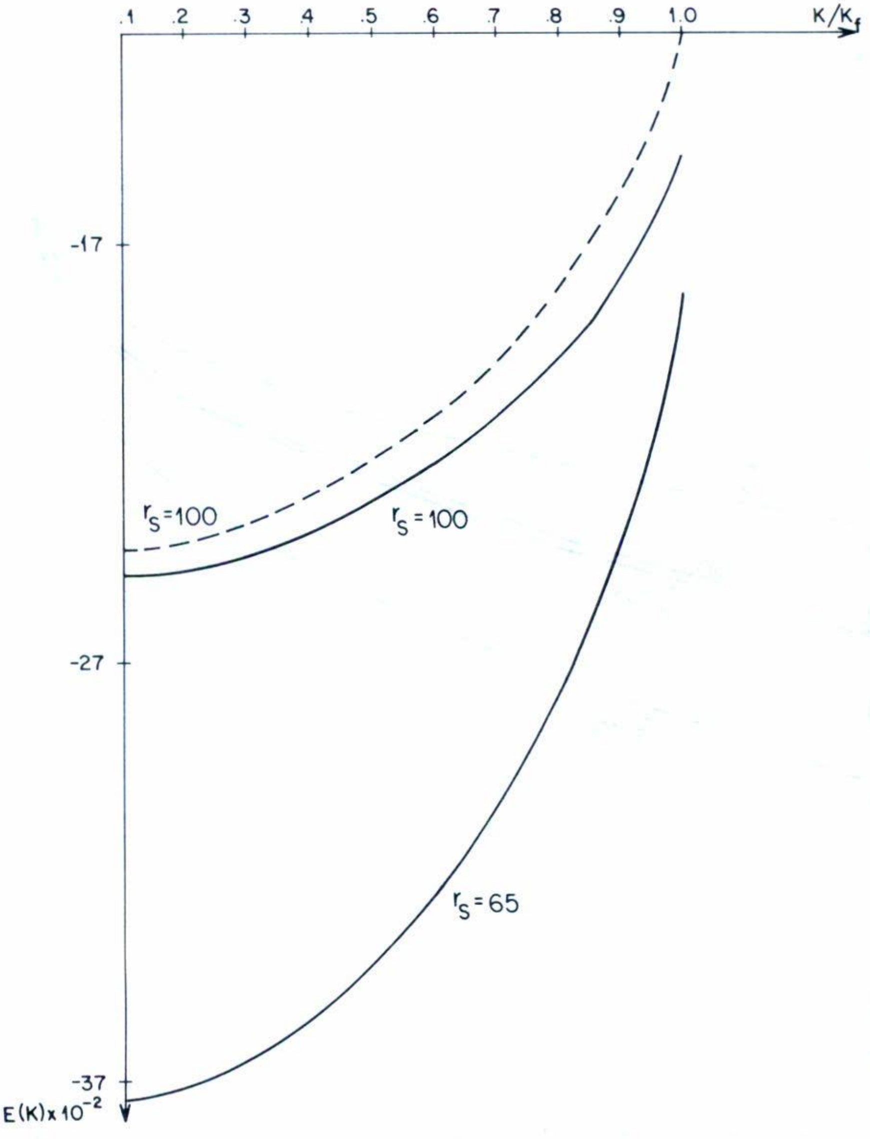

Fig. 1. One electron energy spectrum in terms of the wave number, k. Full curves are for calculations with periodic functions, dashed curves are for PW results.

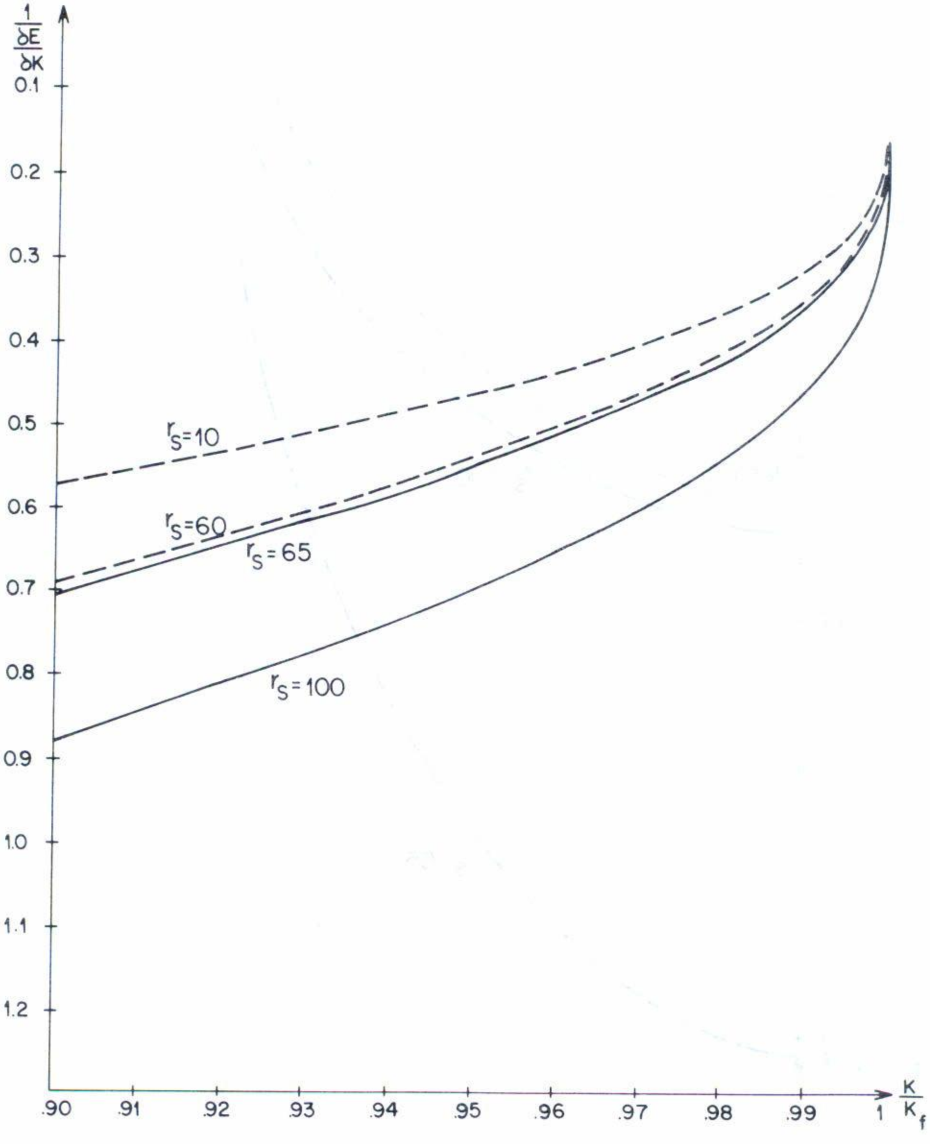

Fig. 2. Electronic density in terms of the wave number, k. Full curves are for PF calculations and dashed curves for PW results.

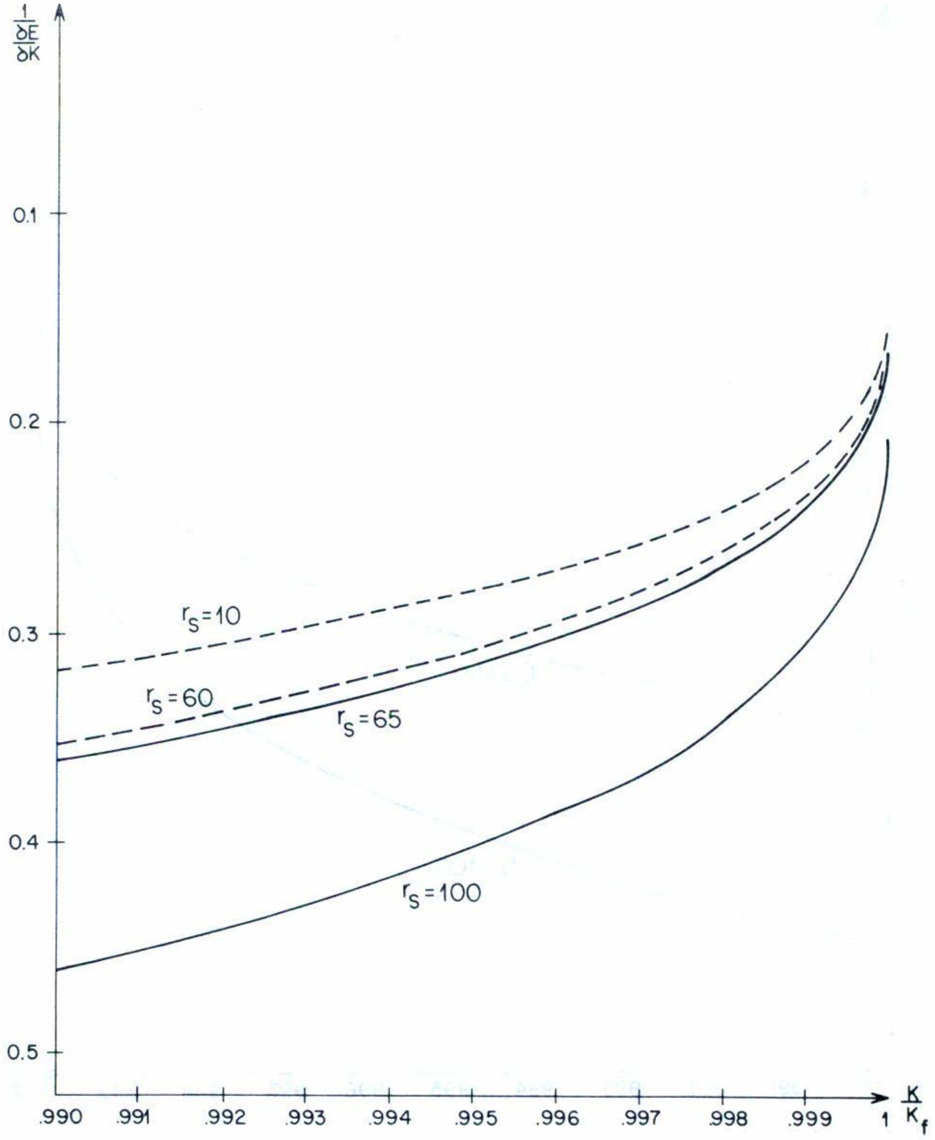

Fig. 3. Electronic density of states in the Fermi level neighboring region. The convention is the same as is Fig. 2.

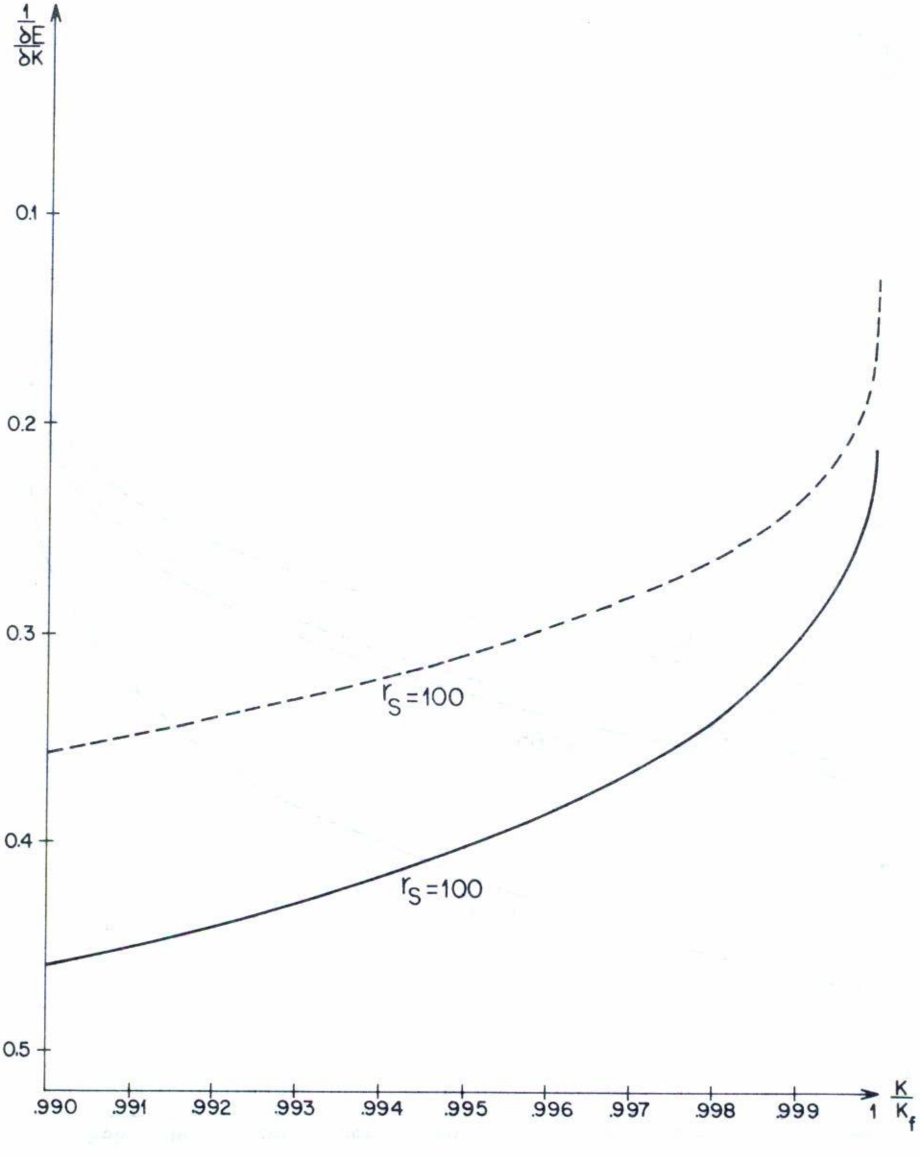

Fig. 4. Electronic density in terms of k for $r_s = 100$. The convention for the curves is the same as in Fig. 2.

gas in the jellium model can be written as

$$E = \langle\psi|\hat{H}|\psi\rangle = \sum_{i=1}^{N} \langle\psi| \frac{p_i^2}{2m} |\psi\rangle + \frac{1}{2} \sum_{\substack{i,j \\ i\neq j}} \langle\psi|V(\underline{r}_i - \underline{r}_j)|\psi\rangle$$

$$- \sum_{i=1}^{N} \int \langle\psi|\eta(\underline{R})\ V(\underline{r}_i - \underline{R})|\psi\rangle d^3R$$

$$+ \frac{1}{2} \int\int \eta(\underline{R})\eta(\underline{R}')\ V(\underline{R} - \underline{R}')\ d^3R\ d^3R' \qquad \text{(A.1)}$$

The application of the Hellman-Feynman theorem to Eq. (A.1), using the background density $\eta(\underline{R})$ as a variational parameter, *i.e.*, $\frac{\partial E}{\partial \eta(\underline{X})} = 0$, gives$^{(5)}$

$$\int \eta(\underline{R}')\ V(\underline{X}, \underline{R}')\ d^3R' = \sum_{i=1}^{N} \langle\psi|(\underline{r}_i, \underline{X})|\psi\rangle \quad . \qquad \text{(A.2)}$$

Equation (A.2) is the condition statisfied by the background density in order to get optimum energy, at first order in $\eta(\underline{R})$.

Now, is the independent particle model, the wave function is given by the Slater determinant of the spin-orbitals of Eq. (1). Using this state function, the ground state energy becomes

$$E = \sum_{i=1}^{N} \langle\underline{n}_i|T|\underline{n}_i\rangle - \frac{1}{2} \sum_{\substack{i,j \\ i\neq j}}^{N} \langle\underline{n}_i, \underline{n}_j|V(\underline{r}, \underline{r}')|\underline{n}_j, \underline{n}_i\rangle \quad , \qquad \text{(A.3)}$$

where $\varphi_{\underline{n}_i} \equiv |\underline{n}_i\rangle$ are the spin-orbitals. This means that the ground state energy is only given by the kinetic energy and the exchange terms.

On the other hand, in the independent particle model, Eq. (A.2)

$$n(\underline{R}) = \sum_{i=1}^{N} \varphi^*_{\underline{n}_i}(\underline{R})\ \varphi_{\underline{n}_i}(\underline{R}) \quad , \qquad \text{(A.4)}$$

that means that the background is deformed according to the electron's density. Then, we have local neutrallity as it can be expected. Now in Eq. (A.3), we use the orbitals of the type given by Eqs. (2) and (3) obtaining for the energy

$$E= \sum_{\underline{k},\lambda_1\lambda_2} \sum_{\substack{n_{1x},n_{1y},n_{1z}\\ n_{3x},n_{3y},n_{3z}}} C^*_{n_{1x}n_{1y}n_{1z}} <\underline{n}_1\underline{k}\lambda_1 |T| \underline{n}_3\underline{k}\lambda_2> C_{n_{3x}n_{3y}n_{3z}}$$

$$-\frac{1}{2} \sum_{\underline{k}_1\underline{k}_2} \sum_{\lambda_1\lambda_2} \sum_{\substack{n_{1x},n_{1y},n_{1z}\\ n_{3x},n_{3y},n_{3z}}} \sum_{\substack{n_{2x},n_{2y},n_{2z}\\ n_{4x},n_{4y},n_{4z}}} C^*_{n_{1x},n_{1y},n_{1z}} C^*_{n_{2x},n_{2y},n_{2z}} \cdot$$

$$<\underline{n}_1\underline{k}_1\lambda_1,\underline{n}_2\underline{k}_2\lambda_2|V|\underline{n}_4\underline{k}_2\lambda_2,\underline{n}_3\underline{k}_1\lambda_1> C_{n_{4x},n_{4y},n_{4z}} \quad C_{n_{3x},n_{3y},n_{3z}} . \qquad (A.5)$$

Taking the variation with respect to the coefficients C_n and using the orthonormality condition we get the HF equations given by Eq. (5).

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