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Ground state energy of the electron gas in jellium

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Abstract. A self-consistent Hartree-Fock analysis for the ground state energy per particle for the electron gas in jellium is carried out. The low, intermediate, and high density regions are considered. The paramagnetic and ferromagnetic states are studied to determine the nature of the ground state. Wigner crystallization at zero temperature in the low density region is observed in all the cases studied. Our results are compared to recent calculations.

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1. Introduction

The electron gas in jellium is a useful model for many body systems. It is a simplified and interesting model for metals [1,2] and even for stellar matter [2,3]. Since many years ago, much effort has been devoted toward theoretical understanding of the phase properties of the electron gas in its ground state [4,5]. As it is well known, calculations with this model have established that at high densities, where the electron-electron interactions can be considered like small perturbations, the system approaches a perfect gas [6]. At low densities, the electron-electron interactions are more relevant and the electrons crystallize in a body-centered-cubic structure [7].

Only for these extreme densities the properties of the ground state have rigorously been established. It would be interesting to have a method that includes the intermediate density region. Among other propositions at intermediate densities, in order to seek whether there are precursors to the crystallized phase. Overhauser considered the so called charge density waves [8,9] (CDW), which are periodic solutions and the electron density is non-uniform, but varies periodically. In this model the background is not rigid, but completely deformable (deformable jellium model), and this fact guarantees local neutrality and lowers the energy. It had also been suggested that at intermediate densities the ferromagnetic state (all spins up) is more stable than the normal paramagnetic (as many up as down spins) [10]. In fact, exchange interactions among itinerant electrons always favor the parallel alignment of spins. However correlation corrections to the independent particle model cancel substantially the effects of exchange [8]. Certainly there are marked differences between the magnetic character of the ground state of the metals and some results obtained in the independent particle model at high densities [11]. Then in order to determine the regions of stability of the different phases, it is necessary to do a calculation for all densities.

In this work a self-cosistent Hartree-Fock (HF) calculation of the ground state energy per particle for the electron gas in the deformable jellium, is presented as a function of the interparticle distance, r_s. The high, intermediate and small density regions are considered. We are looking for the possibility of paramagnetic or ferromagnetic states, as well as the possibility of periodic density. As ground state function it is used an Slater's determinant of the orthonormalized spin-orbitals. For the orbitals it is proposed an expansion in terms of periodic functions, and the coefficients of this are self-consistently determined.

In the paramagnetic fluid, as well as in the ferromagnetic, it is observed a transition from uniform to non-homogeneous, periodic particle density in the low density regimen. The energies for the ground state are compared to recent results that employ the Green function Monte-Carlo method [12], and to results obtained with the integral approximant method [13].

2. The model

The Hamiltonian for the electron gas in the jellium is well know [2,14]. When the deformable jellium model is used in the independent particle approximation, the cancelation of the background and direct electron energy terms has been imposed in similitude to the HF results using plane wave (PW) solutions in the jellium model. However it was shown [14], that this cancelation of energy terms can be obtained from a variational principle giving, in this way, formal justification to the deformable jellium model. Then in order to evaluate the ground state energy, it is necessary to handle only with the kinetic and exchange energy terms, *i.e.*

$$E_{\mathrm{HF}} = \sum_{i=1}^{N} \langle \phi_i \left| \frac{p^2}{2m} \right| \phi_i \rangle - \frac{1}{2} \sum_{i \neq j=1}^{N} \langle \phi_i \phi_j | V(\mathbf{r} - \mathbf{r}') | \phi_j \phi_i \rangle, \tag{1}$$

where ϕ_i is the notation for the spin-orbitals. The orbitals used in this work are expanded in terms of periodic functions. So, we used the next spin-orbitals

$$\phi^1_{\mathbf{k},\lambda}(\mathbf{r}) = \chi_\lambda e^{i\mathbf{K}\cdot\mathbf{r}} \sum_{n=-N}^{N} C_n e^{in\mathbf{q}_0\cdot\mathbf{r}}, \tag{2a}$$

$$\phi^2_{\mathbf{k},\lambda}(\mathbf{r}) = \chi_\lambda e^{i\mathbf{K}\cdot\mathbf{r}} \sum_{n_i=-N}^{N} \sum_{n_j=-N}^{N} C_{n_i n_j} e^{iq_0(n_i x_i + n_j x_j)}, \tag{2b}$$

and

$$\phi^3_{\mathbf{k},\lambda}(\mathbf{r}) = \chi_\lambda e^{i\mathbf{K}\cdot\mathbf{r}} \sum_{\mathbf{n}=-\mathbf{N}}^{\mathbf{N}} C_{\mathbf{n}} e^{iq_0(\mathbf{n}\cdot\mathbf{r})}, \tag{2c}$$

with $\mathbf{r} = \hat{e}_1 x_1 + \hat{e}_2 x_2 + \hat{e}_3 x_3 = \sum_{i=1}^{3} \hat{e}_i x_i$ and $\mathbf{n} = \sum_{i=1}^{3} \hat{e}_i n_i$. With these spin-orbitals it is possible to describe systems with different symmetries. So, with equa-

tion (2*a*) the system may present periodic density along one axis (the direction of $\mathbf{q}_0$).

Equation (2*b*) describes a system which may have periodicity along two orthogonal directions. Finally, equation (2*c*) describes a system which can have periodic non-homogeneous density along three orthogonal directions. In Eq. (2*c*), $\sum_{\mathbf{n}}^{N}$ is a simplified notation ($\sum_{n_1=-N}^{N}\sum_{n_2=-N}^{N}\sum_{n_3=-N}^{N}$), where all the sums run from $-N$ up to N. Also $C_{\mathbf{n}}$ is a compact notation for C_{n_1,n_2,n_3}. The electron density obtained with these functions is given by

$$\rho = \rho_0 \sum_{\mathbf{n}_1}\sum_{\mathbf{n}_2} C^*_{\mathbf{n}_1} C_{\mathbf{n}_2} \cos[(\mathbf{n}_1 - \mathbf{n}_2) q_0 \cdot \mathbf{r}], \tag{3}$$

where ρ_0 is the PW density.

With any of the three functions proposed by equations (2), the total momentum of the system is equal to zero, in similitude with PW results. To determine the coefficients of the state function, it is necessary to solve self-consistently the corresponding HF equations [15]. Once the coefficients $C_{\mathbf{n}}$ and the parameter q_0 are determined, substitution in equation (1) gives the ground state energy. We consider two cases, the paramagnetic state with both spin states for each one-electron orbital, and the ferromagnetic state for an electron gas of identical particle density.

3. Results and discussion

We will now show the results for the ground state energy per particle, in Rydbergs, as a function of the parameter r_s (in Bohr radius). The value of the parameter q_0 must be $q_0 \geq 2k_F$ in order to satisfy the HF equations, as was shown in reference 16. From our calculation we find that $q_0 = 2k_F$ gives the best energy for both, the paramagnetic and ferromagnetic states at all densities and for the three symmetries considered by equations (2*a*) to (2*c*). This optimum value of q_0 was also found in reference 17, where they use particular cases of the expansion given by equation (2*a*), as state functions. In reference 18 this value was also obtained in calculations for the fermion gas in jellium, interacting via screened Coulombic interactions.

At high densities, r_s small, the self-consistent HF solution both in the paramagnetic and ferromagnetic cases becomes a plane-wave (PW). That means that all the $C_{\mathbf{n}}$ self-consistently determined are zero, except C_0. When r_s increases, the electronic density will acquire periodic character. With the paramagnetic state, the HF solution is different from PW beginning at $r_s = 32$, and this result is the same for the three symmetries considered in this work, equations (2*a*) to (2*c*). With the ferromagnetic state the transition from PW to periodic fuctions (PF) happens at $r_s = 40.33$, and this result is also the same for the three symmetries. Then, the HF state function for small r_s (from $r_s \ll 1$ until $r_s = 32$) is the PW both, in the paramagnetic and ferromagnetic cases.

As it is well known, when it is used the PW as state function for the electron gas, the ground state has paramagnetic character until $r_s = 5.47$, and starting with this value the ground state becomes ferromagnetic [10,19,20]. So, the HF ground state in this work is paramagnetic PW (PPW) until $r_s = 5.47$, from this value just up to $r_s = 40.33$ the ground state is ferromagnetic PW (FPW). At $r_s = 32$ the paramagnetic state is a PF, while the ferromagnetic remains a PW; however in the region between $32 \leq r_s \leq 40.33$, the energy with the FPW is lower than the energy obtained in the paramagnetic case, as can be seen from table I. That fact let us conclude that the ferromagnetic PW is the ground state up to $r_s = 40.33$.

r_s	$E_{fer.}$	$E_{par.}$
32	-3.264	-2.745
34	-3.091	-2.656
40	-2.666	-2.424
50	-2.431	-2.113
60	-2.165	-1.867
70	-1.967	-1.669

TABLE I. Paramagnetic and ferromagnetic HF energies at intermediate values of r_s. The energy is in Rydbergs $\times 10^{-2}$ and the r_s in Bohr radius. The state function we use for this calculations is given by Eq. (2*c*).

Beginning at $r_s = 40.33$ the ground state of the system presents non-homogeneous, periodic density, according to the Wigner hypothesis. Direct substitution of the self-consistent determined coefficients $C_{\mathbf{n}}$ in equation (3), shows that this behavior becomes more pronounced when the density diminishes, *i.e.*, when r_s increases. The transition from PW to PF at $r_s = 40.33$ is between the values of r_s given by references 21 and 22. In reference 21, using the density functional method, they get $r_s = 26$. While in reference 22, with the variational Monte-Carlo method, they get $r_s = 67$. These results are different from those of references 12, 13 and 23, since they get $r_s = 100$ as the point where the Wigner transition takes place. Our transition value is under the lower limit given by Wette [24,25]. As it is well known the value of the transition point, at which periodic density takes place, is a subject that remains rather open. As a matter of fact, previous estimates of r_s ranged from $r_s \simeq 2$ to $r_s \simeq 700$ [25,26].

As can be seen from table I the ground state above $r_s = 40.33$ has ferromagnetic character, since the ferromagnetic PF (FPF) gives lower energy than the corresponding paramagnetic PF (PPF), for the three symmetries considered in this work.

In figures 1 and 2 we show the results for the ground state energy per particle, in the density regions where we get better solutions than PW. In figure 1 is displayed the ground state energy at intermediate and small densities, for the three symmetries represented by the state functions given by equations (2*a*) to (2*c*). As was said before, in this region the ground state is a ferromagnetic PF.

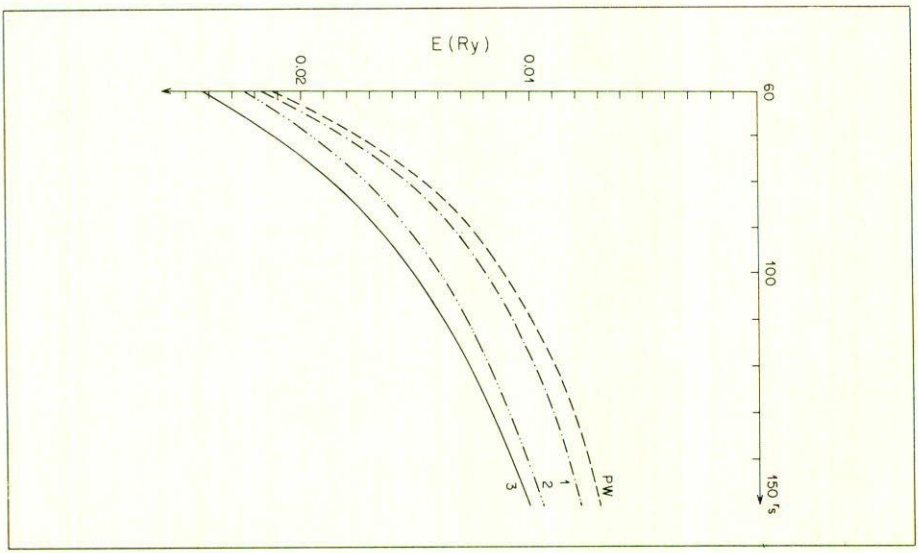

FIGURE 1. Ground state enrgy per particle, as a function of r_s, in Bohr radius, for the three symmetries considered in this work. Curve 3 is the energy with state function (2*c*). Curve 2 shows the results with function (2*b*), and curve 1 is the energy obtained with function (2*a*). These results are compared to the energy obtained with the ferromagnetic PW, dashed curve.

The curves 1 and 2 are the results with the functions in equations (2*a*) and (2*b*) respectively. With equation (2*a*), we use $N = 5$, *i.e.* an expansion with 11 terms. Using this state function the convergence for the energy is good, because the difference with the results for $N = 6$ is less than 10^{-6}. Using the state function in equation (2*b*) good convergence for the energy is obtained since $N = 2$, having in that way 25 terms in the expansion. The lowest energy, curve 3, is for the function in equation (2*c*) where we took $N = 1$, *i.e.* an expansion with 27 terms. With this function we have good convergence for the energy results. As can be seen from figure 1, the energy with the three functions proposed is lower than the energy with the FPW state function.

In figure 2 we compare with recent results our lower ground state energy obtained with the symmetry given by equation (2*c*), which have periodic non-homogeneous density along three orthogonal directions. We consider the intermediate and low density regions. The full curve represents our results, while dashed curve is for results with the Green function Monte-Carlo method [12], where they used a variational wave function of the Bijl-Jastrow-Slater type. The point-dashed curve represents the results with the integral approximant method [13]. In reference 12 we took the results that appear in table I. On the other hand, the results taken from reference 13 are those that appear explicitly in their highly schematic figure 3. As can be seen, both curves coincide at $r_s = 100$. This is because au-

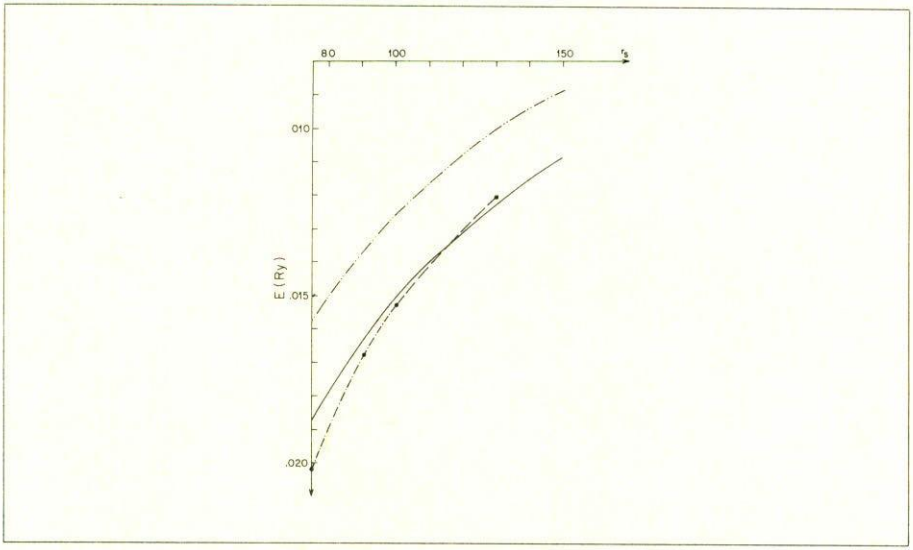

FIGURE 2. Energy per particle, in the intermediate and low density regions, as a function of the parameter r_s. Full curve are the results in this work with state function (2*c*). The point-dashed curve is the energy obtained with the integral approximant method. The dashed curve are the results with the Green function Monte-Carlo method. The double point-dashed curve is the energy per particle obtained with the paramagnetic state.

thors in reference 13 choose their ferromagnetic fluid parameter to reproduce the Monte-Carlo energy [12] at $r_s = 100$. It is interesting to see that our results for the energy in this region are good, however we are using an independent particle model as method of calculation. We also draw the HF results for the paramagnetic PF energy, double point-dashed curve. These are sensibly above the ferromagnetic energy.

In the high density region, $r_s \leq 40.33$, our energy results are not as good as those in references 12 and 13. This is because our state function becomes PW, both in the paramagnetic $r_s \leq 5.47$, as in the ferromagnetic ($5.47 < r_s < 40.33$) cases.

In this work we have presented a systematic method to evaluate the ground state energy for the electron gas in jellium, at all densities. With this method the Wigner crystallization is obtained in a natural way at low densities. The magnetic character of the ground state had also been investigated. According to our results, the ground state is paramagnetic PW until $r_s = 5.47$. From this value until $r_s = 40.33$, it is ferromagnetic PW. This result disagree with other calculations where the paramagnetic state is more stable at all densities [5,27]. At $r_s = 40.33$ the density of the system becomes periodic, and this characteristic, as was said before, becomes more pronounced when the density diminishes. Finally, it is interesting

that notwithstanding we are using an independent particle approximation, our results for the ground state energy in the intermediate and low density regions, are good compared with others that take correlations into account.

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Resumen. Se efectúa un análisis Hartree-Fock autoconsistente para la energía del estado base por partícula del gas de electrones en el modelo de jalea. Se consideran las diferentes regiones de densidades de partículas, desde altas hasta muy bajas densidades. Con el propósito de determinar la naturaleza del estado base, se consideran tanto los estados paramagnéticos como ferromagnéticos. La cristalización de Wigner a temperatura cero se observa en la región de densidades bajas en todos los casos estudiados. Nuestros resultados son comparados con otros cálculos recientes.