Magnetic character of the deformable jellium

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Ground-state properties for the electron gas, in the deformable jellium, are obtained. Periodic expansions for the state function, with fermion density centered around a cubic lattice, are introduced. The paramagnetic and ferromagnetic ground-state energies are calculated and compared at each density to determine the magnetic character of the deformable jellium. More than one transition point between different magnetic phases are obtained and compared with those reported in the literature with different models. A paramagnetic region at intermediate densities, in the self-consistent Hartree-Fock approach, is recovered. At these densities a symmetry transitions from homogeneous to localized solutions is obtained for both magnetic phases, and at lower densities the electrons are localized into a paramagnetic or ferromagnetic *Wigner-like crystal*, respectively. [S0163-1829(96)03427-3]

I. INTRODUCTION

The electron gas in jellium is a simplified many-body system consisting of electrons moving in a background of neutralizing positive charge. This model provides a theoretical approach to describe important electron gas properties in two and three dimensions.[1] In the ordinary or uniform jellium model (UJM) the essential approximation is to assume that the electrons interact through Coulomb forces in a uniform, nonresponsive, positive, neutralizing background.[2,3] Calculations in UJM require only one input parameter, namely, the average electron density in the bulk. The stabilized jellium model[4] (SJM) is a model in which, in addition to the total energy of the UJM, a structureless pseudopotential is introduced. Applied to the metal-surface problem the SJM adequately describes the basic features of the inhomogeneous electron gas near the metal surface.[5] In the SJM the properties depend upon the average electron density as a function of the interparticle distance in units of Bohr radius (r_s), and upon the valence Z and the crystal structure.

A different model is the deformable jellium (DJM) in which the background is statically deformed in order to *locally* neutralize the electron gas charge density.[6,7] This fact implies a lower energy per particle and therefore a more stable system, if a deviation of the homogeneous solution is energetically favored. In this model the background shows its response by deforming itself to preserve local charge neutrality, so that the long-range Coulomb interaction is diminished. The DJM retains the simplicity and universality of the UJM; i.e., all the properties depend on r_s only. A remarkable achievement of the electron gas in the DJM is the description of the symmetry transition from the homogeneous phase at high densities into localized states at intermediate densities.[6,8] Then at intermediate and low electron density regions, when the electronic part of the system develops long-range order, e.g., charge-density waves or Wigner crystallization, it is convenient to consider the DJM.

The DJM and the Hartree-Fock (HF) approximation have been exploited by us in the study of the paramagnetic electron gas.[6] Our approach has been to obtain self-consistency with a set of modulating functions that contain the trivial plane wave (PW) as a possible solution. This has turned into a very powerful technique that has the capability of describing both the metallic and the low-density regions in a unified nonperturbative fashion, which also includes the intermediate density region. At large densities the strong electrostatic interaction among the ions will prevent the background from accommodating into the required uniform or deformed structure. In this region the PW solution is the self-consistent HF ground state in the DJM as well as in the UJM. At low densities, on the other hand, the ions and the electrons are approximately equivalent except for their masses. In this sense the DJM is expected to give a better approximation to the physical system. Accordingly it allows for a lower energy per particle. The long-range-order solutions obtained in the DJM imply that the DJM introduce more correlations than the spin correlations introduced by the HF method in the UJM.

The magnetic character of the electron gas ground state is also a matter of interest. Many powerful methods have been developed to calculate the properties of the electron gas in the paramagnetic and ferromagnetic phases. Several approaches can be found in the literature with different approximations. In 1929, Bloch[9] considered paramagnetic and ferromagnetic states in the electron gas described by a PW's determinant. For $r_s < 5.47$ the paramagnetic PW solution is

more stable than the ferromagnetic one, but for $r_s > 5.47$, Bloch obtained a ferromagnetic fluid. In the HF approximation with PW solution this is the only magnetic transition. Then it is relevant to improve the approach in discussing the magnetic character of the electron gas ground state.

In the present work, the self-consistent HF ground-state energy and the ground-state function for the normal and the fully spin-polarized phases of the electron gas are obtained. In Sec. II the DJM is introduced and a periodic expansion is proposed for both magnetic phases. To determine the magnetic character of the ground state, in Sec. III we compare, at each density, the energies obtained in both phases. Our results are compared with those reported in the literature with different models. Atomic units are used throughout this work with the energy in Rydbergs.

II. THEORY

The defining condition of the DJM is to preserve local charge neutrality in the system. In order to locally neutralize the electron gas charge density the background is statically deformed. In the independent particle approximation, the mathematical expression that defines the DJM is

$$\langle V_d \rangle + \langle V_{e\text{-}b} \rangle + \langle V_{b\text{-}b} \rangle = 0, \tag{1}$$

where $\langle V_d \rangle$ is the energy contribution from the direct term of the electron-electron interaction, $\langle V_{e\text{-}b} \rangle$ and $\langle V_{b\text{-}b} \rangle$ are the electron-background and the background-background interactions, respectively. When a deviation of the homogeneous solution is energetically favored the condition that defines the DJM implies a lower energy per particle and therefore a more stable system. Additionally, the divergences associated with the long-range Coulomb potential in the calculation of the ground-state energy cancel automatically for any solution in this model. The consequences of the DJM and the conditions under which it is satisfied have been discussed in previous works.[6,8] The DJM together with the HF approximation provide a systematic method to describe the ground-state properties of the electron gas at all densities.

For the state functions in the Slater determinant the usual PW's, multiplied by modulating functions are proposed. Constrained by the orbitals orthogonality and to satisfy the HF equations the modulating frequency q_0 must satisfy $q_0 \geqslant 2k_F$. The minimum energy is obtained when $q_0 = 2k_F$. The proposed functions are

$$\phi_k(\mathbf{r}) = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{\Omega}} \sum_{n_x=0}^{N} \sum_{n_y=0}^{N} \sum_{n_z=0}^{N} C_{n_x n_y n_z} \times \cos(q_0 n_x x)\cos(q_0 n_y y)\cos(q_0 n_z z). \tag{2}$$

In this expression the vectors $\mathbf{k} = \hat{\mathbf{i}}k_x + \hat{\mathbf{j}}k_y + \hat{\mathbf{k}}k_z$ and $\mathbf{r} = \hat{\mathbf{i}}x + \hat{\mathbf{j}}y + \hat{\mathbf{k}}z$. $\mathbf{\Omega}$ is the volume in which periodic boundary conditions are imposed. The single-particle state functions are obtained when the coefficients $C_{n_x n_y n_z}$ are self-consistently determined by solving the HF equations with the orthonormality condition. The coefficients $C_{n_x n_y n_z}$ are considered independent of $\mathbf{k}$, the $\mathbf{n} = \hat{\mathbf{i}}n_x + \hat{\mathbf{j}}n_y + \hat{\mathbf{k}}n_z$ values determine the crystalline structure, and the term with $n_x = n_y = n_z = 0$ is the PW solution. In this approach, it was obtained that the simple cubic (sc) lattice is the energetically more stable lattice,[10] then this crystalline structure with $(N+1)^3$ terms is proposed in this work.

Generalized Fermi surfaces have been successfully introduced to describe the electron gas;[11,12] the Fröhlich Fermi sea is a relevant example that preserves spherical symmetry.[13] In this work spherical occupation is proposed for both magnetic phases. The paramagnetic state is a Slater determinant, with the state functions given by Eq. (2), having occupied all one-electron states with wave vector $\mathbf{k}$ lying within a Fermi sphere of radius k_F, for both spin states. Formally $n_k = \theta(k_F - k)$, where θ is the step function and $\mathrm{N} = \Sigma_{k,\lambda} n_{k,\lambda}$. The ferromagnetic state is a Slater determinant having all the electron states within a sphere of radius $2^{1/3}k_F$ occupied, with single occupied spin states. This system is an example of anomalous occupation in spin space,[14] characterized by $n_k = \theta(2^{1/3}k_F - k)$ and $\mathrm{N} = \Sigma_k n_{k,\lambda_1}$.

To calculate the ground-state energy per particle, using the state function of Eq. (2), it is necessary to evaluate for the kinetic energy terms of the form

$$\frac{\langle T \rangle}{\mathrm{N}} = \frac{A_0}{r_s^2} \sum_{\mathbf{n}}^{\mathbf{N}} |C_{n_x n_y n_z}|^2 \left[1 + \frac{20}{3}(n_x^2 + n_y^2 + n_z^2) \right], \tag{3}$$

and for the exchange energy

$$\frac{\langle V \rangle}{\mathrm{N}} = -\frac{A_1}{8^3 r_s} \sum_{\mathbf{n}_1}^{\mathbf{N}} \sum_{\mathbf{n}_2}^{\mathbf{N}} \sum_{\mathbf{n}_3}^{\mathbf{N}} \sum_{\mathbf{n}_4}^{\mathbf{N}} C^*_{\mathbf{n}_1} C^*_{\mathbf{n}_2} C_{\mathbf{n}_3} C_{\mathbf{n}_4} I(\mathbf{n}_1, \mathbf{n}_4) \times F(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3, \mathbf{n}_4). \tag{4}$$

The symbol $\Sigma_{\mathbf{n}}^{\mathbf{N}}$, with $\mathbf{N} = N(\hat{\mathbf{i}} + \hat{\mathbf{j}} + \hat{\mathbf{k}})$, has been used for $\Sigma_{n_x=0}^{N} \Sigma_{n_y=0}^{N} \Sigma_{n_z=0}^{N}$, and $C_{\mathbf{n}}$ for $C_{n_x n_y n_z}$. $A_0 = 2.21$ and $A_1 = 0.611$. When the self-consistent solutions are PW the r_s^{-1} coefficient reduces to the usual value, 0.916. F is a sum of terms that are products of Kronecker δ functions, and the function I stems from the integrals of the Coulomb potential.

III. RESULTS AND CONCLUSIONS

The single-particle state functions and the ground-state energy per particle for the electron gas were evaluated in terms of r_s. Calculations were done in the DJM, at high, intermediate, and low densities. The coefficients $C_{\mathbf{n}}$ in Eq. (2) were determined self-consistently with a precision of 10^{-5} with respect to the previous iteration for both magnetic phases. In order to obtain ground-state energy results independent of N, the upper limit in the expansion of Eq. (2) was changed from 1 up to 5. The results are shown for the functions with $N = 5$ (this function has 216 terms). With this state function we get convergence for the energy results, i.e., independence in N for $r_s \leqslant 50$ in the paramagnetic phase,[6] and for $r_s \leqslant 63$ in the ferromagnetic one.

Within the HF approach with the single-particle state functions of Eq. (2), the electron gas behavior in both magnetic phases is qualitatively equivalent. In the high-density region the PW's are the self-consistent HF solutions for these systems; at intermediate densities a symmetry instability is found and long-range order solutions are obtained for both phases. At $r_s \approx 26$ a symmetry transition from the homogeneous to the corrugated state is obtained in the paramagnetic

TABLE I. Symmetry transitions from homogeneous paramagnetic (PW-P) and homogeneous ferromagnetic solutions (PW-F) to localized solutions (L-P) and (L-F), respectively.

r_s	Symmetry transitions
26.0	PW-P to L-P
32.8	PW-F to L-F

phase[6] (localized-P). In the polarized phase the change from PW to the localized solution (localized-F) is obtained at $r_s \approx 32.8$. At very low densities the electrons crystallize in a *Wigner-like crystal* with the sc symmetry of the state functions proposed. In Table I the r_s values for the symmetry transitions previously reported are shown.

From the energies obtained, for the two phases the magnetic character of the electron gas ground state is determined at each r_s value. The magnetic character of the ground state is the same as the one obtained by Bloch[9] until intermediate densities. The self-consistent state function obtained here for both magnetic phases at this region is the PW. In the high-density region ($1 < r_s < 5.47$) the ground state is paramagnetic (PW-P) and there is a transition to a polarized state (PW-F) at $r_s = 5.47$. For $5.47 \leqslant r_s < 36$ the ferromagnetic solution is more stable than the paramagnetic one. In the interval $5.47 \leqslant r_s < 32.8$ the ferromagnetic PW solution is the ground state. After the symmetry transition in the polarized phase, for $32.8 \leqslant r_s < 36$ the localized-F is energetically favored.

In Fig. 1 the ground-state energy per particle in terms of r_s is plotted at intermediate and low densities. The continuous line shows the paramagnetic energy and the dashed line the ferromagnetic energy. As can be seen in Fig. 1, at $r_s \approx 36$ a *magnetic* transition is obtained, because the paramagnetic solution is more stable than the ferromagnetic one. Then a more stable paramagnetic region at intermediate densities is recovered in the HF approach. At lower densities, for $r_s \approx 47.5$, the last *magnetic* transition is obtained and the localized-F state is energetically more stable for $r_s \geqslant 47.5$. Finally at very low densities the electrons crystallize and the ground state is a ferromagnetic *Wigner-like crystal.*

TABLE II. Ground-state transitions. At $r_s = 5.47$ the Bloch magnetic transition is obtained from PW-P to PW-F solution. A symmetry transition at $r_s = 32.8$ changes the ground state from PW-F to L-F. At $r_s = 36$ a magnetic transition changes the ground state from L-F to L-P solution. Finally at $r_s = 47.5$ the last magnetic transition is obtained, from L-P to L-F ground state.

r_s	Ground-state transitions
5.47	PW-P to PW-F
32.8	PW-F to L-F
36	L-F to L-P
47.5	L-P to L-F

In Table II the r_s values for the ground-state transitions are shown. The last results can be compared with others reported in the literature, for the electron gas in the UJM, which include explicitly a two-body correlation function. We compare our results with Monte Carlo calculations by Ceperley and Alder.[15] They have obtained a paramagnetic fluid in the intermediate region, and a paramagnetic to ferromagnetic transition at $r_s = 75 \pm 5$. In Ref. 16, using Padé approximants a paramagnetic system in the intermediate density region is obtained and one parameter was taken so as to reproduce the magnetic transition point obtained in Ref. 15 at $r_s = 75$. The behavior of the electron gas in this work is qualitatively similar, nevertheless the last magnetic transition is obtained at $r_s = 47.5$. In Ref. 17 a different expansion scheme is introduced, where the symmetry effect has been neglected, nevertheless they use the results obtained in Ref. 15.

In Fig. 2 the ground-state energy per particle in terms of r_s is plotted. The energy scale allows us to introduce the energy values obtained in Refs. 15, 16, and 17. The continuous line shows the paramagnetic energy and the dashed line the ferromagnetic one. At the range shown, the best results in

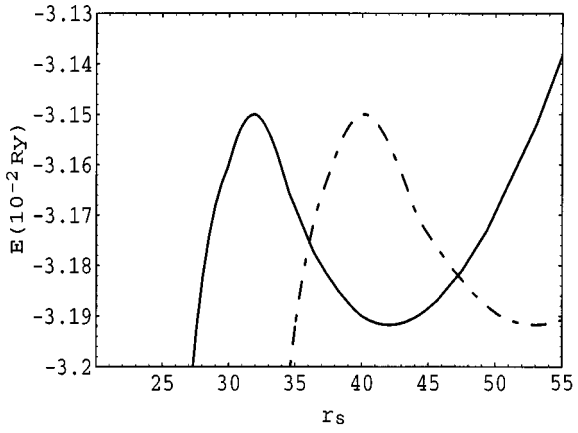

FIG. 1. Ground-state energy per particle of terms of r_s. The continuous line shows the paramagnetic energy and the dashed line the ferromagnetic one. From $5.47 < r_s < 36$ the ground state is ferromagnetic. At $r_s \approx 36$ up to $r_s = 47.5$ the self-consistent solution is paramagnetic, and finally for $r_s > 47.5$ the ground state is ferromagnetic.

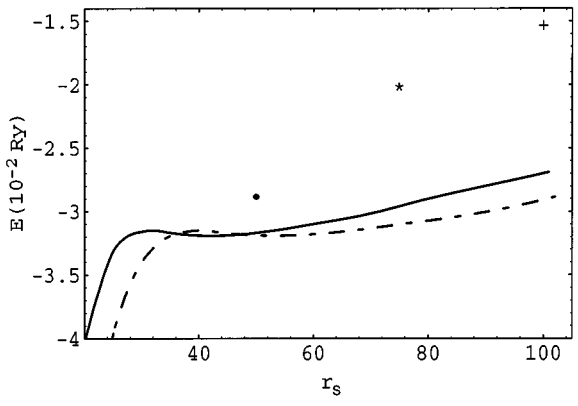

FIG. 2. Ground-state energy per particle of terms of r_s. The continuous line shows the paramagnetic energy and the dashed line the ferromagnetic one. At this range, the best results in Refs. 15, 16, and 17 are the Monte Carlo calculations of Ceperley and Alder's. At $r_s = 50$ the dot corresponds to a paramagnetic fluid. The * at $r_s = 75$ points the paramagnetic-ferromagnetic transition. Finally the + at $r_s = 100$ corresponds to a ferromagnetic phase.

the last references are those in Ref. 15. At $r_s=50$ (the dot in Fig. 2) they obtain a paramagnetic fluid. At $r_s=75$ (the asterisk) a paramagnetic-ferromagnetic transition is reported. Finally at $r_s=100$ (the plus) they report a ferromagnetic fluid. The other results obtained in Refs. 15, 16, and 17 at these densities are very near the points shown in the figure, but in this scale, it is impossible to distinguish among them.

A very powerful nonperturbative technique, which allows a direct evaluation of the ground-state properties of the electron gas, has been developed. In a unified approach the low-, intermediate-, and high-density regions are considered. The self-consistent energies obtained in both phases are compared at each r_s, and the magnetic character of the DJM was determined. Within this approach, several magnetic regions were obtained, a paramagnetic region at intermediate densities is recovered and a last magnetic transition is obtained in the low-density region. The symmetry transition to the corrugated state is localized at $r_s\approx 32.8$ and at very low densities the electrons crystallize into the *Wigner-like crystal* as was to be expected. It is well known that in the UJM the ground-state structure of the Wigner crystal is bcc. Here the state functions proposed in the DJM have sc symmetry, as a consequence a Wigner-like crystal is obtained with sc structure. Nevertheless the background deformations in the DJM with the HF approach produce lower energy than the one obtained with bcc symmetry in the UJM including explicit two-body correlations. On the other hand, the DJM self-consistent calculation in the HF approach reproduces similar magnetic behavior of the electron gas at intermediate and low densities, as compared to the one obtained when explicit two-body correlations are introduced into the UJM.

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