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Ground-state properties of the deformable jellium

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A self-consistent calculation is done to evaluate relevant ground-state properties of the electron gas in the deformable-jellium model. We get the melting point of the Wigner crystal and the ground-state energy per particle at all densities. The single-particle state function in the Slater determinant is expanded in a basis of periodic functions. This expansion guarantees the existence of a particle density centered on a simple-cubic lattice. The transition to the Wigner crystal is obtained as the value of the Wigner-Seitz parameter at the point where the state function changes from a periodic density to a plane-wave density. Our results for the transition density to the Wigner crystal are close to values obtained using alternative methods. The ground-state energy obtained in this work is compared to recently reported theoretical predictions.

I. INTRODUCTION

The ground-state properties of the electron gas have been a matter of increasing interest. Beginning with the pioneering work of Wigner,[1] who predicted crystallization at low densities, many methods have been proposed in order to obtain these properties, in particular, the Wigner crystal melting point. The reported values of the transition point are very different depending on the model and the method used.[2,3] They range from about $r_s=6$ up to 700, where the Wigner-Seitz parameter r_s is the interparticle distance, in units of the Bohr radius. The theoretical methods include the random-phase approximation;[4] analysis of the behavior of the free energy for both the crystal and the fluid phases;[5,6] and variational calculations[7,8] and Monte Carlo variational calculations,[9] where the authors compare directly the energies of different states. Stochastic simulation of the Schrödinger equation[10] and the integral-approximant method[11] have given similar results for the melting point. The density-functional formalism for jellium[12–14] and self-consistent calculations for the electron gas in deformable jellium[15] can be mentioned among the relevant methods used to find the transition point of the Wigner crystal.

Jellium is a simplified and useful model to describe many-body systems in which the neutralizing background is assumed to be uniform.[12,13,16] In the deformable jellium, instead, the neutralizing background is deformed in order to get local neutrality and consequently diminish the energy of the system.[17,18] The basic idea of a deformable background was first introduced by Overhauser,[19] and has provided interesting descriptions for the ground states of many-particle systems, in particular in the electron gas.[15,16] In the past some of us have reported Hartree-Fock (HF) self-consistent calculations to solve the fermion gas in deformable jellium using an exponential basis for the orbitals in the Slater determinant.[20]

In this work a different and more refined self-consistent HF calculation is performed for the electron gas. Our aim is to obtain the transition point (melting point) from periodic solutions—which are charge-density waves (CDW's)—to plane waves (PW's). The ground-state energy is also evaluated. The general method used has been described in Ref. 20. The deformable jellium, as defined in Ref. 18, is used in order to attain lower values for the energy of the system. The spatial factor of the spin orbitals is proposed to be a periodic expansion in terms of cosine functions. This expansion is given in such a way that it guarantees the possibility for periodic nonhomogeneous density centered on a simple-cubic lattice. The algebraic form in terms of cosine functions lets one handle a larger number of terms than the exponential form, with a considerably diminished computational effort. Our results are compared with other theoretical models recently reported for the electron gas. Some conclusions about the convergence of the proposed expansion are also made.

II. THE MODEL

In the deformable jellium it can be shown that the equations for the ground-state HF energy only have the particle kinetic energy and the exchange terms.[15] The HF equations are written including the orthonormality condition for the HF doubly occupied orbitals. The spin orbitals in the Slater determinant are expanded in terms of a cosine function series

$$\phi_{\mathbf{k},\lambda}(\mathbf{r})=\chi_\lambda\frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{V}}\sum_{n_x=0}^{\mathcal{N}_x}\sum_{n_y=0}^{\mathcal{N}_y}\sum_{n_z=0}^{\mathcal{N}_z}C_{n_xn_yn_z}\cos(q_0n_xx)\times\cos(q_0n_yy)\times\cos(q_0n_zz)\ , \quad (1)$$

where χ_λ is the spin function and V is the volume in which normalization conditions are imposed. The first term in this expansion ($n_x = n_y = n_z = 0$) corresponds to the PW solution. The expansion gives the possibility to describe a lot of systems with different symmetries. In this work, we study a system that may present periodic density centered on a simple-cubic lattice. Therefore we selected $\mathcal{N}_x = \mathcal{N}_y = \mathcal{N}_z = \mathcal{N}$. Consequently, all the sums run from 0 up to the same positive value $\mathcal{N}$. In this way the number of terms in the expansion of Eq. (1) is equal to $(\mathcal{N}+1)^3$ The coefficients C_{n_x,n_y,n_z} are self-consistently determined, and the value of q_0 is selected in order to satisfy the HF equations.[20]

With the proposed HF basis of states, it is possible to obtain the periodic density

$$\rho = \rho_0 \left[\sum_{n_x}^{\mathcal{N}} \sum_{n_y}^{\mathcal{N}} \sum_{n_z}^{\mathcal{N}} C_{n_x n_y n_z} \cos(q_0 n_x x) \times \cos(q_0 n_y y) \cos(q_0 n_z z) \right]^2 , \quad (2)$$

where ρ_0 is the PW density.

In order to calculate the ground-state energy per particle, using Eq. (1) for the spin orbitals, it is necessary to evaluate terms of the form

$$\frac{\langle \hat{T} \rangle}{N} = A_0 \sum_{\mathbf{n}}^{\mathcal{N}} |C_{\mathbf{n}}|^2 [1 + \tfrac{20}{3}(n_x^2 + n_y^2 + n_z^2)] \quad (3)$$

for the kinetic energy and for the exchange energy

$$\frac{\langle \hat{V} \rangle}{N} = -\frac{A_1}{512} \sum_{\mathbf{n}_1} \sum_{\mathbf{n}_2} \sum_{\mathbf{n}_3} \sum_{\mathbf{n}_4} C^*_{\mathbf{n}_1} C^*_{\mathbf{n}_2} C_{\mathbf{n}_3} C_{\mathbf{n}_4} I(\mathbf{n}_1, \mathbf{n}_4) \times F(\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3, \mathbf{n}_4) , \quad (4)$$

where N is the number of particles and $C_{\mathbf{n}} \equiv C_{n_x n_y n_z}$. We have used $\sum_{\mathbf{n}}$ for $\sum_{n_x} \sum_{n_y} \sum_{n_z}$ and $\mathbf{n} = n_x \mathbf{i} + n_y \mathbf{j} + n_z \mathbf{k}$. F is a sum of terms which are products of Kronecker δ functions in the components n_x, n_y, and n_z of the four $\mathbf{n}_i$'s. Finally, I is a function that stems from the integrals of the Coulomb potential in terms of the components of $\mathbf{n}_1$ and $\mathbf{n}_4$.

It is interesting to notice that the exchange term, Eq. (4), has been greatly simplified taking into account symmetry considerations: We have to evaluate 8^3 terms instead of 8^4 for each triad of values (n_x, n_y, n_z) in the sums. With a basis in terms of cosine functions the matrices have dimension $(\mathcal{N}+1)^3$, instead of $(2\mathcal{N}+1)^3$, which is the matrix dimension with the exponential expansion.[20]

III. DISCUSSION

Self-consistent calculations were done to determine the coefficients $C_{\mathbf{n}}$, for a different number of terms in the expansion of Eq. (1). The values considered for $\mathcal{N}$ range from 1 up to 5. In the first two cases, the coefficients in the state function were determined with an approximation of 10^{-6} with respect to the last iteration. In the largest expansions, $\mathcal{N}=3$ up to 5, the coefficients were determined with an approximation of 10^{-5}. The number of iterations needed in each case to get self-consistency in the accuracy required explodes near the transition point. Naturally the results for the melting point and the ground-state energy depend on the number of terms in the expansion for the state function. However, due to the fact that the proposed basis is adequate to describe this system, we expect that the results converge rapidly starting with a given value of $\mathcal{N} = \mathcal{N}_{\max}$. This fact justifies the cutting in the number of terms for that value of $\mathcal{N}$.

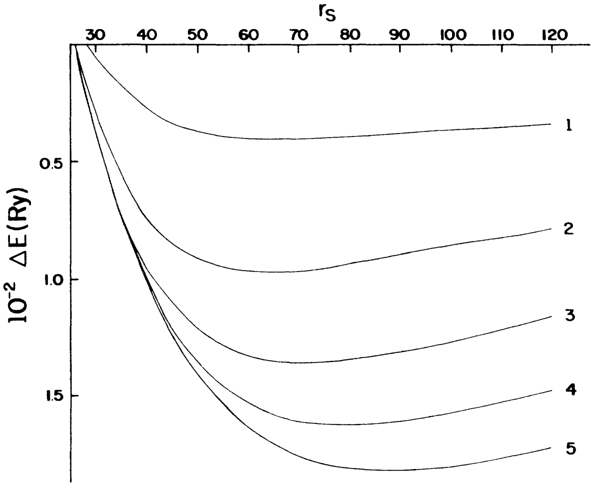

FIG. 1. Energy difference per particle between the trivial PW and the expansion in Eq. (1) as a function of the parameter r_s. The results for $\mathcal{N}=1$ up to $\mathcal{N}=5$ are shown in curves 1–5.

For all the expansions we have considered, it is observed that the self-consistently determined state function is a CDW in the low- and intermediate-density regions. But it reduces to a PW for high densities. The value of the parameter r_s where the solutions transform from CDW to PW will be taken as the melting point.[15] This criterion is similar to that given in Ref. 12, where the authors consider a CDW instead of a close-packed structure. It is worthwhile to comment that near the transition, $r_s \gtrsim r_s$(melting), the electrons are not strongly localized. That result was also reported in Refs. 12 and 13. However, as the value of r_s increases, the electron's density rapidly resembles a close-packed structure.

The difference in energy per particle ΔE between the results with the trivial PW solution and the state function in Eq. (1) is displayed in Fig. 1. The results are given in rydbergs in terms of the interparticle distance r_s. We show the results for expansions with values of $\mathcal{N}$ from 1 up to 5. The matrix dimensions in all cases are given in Table I, and these values are compared with those corre-

TABLE I. Number of terms for the equivalent state functions with the exponential and the cosine basis.

$\mathcal{N}$	Exponential basis	Cosine basis
1	27	8
2	125	27
3	343	64
4	729	125
5	1331	216

TABLE II. Energy difference per particle in units of 10^{-2} Ry for three values or the parameter r_s, as a function of the number of terms in the state function.

$\mathcal{N}$	$\Delta E(r_s=30)$	$\Delta E(r_s=70)$	$\Delta E(r_s=120)$
1	0.04	0.04	0.037
2	0.29	0.96	0.78
3	0.36	1.36	1.16
4	0.37	1.61	1.47
5	0.37	1.76	1.71

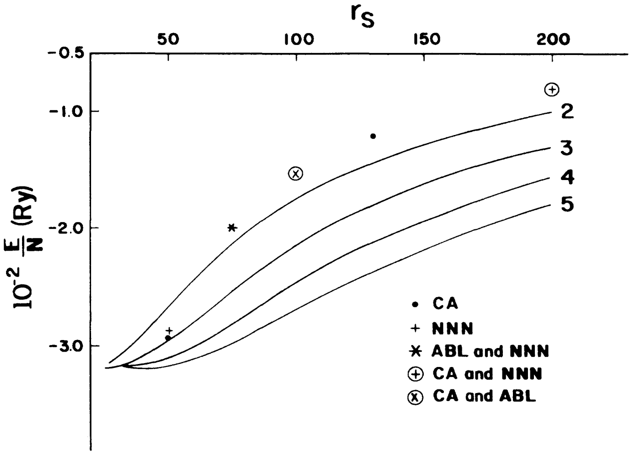

FIG. 2. Ground-state energy per particle in rydbergs as a function of r_s. The solid curve shows the results obtained in this work with $\mathcal{N}=2$, 3, 4, and 5. The value of $\mathcal{N}$ labels the curves. The points (●) show the results of Ceperly and Alder (Ref. 10). The results of Aguilera-Navarro, Baker, and de Llano (Ref. 11) are indicated by ×. The results of Nagara, Nagata, and Nakamura (Ref. 6) are indicated by +.

sponding to the exponential basis. It follows from Fig. 1 that the transition from periodic to homogeneous density occurs at $r_s=28.8$, 26.2, and 26.1 for the cases with $\mathcal{N}=1$, 2, and 3, respectively. And it occurs at $r_s=26$ for $\mathcal{N}=4$ and 5. When the state function has more terms, the transition point converges to a value of the density parameter $r_s=26$. As the values of the melting point using alternative models fall in a wide interval ($6 \le r_s \le 700$), it is interesting to comment about some results similar to ours. Our HF, deformable-jellium value of the melting point is near the result of Van Horn[21] of $r_s=27$, obtained by an improvement of the de Wette stability criterion for the Wigner lattice.[22] In Ref. 14, Das and Mahanty, using the density-functional method for the jellium, obtained a value of $r_s=30$ for the transition point with a fcc structure. Our results are also near to those of Refs. 12 and 13, where $r_s=25$ and 26 are obtained, using the density-functional method and the jellium model.

It is worthwhile to comment that a greater numerical precision, in the determination of the C_n coefficients, is required to evaluate the energy in the region near the melting point than far from it. This fact, together with the greater number of iterations needed near the melting point, makes the evaluation of the energy in the region of the Wigner transition extremely expensive.

As can be seen from Fig. 1, the difference in energy ΔE increases with the number of terms in the expansion of the state function. In table II we show some energy results in terms of r_s for a different number of terms in the expansion. Then, the lowest energy is obtained with the greatest expansion for the state function. From the results in Fig. 1 and Table II, we can expect that our energies converge rapidly to limiting values when $\mathcal{N}$ increases. Notice that, even with an expansion in which $\mathcal{N}=1$, we have good energy results as compared with other values obtained with the deformable jellium.[18] With $\mathcal{N}=5$ our energy results converge in the intermediate-density region $26 \le r_s \le 60$.

In Fig. 2, the ground-state energy per particle in rydbergs is shown, in terms of r_s. Our results are given for the orbitals with 27, 64, 125, and 216 terms in the expansion. We also show other recent results for the ground state of the electron gas in jellium.[6,10,11] From Ref. 6 we took the values that correspond to the ground-state energy of the solid, for the higher approximation. As can be seen from Fig. 2, our energy values are close to those of Ref. 6 and the "exact" solutions of Ref. 10 at $r_s=50$. At other densities it is seen that with the function with 27 terms, curve 2, we are close to the energies in Refs. 6, 10, and 11. Naturally, if we use larger expansions our results converge to a lower energy, because of the characteristics of the deformable jellium used in this work. If correlation corrections to the HF approximation of this work are taken into account, the energy curves in Fig. 2 are expected to move up, becoming nearer to the results in the above-mentioned references. It is worthwhile to remark that we are comparing results of different models of the same physical system: the electron gas. Different models clearly contain distinct approximations. Therefore this comparison reflects the differences between the physical assumptions.

From a technical perspective the main difference with other self-consistent HF calculations is the use of an improved basis of state functions. In particular, we have to handle matrices of dimension $(\mathcal{N}+1)^3$, instead of $(2\mathcal{N}+1)^3$, as would be the case with an exponential basis. These expansions are excellent, as can be observed from the rapid convergence of the energy results in the intermediate-density region. Finally, the results for the melting point of the Wigner crystal obtained in this work are close to other results obtained with the density-functional method.

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