Ground-state properties of a strongly coupled one-component plasma

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The ground state of a quantum strongly coupled one-component plasma, with planar symmetry, is analyzed. The analysis was done working with the deformable jellium model and the particle-particle interaction as a screened Coulombic potential. For the single-particle state functions, two different periodic expansions were used. We obtained the behavior of the ground-state energy per particle, the coupling parameter Γ, the particle localization, and the density of states as functions of the interparticle distance r_s.

INTRODUCTION

A homogeneous one-component plasma (OCP) is a system consisting of charged particles of a single species in a neutralizing background. It is a simplified model which nevertheless manifests fundamental characteristics of a Coulomb system. The OCP is characterized by the dimensionless coupling parameter Γ,[1,2] which is a measure of the ratio of the average potential energy to the average kinetic energy. The Γ values classify the plasma in strongly coupled, if $\Gamma > 1$, and weakly coupled, if $\Gamma < 1$. Examples of strongly coupled plasma are the system of ions inside a highly evolved star,[3] and the system of valence electrons in the metal.[4]

A number of special models that concentrate upon some physical properties of the system have been developed to bring out more clearly the physical characteristics involved or to give alternative viewpoints. Estimates of static and dynamic properties of a quantum OCP have been clarified through various theoretical approaches. Among the analytic theories reported in the literature one can mention the Green's-function method,[5] the dielectric formulation,[6] the variational methods in terms of a trial wave function,[7] the density-functional method,[8] and Hartree-Fock[9] calculations. Also, Monte Carlo variational calculations,[10–11] thanks to the development of fast computers and the rapid progress of computational technique, constitute useful tools in the study of these systems.

In the Coulombic systems at low densities, the potential energy becomes relatively more important than the kinetic energy, and it is expected that the spatial density becomes nonuniform to minimize the energy. Then the particles that are nearly free at high densities are expected to form a periodic crystalline array at low densities. Therefore it is valuable from a theoretical standpoint to predict the properties and phases of a quantum OCP for the complete range of densities.

Historically, Wigner[12] first proposed in 1934 a phase transition in the electron gas at low densities. In this density region the electron gas is a strongly coupled OCP. Since this pioneering work, the phases of the electron gas have attracted a great deal of interest. The arguments for lattice formation and the condition under which it is expected to occur are elaborated in various directions, and there are many different estimates for the critical interparticle distance at which the electron gas will condense into the ordered Wigner lattice.[13] Almost all these analyses were done for systems in three dimensions (3D); for these systems, the exact Monte Carlo results obtained by Ceperley and Alder[10] provide an upper bound to the ground-state energy. In the literature, there are also analysis of the ground-state properties of the two-dimensional (2D) electron gas,[14] because it is a fundamental model in many body physics and has several important applications. There are laboratory reports of Coulombic systems with crystalline array in 2D and 3D: electrons deposited on the surface of liquid helium,[15] the crystallized suspensions of polystyrene spheres,[16] and colloidal crystals.[17]

In a theoretical approach to 3D systems, Overhauser[18] considers a model in which the background is deformable, as the ions in the alkali metals might be. At low densities this system is unstable against charge-density waves (CDW) and this transition is considered as a precursor to the Wigner crystallization. This model, the deformable jellium model, has been extensively used. Initially in the Overhauser's model, the CDW are presented in only one direction, and it was an important problem to determine the optimum direction for the CDW in a particular system. Presently it is usual to find in the literature calculations which present CDW in one, two, and three directions,[19] in order to obtain an adequate description of systems with linear, planar, or three-dimensional symmetry, respectively.

In this paper we analyze a 3D strongly coupled quantum electron OCP (QEOCP) in the deformable jellium model. We are interested in the ground-state properties of systems with planar symmetry. The state function is evaluated by a self-consistent Hartree-Fock (HF) method. The single-particle state functions proposed are two alternative periodic expansions such that the self-consistent calculations may produce a CDW in two directions, for both expansions.

It is well known that at metallic densities, the self-consistent HF solution for a QEOCP is the plane-wave (PW) solution.[5] If the system is unstable against a two-dimensional CDW, there will be a phase transition at a

characteristic interparticle distance, and the self-consistent solution obtained in this region will be a CDW. Therefore the particles density will be periodic along two orthogonal axes starting at a critical interparticle distance. It is interesting to see how the particle localization changes as the interparticle distance increases from the transition point.

The ground-state energy and the coupling parameter Γ are calculated as functions of the interparticle distance. The behavior of both are very useful to determine the plasma stability. A discontinuity in the function Γ as well as the energy criterion are used to characterize the fusion point for the Wigner crystal.[13,20]

The electronic density of states, specially near the Fermi level, is essential to obtain transport properties of the system: therefore it is convenient to remove the pathological logarithmic zero found for Coulombic systems with a PW solution[21] in the HF approximation. In order to analyze the system behavior for different interaction ranges and to remove the divergence in the density of states at the Fermi level, the proposed interaction is a screening Coulombic potential.[22]

THE MODEL

The Hamiltonian for a 3D strongly coupled QEOCP has the general form

$$H=T+V_{e\text{-}e}+V_{e\text{-}b}+V_{b\text{-}b} \ .$$

T is the kinetic energy of the electrons, $V_{e\text{-}e}$ is the electron-electron interaction, $V_{e\text{-}b}$ is the electron-background interaction, and finally $V_{b\text{-}b}$ is the background-background interaction. The deformable jellium in the single-particle approximation is defined by the condition[23,24]

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

where $\langle V_d \rangle$ is the energy contribution from the direct term of the electron-electron interaction.

In this work, the single-particle state functions in the Slater determinant have the general form

$$\Phi_{k,\lambda}=\chi_\lambda \mathcal{V}^{-1/2}\exp(i\mathbf{k}\cdot\mathbf{r})F_k(\mathbf{r}) \ ,$$

where χ_λ is the spin function, $\mathcal{V}$ is the volume in which normalization conditions are imposed, and $F_k(\mathbf{r})$ is a function with the symmetry of the system. As a first approximation we propose $F_0(r)$, and the specific form is determined by means of the HF equations with the orthonormalization condition included. All the calculations are performed for the two following alternative periodic expansions, proposed for the single-particle state functions:

$$\Phi_{k,\lambda}=\chi_\lambda \mathcal{V}^{-1/2}\exp(i\mathbf{k}\cdot\mathbf{r}) \times \sum_{n_x=0}^{N}\sum_{n_y=0}^{N} C_{n_x n_y}\cos q_0(n_x x+n_y y) \ , \tag{1}$$

$$\Phi_{k,\lambda}=\chi_\lambda \mathcal{V}^{-1/2}\exp(i\mathbf{k}\cdot\mathbf{r}) \times \sum_{n_x=0}^{N}\sum_{n_y=0}^{N} C_{n_x n_y}\cos(q_0 n_x x)\cos(q_0 n_y y) \ . \tag{2}$$

The C_n coefficients are determined by means of the HF equations, with the orthonormalization condition included. In order to satisfy the HF equations, the parameter q_0 must be equal to or greater than $2k_f$; here it is selected as the energetically favored value $q_0=2k_f$.[23]

If the system is unstable against a CDW, then it is possible to obtain in the low-density region, a CDW in two directions, with each of the proposed expansions, i.e., periodic particle density along the X and Y axes, and homogeneous density along the Z axis. The HF equations to be solved are

$$\sum_{\mathbf{n}_3}\left[\langle \mathbf{n}_1\mathbf{k}_1|T|\mathbf{n}_3\mathbf{k}_1\rangle - \sum_{\mathbf{n}_2}\sum_{\mathbf{n}_4}\langle \mathbf{n}_1\mathbf{k}_1,\mathbf{n}_2 kec_2|V|\mathbf{n}_4\mathbf{k}_2,\mathbf{n}_3\mathbf{k}_1\rangle C^*_{\mathbf{n}_2}C^*_{\mathbf{n}_4}\right]C_{\mathbf{n}_3}=\epsilon_{\mathbf{n}_1}C_{\mathbf{n}_1} \ ,$$

where the orthogonality condition of the spin-orbitals is included, the $\sum_{\mathbf{n}}$ replaces $\sum_{n_x}\sum_{n_y}$ and the coefficients $C_{\mathbf{n}}$ are used instead of $C_{n_x n_y}$.

These coefficients are self-consistently determined with an approximation of 10^{-6} with respect to the last iteration. The plasma density is characterized by the interparticle distance r_s in Bohr radius, and the self-consisting calculations can be performed for every r_s value. In this work we are interested in the density range[20] $1 \le r_s \le 100$. The screened Coulombic potential used in the calculations is the following:

$$V(r)=e^2\exp(-\mu r)/r \ ,$$

where μ is the screening parameter in units of $2k_f$. With the self-consistent state functions other physical properties of the corresponding ground states can be calculated.

RESULTS AND DISCUSSION

The behavior of a strongly coupled QEOCP with planar symmetry at the intermediate and low densities was analyzed. These systems are characterized by the state function and by their interaction ranges. The analysis indicate that the behavior of some properties are qualitatively equivalent, for both expansions and for every value of the screening parameter μ. The analysis also indicates that all these systems are unstable against a two-dimensional CDW in the low-density region, but the energy gain and the transition point from PW to CDW are characteristic for each system.

As it is usual, we take as energy reference the corresponding PW ground-state energy per particle in rydbergs. In this work, the melting point for the Wigner crystal is determined by means of the unstability against

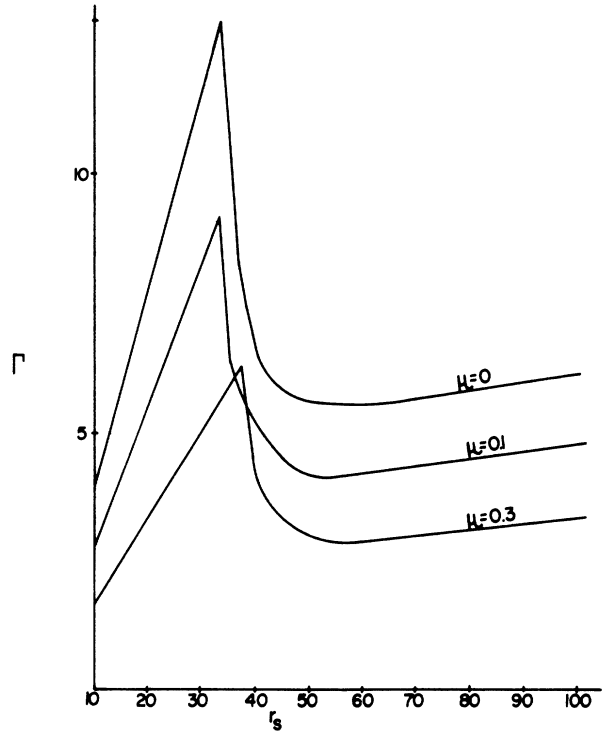

FIG. 1. The coupling parameter Γ corresponding to expansion (1) as a function of the interparticle distance r_s for $\mu=0$, 0.1, and 0.3; μ is in units of $2k_f$.

a CDW, and this is characterized by the following criteria: (a) the singular coupling parameter behavior, (b) the ground-state energy gain with respect to the PW, $\Delta E=E(CDW)-E(PW)$, and (c) the particle localization.

The self-consistent calculations were performed with state functions for which the upper limit in the expansions is $N=6$, because with this value the convergence in energy is reached. It means that starting with $N=6$ the properties evaluated are independent of the value N. As it is expected, we obtain the PW as the self-consistent solution in the high-density region, up to a characteristic interparticle distance r_s. Starting at this critical density the HF solution is a periodic function, therefore the energy difference $\Delta E=E(\text{CDW})-E(\text{PW})$ is different from zero. This freezing density is different for each expansion, and it is found that the critical r_s value increases with the screening parameter μ.

In Fig. 1 we show the coupling parameter Γ as function of the interparticle distance r_s for the complete range of densities. The results corresponding to expansion (1) for $\mu=0$, 0.1, and 0.3, μ in units of $2k_f$, are reported. In the high-density region the $\Gamma(r_s)$ functions obtained, for each μ value, are linear functions, as it is expected for PW. The figure shows that the slope of these curves decreases as the screening parameter μ increases. The singular point in each curve determines the melting point of the corresponding Wigner crystal, this criterion is very useful because as it can be seen in the figure this critical point is precisely determined.

In Table I we display the critical r_s and the Γ values for the melting point obtained with expansion (1) for systems with screened potentials corresponding to $\mu=0$, 0.1, and 0.3. The Γ behavior for expansion (2) is qualitatively equivalent. In Fig. 2 we show ΔE in rydbergs for the two expansions and for three different values of the screening parameter $\mu=0$, 0.3, and 1.0. It is found that for all the μ values, expansion (2) with $4(N+1)^2$ terms is energetically more stable than expansion (1) with $2(N+1)^2$ terms, as expected. The Fig. 2 also shows that for both expansions, the energy gain obtained is greater for the long-range interactions, i.e., for small screening parameters.

TABLE I. Γ and r_s values for the melting point of the Wigner crystal, obtained for expansion (1) with $\mu=0$, 0.1, and 0.3; μ in units of $2k_f$.

μ	r_s	Γ
0	31.5	13.02
0.1	32.3	9.28
0.3	37.3	5.85

The anisotropy of the systems here analyzed is manifested in the resulting particle density variation. The density is homogeneous along the Z axis for every r_s, but along the X or Y axes, the particles are localized after the melting point. This localization is more pronounced for greater values of r_s. This behavior is qualitatively equivalent for every μ and for both expansions. In Fig. 3 we show the particle localization for expansion (1) in the XY plane, in Fig. 3(a) at $r_s=60$ and in Fig. 3(b) at $r_s=100$.

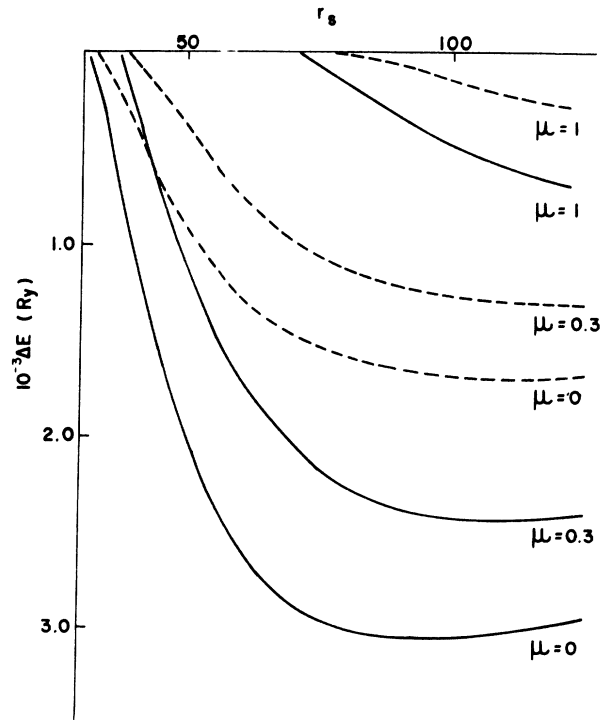

FIG. 2. Energy gain ΔE per particle for the screening parameter $\mu=0$, 0.3, and 1. The continuous curves correspond to expansion (2) and the dashed curves to expansion (1). In both cases the upper limit in the expansions is $N=6$, and μ is in units of $2k_f$.

A very important result for the electronic density of states near the Fermi level is obtained. The pathological logarithmic zero found for the density of states with a Coulombic potential in HF calculations and PW solutions make this approach inadequate to evaluate transport properties or any other properties that are sensitive to the number of states at the Fermi level.

It is known that for Coulombic systems in the HF approach this divergence cannot be removed by means of a state function different from the PW one, but it can be removed by means of a screened interaction because the logarithmic form of the density of states is a signature of the long-range interaction. Thus with the state functions here proposed and $\mu=0$, the divergence in k_f remains; nevertheless, the density of states goes to zero more slowly than with the PW solution.[24] For any other values of the screening parameter as small as 10^{-9} the logarithmic divergence at $k=k_f$ is removed because the μ dependence of the density of states appears in terms of the form $\ln[\mu^2/(1+\mu^2)]$.

In order to show this logarithmic behavior we follow the approximations suggested by Harrison in Ref. 25 for the calculation of $k^2/|\nabla E_k|$. The curvature of the functions obtained for small μ values is similar to the corresponding $\mu=0$ curve, but as μ increases the curvature changes slowly, up to a μ value of about 0.03. Starting with this value of the screening parameter, the slope of the curve and consequently the behavior of the density of states change drastically. The curves corresponding to expansions (1) and (2), for $\mu=0.01$, and 0.03 at $r_s=35$, are shown in Fig. 4.

The behavior for $\mu=0.03$ or greater is the same as reported in the literature when the local-spin-density approximation[23] (LSDA) is used, because in this approximation the electron gas is subjected to an effective screening of the interparticle interaction.

For $\mu \leq 0.03$ our results are qualitatively equivalent to

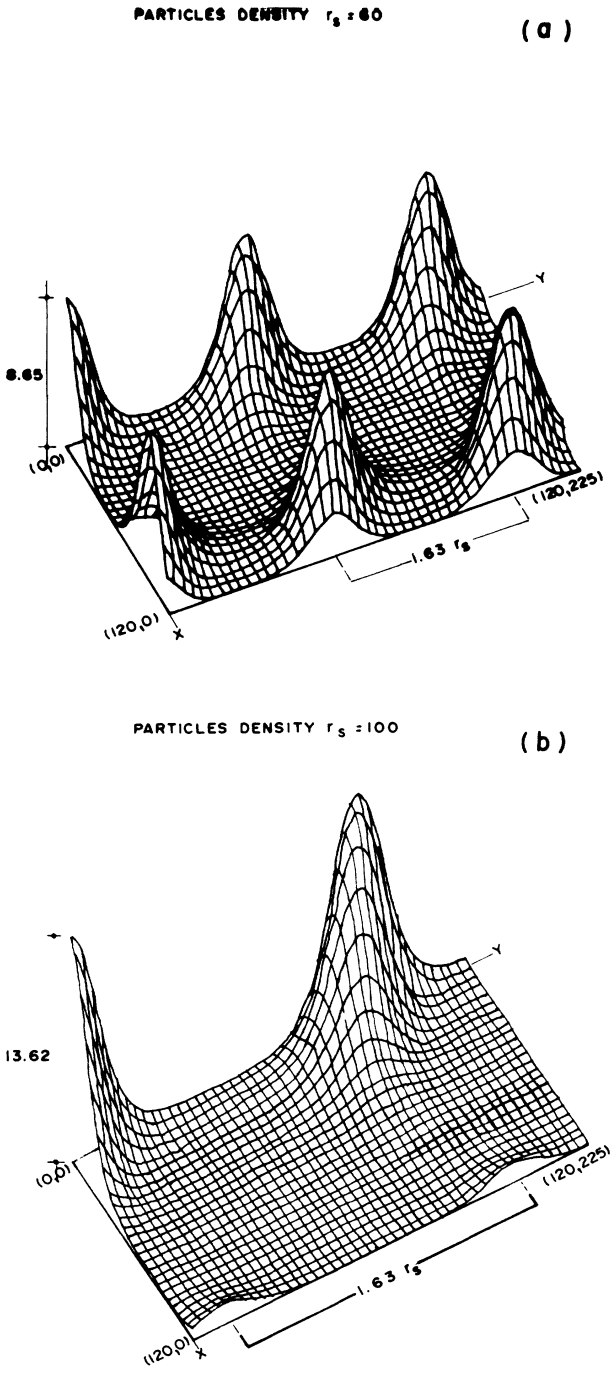

FIG. 3. Particles localization in the XY plane for expansion (1), (a) at $r_s=60$, and (b) at $r_s=100$.

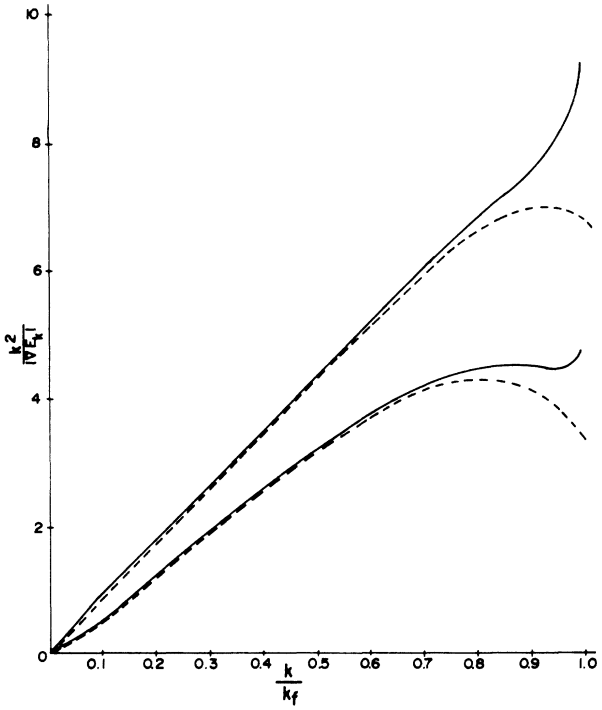

FIG. 4. Qualitative behavior of the density of states for $r_s=35$ corresponding to the state functions (1) and (2). The lower curves show the results with expansion (1) and the upper ones with expansion (2). The continuous curves correspond to $\mu=0.03$ and the dashed curves to 0.01; μ is in units of $2k_f$.

the one obtained with the orbital self-interaction correction (SIC) to the LSDA because it has a reduction of the effective screening that is introduced in the LSDA.

In summary, we obtained some ground-state properties of a strongly coupling QEOCP with planar symmetry. The localization of the particles shows the characteristic symmetry of the system. The more stable state function corresponds to expansion (2). The best results, for both expansions, are obtained for those systems described by means of a screening Coulombic potential, but with μ near zero.

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