Fermion gas with screened interactions

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(Received 12 March 1987)

We consider an interacting fermion system in jellium. The particle-particle interaction is taken as a screened Coulombic one. The behavior of the ground-state energy per particle as a function of the screening and the interparticle distance r_s is obtained. The density of states at the Fermi level as a function of the Wigner-Seitz distance and the screening parameter is calculated. In all the cases considered in this work, the localization of the particles in the system is obtained in a natural way in the low-density region, in agreement with Wigner's prediction. Our results, obtained using as state function an expansion of periodic functions, are compared to the usual plane waves and to similar calculations with the same potential.

I. INTRODUCTION

Calculations for fermion systems in which the particle-particle interaction is a screened Coulomb potential appear often in the literature. Sometimes this type of interaction is considered as a powerful way of accounting for some correlation effects in the fermion gas.[1] Physically the effective interaction between electrons in a plasma (quantum or classical) is not a particularly long-range one; for this reason screened potentials that cut out the long-range interactions have been extensively used.[2,3] In a quantum plasma the effective interaction between a pair of electrons will be screened as a result of the polarization cloud which surrounds any electron.[2] In two-dimensional electron layers, calculations with screened potentials have been extensively done.[4] In connection with an evaluation of the nuclear reaction rate in a compressed star, screened potentials have also been used.[5,6]

Jellium is a relevant model for the study of many-body systems such as metals[2] or stellar matter.[7] There are many calculations that use this model, such as variational calculations,[8] the plane-wave Hartree-Fock (HF) method,[9] density-functional calculations,[10,11] and numerical methods such as Monte Carlo simulations,[12,13] in order to get ground-state energies or other properties of the system.

Despite its simplicity, the HF approximation has been successfully used to evaluate one-particle properties of many-body systems.[3,7] It is also useful as a starting point to more complex approximations.[3] However, in the calculation of the HF energy of the electron gas with a plane-wave solution (PW) there is an alarming feature occurring in the derivative $\partial E/\partial k$ at the Fermi level: it becomes logarithmically infinite.[14] It must be remarked that this singularity is also obtained with other nontrivial solutions for the state function when the Coulomb potential is used.[15] This behavior can be traced back to the long-range nature of the Coulomb potential because it does not occur for other short-ranged potentials like the Yukawa interaction. For these potentials, the elimination of the divergence allows the description of transport properties of the system.

In this work we consider a fermion system in jellium, interacting via screened Coulombic interactions of Yukawa type, with the purpose to cut the long range of the interaction. As a particular case the Coulomb potential is considered. In order to obtain an adequate description of the behavior of the system at all densities, the trial state function is taken as an expansion of periodic functions; as is well known,[16] in the low-density region, periodic solutions (charge-density waves) are found to be better than PW's. The state functions in this work have periodicity in one, two, or three orthogonal directions, potentially describing in this way some systems with different symmetries. The state function was also selected so that it gives the same value for the total momentum at any density.

In this work a HF calculation is done for the ground-state energy, and the coefficients in the expansion of the wave function are self-consistently determined. The behavior of the ground-state energy is obtained as a function of the screening μ and the density parameter r_s. In agreement with the Wigner prediction,[17] we get localization for the particles in all these systems starting with some critical values of the parameter r_s. The dependence of this critical value on the type of system is displayed. Our results are compared with others that use different state functions. In order to see the effect of the screening in the elimination of the divergence in $\partial E/\partial k$ at the Fermi level, we evaluate the density of states at $k=k_F$.

II. THEORY

The Hamiltonian of a fermion gas in jellium has a kinetic energy term for the fermions and fermion-fermion, fermion-background, and background-background potential-energy terms.[7] All these interaction terms are supposed to have the same functional form. According to a theorem for the jellium model,[18] the background terms cancel with the direct term of the fermions, so we only have the kinetic energy and the exchange term.

We select as single-particle state function an expansion

in terms of periodic functions of the form

$$\phi_{\mathbf{k},\lambda}(\mathbf{r})=\chi_\lambda \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{V}} \sum_{n_x=-N}^{N} \sum_{n_y=-N}^{N} \sum_{n_z=-N}^{N} C_{n_x n_y n_z} e^{iq_0 \mathbf{n}\cdot\mathbf{r}}, \tag{1}$$

with $\mathbf{n}=\hat{\mathbf{i}}n_x+\hat{\mathbf{j}}n_y+\hat{\mathbf{k}}n_z$, χ_λ is the spin function, and q_0 is a parameter to be determined. As interaction potential we propose a screened Coulombic, Yukawa-type potential $V(r_{ij})=e^2\exp(-\mu r_{ij})/r_{ij}$, where $r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|$.

The selected state function guarantees the periodic character in three independent directions. As a particular case, we can describe systems which present periodic behavior in one or two directions.[19] With this kind of expansion the total momentum is always zero at all densities.

In order to get the coefficients in the expansion (1), the HF equations must be solved self-consistently, i.e.,

$$\sum_{\mathbf{n}_3} \left[\langle \mathbf{n}_1\mathbf{k}_1 | \hat{T} | \mathbf{n}_3\mathbf{k}_1 \rangle - \sum_{\mathbf{n}_2} \sum_{\mathbf{n}_4} \langle \mathbf{n}_1\mathbf{k}_1, \mathbf{n}_2\mathbf{k}_2 | \hat{V} | \mathbf{n}_4\mathbf{k}_2, \mathbf{n}_3\mathbf{k}_1 \rangle C^*_{\mathbf{n}_2} C^*_{\mathbf{n}_4} \right] C_{\mathbf{n}_3} = \varepsilon_{\mathbf{n}_1} C_{\mathbf{n}_1}, \tag{2}$$

where $C_{\mathbf{n}}$ is used instead of C_{n_x,n_y,n_z} and $\sum_{\mathbf{n}}$ replaces $\sum_{n_x}\sum_{n_y}\sum_{n_z}$, with all the sums run from $-N$ up to N. Once we have determined the state function, the ground-state energy per particle of the system is evaluated.

On the other hand, the derivative of the one-particle energy spectrum at the Fermi level does not diverge when a Yukawa-type interaction is used. Then the density of states $N(k)$ at the Fermi level is nonzero. In atomic units the derivative of $E(k)$ is

$$\begin{aligned}
\left.\frac{\partial E(k)}{\partial k}\right|_{k=k_F} &= \frac{3.84}{r_s} \sum_{\mathbf{n}_1} |C_{\mathbf{n}_1}|^2 (1-2n_1 d_{n_1}) \\
&\quad - \frac{1}{\pi} \sum_{\substack{\mathbf{n}_1,\mathbf{n}_2,\\ \mathbf{n}_3,\mathbf{n}_4}}^{(\mathbf{n}_1\neq\mathbf{n}_4)} C^*_{\mathbf{n}_1} C^*_{\mathbf{n}_2} C_{\mathbf{n}_3} C_{\mathbf{n}_4} \delta_{\mathbf{n}_1+\mathbf{n}_2,\mathbf{n}_3+\mathbf{n}_4} \\
&\quad \times \left[\frac{(1+2N_{14}d_N)(2+\mu^2+4N_{14}^2+4N_{14}d_N)}{2(1+4N_{14}^2+4N_{14}d_N)^{3/2}} \ln \left| \frac{[1+(1+4N_{14}^2+4N_{14}d_N)^{1/2}]^2+\mu^2}{[1-(1+4N_{14}^2+4N_{14}d_N)^{1/2}]^2+\mu^2} \right| \right. \\
&\quad \left. + \frac{2(1+2N_{14}d_N)}{1+4N_{14}^2+4N_{14}d_N} \frac{(4N_{14}^2+4N_{14}d_N+\mu^2)^2+4\mu^2(1+4N_{14}^2+4N_{14}d_N)}{(2+4N_{14}^2+4N_{14}d_N+\mu^2)^2-4(1+4N_{14}^2+4N_{14}d_N)} \right] \\
&\quad - \frac{1}{\pi} \sum_{\mathbf{n}_1,\mathbf{n}_2} |C_{\mathbf{n}_1}|^2 |C_{\mathbf{n}_2}|^2 \left[2+\frac{2+\mu^2}{2} \ln \left| \frac{4+\mu^2}{\mu^2} \right| \right],
\end{aligned} \tag{3}$$

where $\mathbf{N}_{14}=\mathbf{n}_1-\mathbf{n}_4=N_{14}\hat{\mathbf{e}}_n$ and $d_n=\hat{\mathbf{e}}_k\cdot\hat{\mathbf{e}}_n$. This equation, as claimed before, does not diverge as in the Coulomb case, even the terms with $\mathbf{N}=\mathbf{0}$, i.e., $\mathbf{n}_1=\mathbf{n}_4$. In fact if the screening is turned off, the last term in Eq. (3) diverges.

III. RESULTS AND DISCUSSION

We now show the results for the ground-state energy per particle as a function of the density. The value of the parameter q_0 in Eq. (1) must be $q_0 \geq 2k_F$ in order to satisfy the HF equations. The q_0 value we use is $2k_F$ since it corresponds to the best energy. We have done calculations using different values of the screening parameter, including the Coulomb case.

The results are obtained for systems with different symmetries. Localization of the particles along three directions is obtained when n_x, n_y, and n_z run from $-N$ up to N. In two directions, localization is obtained when one of the sum indexes is equal to zero and the other two run from $-N$ up to N. Finally, localization in only one direction is obtained when two of the indexes are zero. Because of the symmetrical character of the sum indexes (from $-N$ up to N), we have total momentum equal to zero at any density, even when the HF solution changes from a PW to a periodic function.

In the figures the results for the ground-state energy are shown. We draw the difference in energy ΔE, obtained with the energy per particle using the state function (1) minus the PW energy per particle. In all the cases considered here the self-consistent solution becomes a PW in the high-density region. Starting with a transition r_s value (about 32 or greater), the state function becomes a periodic one, and the system density changes from homogeneous to periodic. This result is consistent with Wigner's prediction.

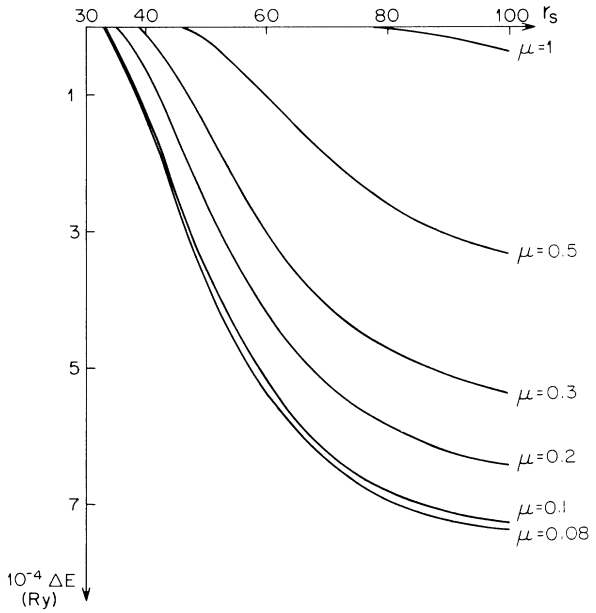

FIG. 1. Energy difference per particle between the function in Eq. (1) with corrugation along one axis and the plane wave as a function of r_s (in units of the Bohr radius). The results for different values of μ are shown.

In Fig. 1 the results for state function (1) with an expansion in which the electron localization is along one axis are shown. In the expansion considered here N is equal to 5, i.e., the state function has 11 terms. With this expansion the convergence for the energy is good because the difference from the results for $N=6$ is less than 10^{-6}.

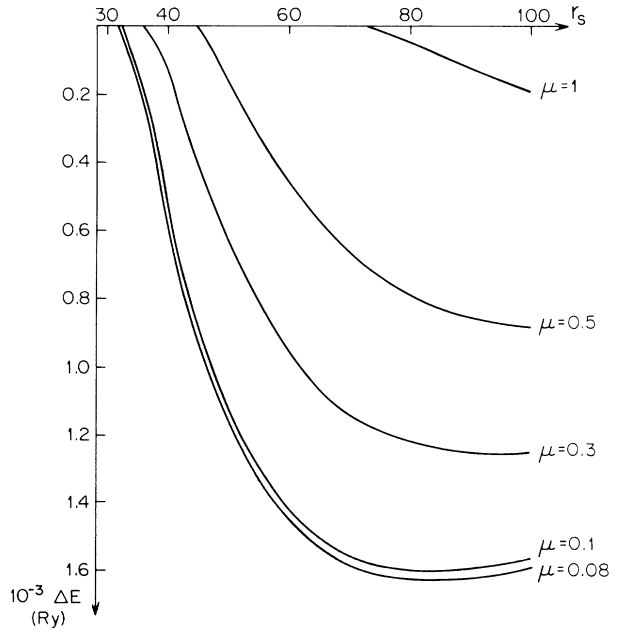

FIG. 2. Energy difference per particle between the function in Eq. (1) with corrugation along two orthogonal axes and the plane wave as a function of r_s. The results for different values of μ are shown.

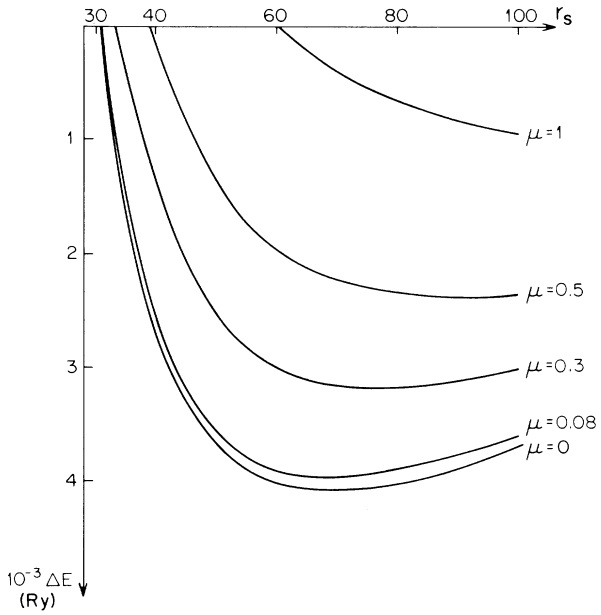

FIG. 3. Energy difference per particle between the function in Eq. (1) with the three sum indexes running from -1 up to 1 and the plane wave as a function of r_s. The results for different values of μ, including $\mu=0$, are shown.

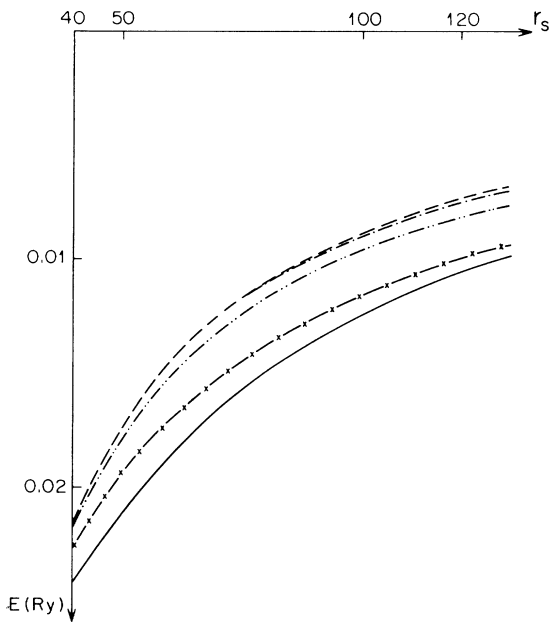

FIG. 4. Energy per particle obtained with different state functions in terms of the variable r_s. The results are shown in the Coulomb case $\mu=0$. The dashed curve is the energy for the plane wave, the dot-dashed curve shows the results for the function in Ref. 20. The double dot-dashed curve shows the results for the function in Eq. (1) with corrugation along one axis. The cross-dashed curve is the energy for the function in Eq. (1) with corrugation along two orthogonal directions. The continuous curve corresponds to the function in Eq. (1) with corrugation along three orthogonal directions.

The energies for different values of the screening parameter are compared. When r_s is small $\Delta E=0$ because the PW is the self-consistent solution, and $\Delta E\neq 0$ at small densities since the self-consistent solution becomes periodic. The r_s transition value increases with the screening parameter. It is equal to 32 in the Coulomb case, but when $\mu=1$ (in units of $2k_F$) it is equal to 77.

The results for an expansion of the state function in which the electron localization is along two independent directions are shown in Fig. 2. Good convergence for the energy is obtained for values of $N\geq 2$, having 25 terms in the expansion in Eq. (1). The results displayed in Fig. 2 are similar to those of Fig. 1. However, the ground-state energy obtained is lower when the system has periodicity along two independent directions. In the Coulomb case it is seen that the transition from PW to periodic function is also at $r_s=32$. But for other values of μ, the transition happens at smaller r_s values than those for the same μ in Fig. 1. The results for the case in which the localization is along three independent directions are shown in Fig. 3. Good convergence for the energy is obtained in this case since $N=1$, i.e., with an expansion of the wave function with 27 terms. The ground-state energy is lower than in the two cases shown before. Again the transition from PW to periodic function is at $r_s=32$ for the Coulomb potential. When $\mu\neq 0$ the transition happens at smaller r_s values than with the other two symmetries for the same μ.

As can be seen from Figs. 1–3, the lowest ground-state energy is obtained for the Coulomb potential. On the other hand, the lowest ground-state energy at any value of μ is obtained with the state function that gives localization along three directions. In fact, calculations were done using the expansion in Fig. 1 with $N=13$, i.e., a state function with 27 terms, and the results are the same as those in Fig. 1 for a function with 11 terms ($N=5$). Then the energy not only depends on the number of terms of the state function, but on the symmetry of the system.

Finally, in Fig. 4 we compare the results for the energy per particle, using three kinds of expansion for the state function, with the results from Ref. 20. As claimed before the lowest energy is obtained using an expansion in the three indexes, and the differences between PW energy and these results are 1 order of magnitude greater than the difference between PW energy and the results from Ref. 20.

We have some final remarks. It has been shown that the transition from PW to periodic function, in the Coulomb case, happens at $r_s=32$ for the three types of state function. When we use a potential with $\mu=0$, the transition occurs at smaller values of the density. However, in these cases it is seen that the transition depends also on the kind of expansion used, as follows from Figs. 1–3.

For all the expansions of the state function considered in this work, the system presents total momentum conservation because the transition is from PW to a function in which $C_{\mathbf{n}}=C_{-\mathbf{n}}$ for all $\mathbf{n}$. This transition, observed in all the cases considered, occurs in a natural way in our calculations at low densities. This is in agreement with the Wigner hypothesis of localization of the particles. With the state functions proposed in this work it is possible to describe systems with different symmetries. The method presented in this work gives a systematic way to do self-consistent calculations which give better results for the ground-state energy than other previous HF calculations.

ACKNOWLEDGMENT

The authors acknowledge the valuable comments of Dr. M. Moreno.

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