Density of states for a fermion gas in the deformable jellium model

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ABSTRACT. The density of states for a fermion gas in the deformable jellium model is evaluated. A screened Coulombic potential is used. The state function is proposed as a cosine series which presents periodic charge density along one axis. Calculations in terms of the polar angle are done in order to find the departure of the density of states from the spherical approximation.

RESUMEN. Se presenta un cálculo de la densidad de estados para el gas de fermiones en el modelo de jalea deformable. Como interacción entre pares de partículas se utiliza un potencial coulombiano apantallado. Como función de estado se propone un desarrollo en términos de cosenos, el cual presenta densidad de carga periódica a lo largo de un eje. Los cálculos se efectúan como función del ángulo polar, con el objeto de determinar la desviación de la densidad de estados de la aproximación esférica.

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1. INTRODUCTION

The deformable jellium model, as was introduced by Overhauser [1] has been successfully used to describe properties of many particle systems as the fermion gas [2]. In the deformable jellium, the particles are immersed in a deformable neutralizing background, in order to get local charge neutrality. This model has been applied, for instance, to evaluate ground state properties of the electron gas [3]. It is worthwhile to mention that particle localization was observed for fermion gases, in particular for the electron gas, at low densities according to the Wigner hypothesis [4].
Using trial state functions with different symmetries, the Hartree-Fock (HF) approximation has been successfully used within the deformable jellium in order to describe three dimensional (3D) systems which present linear, planar or cubic symmetries [5,6,3].

Recently the HF approximation together with the 3D electron gas model have been used in the description of the new high $T_c$ superconductor cuprates [7]. They use plane wave solutions and suppose generalized Fermi surface topologies instead of the normal Fermi surface.

Our purpose in this work is to use the method outlined above (HF and deformable jellium) in order to evaluate the density of states (DOS) for a system of fermions which presents periodic charge density along one direction. Calculations are done in terms of the polar angle in order to see the departure of the density of states from the spherical approximation. We use a screened Coulombic potential as pair interaction in order to remove the divergence in the density of states at the Fermi level. As it is well known this divergence appears from the use of the Coulomb interactions in the HF approximation. The single particle state function proposed is an expansion in terms of cosine functions. This expansion is given in such a way that it guarantees the possibility for periodic non-homogeneous density along one axis. The results for the DOS obtained in this work are compared to recently reported calculations which use the spherical approximation [8].

2. The model

The Hamiltonian for a 3D fermion gas in the jellium model has the form

$$H = T + V_{f,f} + V_{f,b} + V_{b,b},$$

where $T$ is the kinetic energy of the fermions, $V_{f,f}$ is the fermion-fermion interaction, $V_{f,b}$ is the fermion-background interaction and $V_{b,b}$ is the interaction of the background with itself.

The deformable jellium in the single-particle approximation is defined in such a way that [9]

$$\langle V_d \rangle + \langle V_{f,b} \rangle + \langle V_{b,b} \rangle = 0,$$

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

Despite its simplicity, the HF approximation has been successfully used to describe one-particle properties of many-body systems [10]. However, in the calculation of the HF energy of the electron gas there is an alarming feature occurring in the derivative $\partial E/\partial k$ at the Fermi level: it becomes logarithmically infinite. This behavior can be traced back to the long-range nature of the Coulomb potential since it does not occur for other short-ranged potentials like the Yukawa interaction. Therefore we propose for the particle-particle interaction a screened Coulomb potential given by

$$V(r_{ij}) = \frac{e^{-\mu r_{ij}}}{r_{ij}},$$

where $\mu$ is the screening parameter.
For the orbital part of the state function it is proposed the product of the plane wave multiplied by an expansion in terms of cosine functions of the form

$$\psi_k(r) = \frac{e^{i k \cdot r}}{\sqrt{V}} \sum_{n=0}^{N} C_n \cos(q_0 n \cdot r).$$  \hspace{1cm} (4)

In this equation $n = n_k$ and $V$ is the volume in which normalization conditions are imposed. The $C_n$ coefficients are self-consistently determined by means of the HF equations where the orthonormality condition of the spin-orbitals is included. These coefficients were determined with an approximation of $10^{-6}$ with respect to the last iteration. The value of the parameter $q_0$ must be $q_0 \geq 2k_F$ in order to satisfy the HF equation [11]. From energy calculations it is found that $q_0 = 2k_F$ gives the best energy per particle using the state function proposed by Eq. (4) [12]. The value of $N = 6$ gives the minimum number of terms $(N + 1)$, at which we get convergence in the ground state energy of the system at all densities, given by the Wigner-Seitz parameter [13]. The densities at which particle localization is obtained with this state function, for the different potentials, were obtained in Ref. [12].

The one particle energy spectra $E(k)$ for the ground and the first excited states have been reported in a previous work [14].

The density of states is given by

$$D(E) = \frac{4}{3\pi^3} \int \frac{dS}{|\nabla_k E(k)|},$$  \hspace{1cm} (5)

with $\nabla_k E(k)$ in spherical coordinates and the integration is calculated over the surface of constant energy $E$. In general the constant energy surfaces do not have spherical symmetry.

3. Results and Discussion

The behavior of the density of states will be studied in terms of the variation of three parameters. These are the interparticle distance $r_s$, in Bohr ratios, the screening parameter $\mu$, in units of $2k_F$ and the wave-number $k$, in units of $k_F$. Where $k_F$ is the Fermi wave number.

At high densities in the fermion gas, i.e. small values of the interparticle distance, the self-consistent solutions of the HF equations are the plane-waves. In that region the surfaces of constant energy are spheres in the $k$-space and the size of $|\nabla_k E(k)|$ is a constant. For larger values of $r_s$, where the self-consistent solutions given by Eq. (4) are charge density waves, we expect a deformation of the spherical surface in the corrugation direction. Therefore, the calculation of the DOS could be difficult. As a first approximation the departure of the spherical form is supposed small and we evaluate the integral over a spherical surface.
FIGURE 1. The $\nabla_k E(k)$ in terms of its components in the $k_z-k_x$ plane for different values of $r_s$ at the Fermi level.

FIGURE 2. The density of states as function of $k$ for different values of the screening parameter at $r_s = 60$.

Following the spherical approximation suggested by Harrison [8], the DOS was obtained for a system with planar symmetry [6]. In that case the logarithmic behavior of this function was obtained.

In Fig. 1 the components of the $\nabla_k E(k)$ are drawn in the $k_z-k_x$ plane, $\theta$ is the polar angle and $z$ is the direction in which periodic particle density can be obtained. In Fig. 1 the curves are shown for different values of $r_s$ at the Fermi level, i.e. at $k = 1$. We observe that the $|\nabla_k E(k)|$ is minimum for $\theta = \pi/2$ (the $k_z-k_y$ plane), and it is a maximum along the $k_z$ direction.

In Fig. 2 the behavior of the DOS as function of $k$ is shown for different values of the screening parameter at $r_s = 60$. As can be seen from Fig. 2, the pathological logarithmic
zero found for the Coulomb potential is removed. The curvature of the functions obtained for small values of $\mu$, is similar to the curvature of the $\mu = 0$ curve. The behavior of the curves for $\mu = 0.03$ or greater changes drastically.

In Fig. 3 the behavior of the DOS as function of $k$ is shown for different values of $r_s$ for a potential with $\mu = 0.01$.

As can be seen from the figures, our results for values of $\mu > 0.03$, are similar to those with the local spin-density approximation (LSDA) [8]. For smaller values of $\mu$, our results qualitatively correspond to those obtained in Ref. [8] with the orbital self-interaction correction (SIC) to the LSDA. This method is related to a reduction of the effective screening introduced by the LSDA. We can conclude that despite its simplicity, the spherical approximation is good for values of $r_s$, near the transition point to localized solutions, i.e. $r_s \leq 60$.

We could have used more elaborate state functions which give periodic density along two or three perpendicular axes. The state function used however, guarantees the possibility for periodic non-homogeneous density along one axis. This is the more simple function of this type. Nonetheless its simplicity, the results for the DOS obtained with this expansion are qualitatively similar to the results which we would expect from more complicate symmetries. The same behavior has been observed in the evaluation of other properties for the 3D fermion system as ground state energy, particle localization, and one particle energy spectrum.

The method outlined in this work can be generalized for 3D and two dimensional fermion systems with periodic solutions and generalized Fermi surfaces instead of the normal occupancy. This generalization can be useful in order to describe some high $T_c$ superconductor cuprates.

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