Energy of a Fully Spin-Polarized Two-Dimensional Electron Gas Separated from its Jellium Neutralizing Background

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We study a two-dimensional electron gas in which the electrons are separated from the corresponding jellium neturalizing background. For simplicity, we assume that the electrons are fully spin-polarized meaning that they are treated as spinless particles. The current setup implies that the overall energy of the system will depend on both density and separation distance of the electrons from the neutralizing background. The subtle interplay of these two parameters determines the stability of the system. Analytical results for the energy are obtained in the thermodynamic limit by using the Hartree–Fock approach. It is found that, within the framework of this approximation, the effect of separation manifests as an effective increase of kinetic energy.

***Index Terms*—Electron gas, Energy, Jellium, Separation distance.**

I. Introduction

EXPERIMENTAL ADVANCES have led to the creation of many low-dimensional structures under laboratory conditions. This includes two-dimensional electron gas (2DEG) systems which may be fabricated by means of various techniques [1], [2]. A 2DEG system is routinely studied by assuming that the electrons are immersed in a two-dimensional (2D) jellium neutralizing positive background so that overall charge neutrality is imposed. This means that the 2D system of electrons is in the same space layer as the 2D jellium background. It is assumed that the electrons interact via a standard Coulomb pair interaction among themselves and with the background. Many studies of this model have shown that the 2D system of electrons crystallizes in a Wigner solid state at low density, but is a liquid state at high density [3]–[5]. Studies where the interaction potential is different from a Coulomb potential are rare [6]. The simplest treatment of a 2DEG system involves use of an anti-symmetrized Slater determinant wave function [7] which stands at the core of the Hartree-Fock (HF) approximation [8]. This treatment allows one to obtain the total energy of the system as a sum of two competing terms. One being the positive kinetic energy and the other one the negative potential (exchange) energy. The correlation energy is not included in the HF treatment.

In this work, we revisit this model by modifying a crucial part of it. We assume that the 2D system of electrons is parallel and spatially separated from the 2D jellium background layer by a given arbitrary distance. This modification affects the way the electrons interact with the neutralizing background and, thus, it impacts the overall energy stability of the system. For simplicity, we consider the system of electrons to be fully spin-polarized which means that we are treating the electrons as being spinless particles. The (effective) mass of electrons is considered constant and isotropic. For this scenario, one expects that the total energy of the system in the thermodynamic limit will depend on two parameters: (i) the average interparticle distance and (ii) the separation distance between the 2D system of electrons and the 2D jellium background. The subtle interplay of these two parameters determines the overall stability of the system. The key purpose of this study is to calculate the resulting energy in the thermodynamic limit in order to shed more light on how space separation affects the properties of the system.

II. Model and Results

We start with a 2D system of N electrons in which the electrons are separated by an arbitrary distance, d from the neutralizing 2D neutralizing jellium background with area, A. In the thermodynamic limit, both N and A go to infinity. However, their ratio $\rho_0 = N/A$ which represents the electron number density remains constant. One can write:

$$\rho_0 = \frac{N}{A} = \frac{1}{\pi\,(r_s\,a_B)^2} \ , \tag{1}$$

where r_s is the dimensionless Wigner-Seitz parameter and a_B is the Bohr radius. The Hamiltonian of the system reads:

$$\hat{H} = \hat{T} + \hat{V} \ , \tag{2}$$

where

$$\hat{T} = \sum_{i=1}^{N} \frac{|\hat{\vec{p}}_i|^2}{2\,m} \ , \tag{3}$$

is the kinetic energy operator and

$$\hat{V} = \hat{V}_{ee} + \hat{V}_{eb} + \hat{V}_{bb} \ , \tag{4}$$

is the potential energy operator. The kinetic energy operator is the sum of the individual kinetic energies where $\hat{\vec{p}}_i$ is the linear momentum quantum operator and m is the mass of the electrons. The potential operator consists of the sum of electron-electron (ee), electron-background (eb) and background-background (bb) interaction potential energy terms. One has:

$$\hat{V}_{ee} = \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N} v(|\vec{r}_i - \vec{r}_j|) \ , \tag{5}$$

where

$$v(|\vec{r}_i - \vec{r}_j|) = \frac{k_e\,e^2}{|\vec{r}_i - \vec{r}_j|} \ , \tag{6}$$

is the Coulomb interaction potential between two electrons with charge $-e$ ($e > 0$) localized at 2D vector positions $\vec{r}_i$ (and $\vec{r}_j$) and k_e is Coulomb's electric constant. One sees that:

$$\hat{V}_{eb} = -\rho_0 \sum_{i=1}^{N} \int_A d^2r' \, v_d(|\vec{r}_i - \vec{r}\,'|) \ , \tag{7}$$

where

$$v_d(|\vec{r}_i - \vec{r}\,'|) = \frac{k_e \, e^2}{\sqrt{|\vec{r}_i - \vec{r}\,'|^2 + d^2}} \ , \tag{8}$$

with $d \geq 0$ being the separation distance between the layer of electrons and the 2D jellium background layer. The energy term originating from the background is a constant written as:

$$\hat{V}_{bb} = \frac{\rho_0^2}{2} \int_A d^2r \int_A d^2r' \ v(|\vec{r} - \vec{r}\,'|) \ , \tag{9}$$

where $\vec{r}$ and $\vec{r}\,'$ are dummy background 2D vector variables. We adopt a HF approach and start with a normalized N-particle antisymmetric wave function of electrons built as a Slater determinant of the ortho-normalized single-particle space-spin orbitals:

$$|\Psi\rangle = \frac{1}{\sqrt{N!}} \, Det \left\{ \phi_{\vec{k}_1}(\vec{r}_1), \ldots, \phi_{\vec{k}_N}(\vec{r}_N) \right\} \ , \tag{10}$$

where the single-particle states are ortho-normalized 2D plane waves, $\phi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{A}} \, e^{i \, \vec{k} \, \vec{r}}$ with periodic boundary conditions being applied. The total energy of the system is:

$$\langle \hat{H} \rangle = \langle \hat{T} \rangle + \langle \hat{V} \rangle \ , \tag{11}$$

where $\langle \hat{O} \rangle$ is the quantum expectation value of operator $\hat{O}$. The energy per particle in the thermodynamic limit is:

$$\epsilon(r_s, d) = \frac{\langle \hat{H} \rangle}{N} \ , \tag{12}$$

where r_s and d are shown as arguments. The energy is expressed in units of Rydbergs (Ry) which is defined as:

$$1 \, Ry = \frac{\hbar^2}{2 \, m \, a_B^2} = \frac{k_e \, e^2}{2 \, a_B} \ , \tag{13}$$

where $a_B = \hbar^2/(m \, k_e \, e^2)$ is the Bohr radius. The quantity, $\epsilon(r_s, d = 0)$ represents the known result [9] for the energy of a fully spin-polarized 2DEG system:

$$\epsilon(r_s, d = 0) = \left(\frac{2}{r_s^2} - \frac{16}{3\,\pi} \frac{1}{r_s} \right) \frac{k_e \, e^2}{2 \, a_B} \ , \tag{14}$$

where the first term represents the kinetic energy per particle while the second term is the (exchange) potential energy per particle. The calculation of $\langle \hat{T} \rangle / N$ is straightforward. The calculation of $\langle \hat{V} \rangle / N$ requires a rather careful consideration of the thermodynamic limit ($N \to \infty$; $A \to \infty$ with $\rho_0 = N/A$ constant). For the sake of brevity we skip the details of the calculation. The final result obtained for the total energy per particle as a function of r_s and d is:

$$\epsilon(r_s, d) = \left[\left(2 + 4 \frac{d}{a_B} \right) \frac{1}{r_s^2} - \frac{16}{3\,\pi} \frac{1}{r_s} \right] \frac{k_e \, e^2}{2 \, a_B} \ . \tag{15}$$

In Fig. 1 we show the dependence of $\epsilon(r_s, d)$ as a function of r_s for values of $d/a_B = 0, 0.3$ and 0.6. The most important observation is that the effect of space separation between the 2D system of electrons and the 2D neutralizing layer manifests exactly as a positive effective kinetic energy $\propto 1/r_s^2$ modified by a proportionality factor that dependes on d/a_B. The minimum of energy is obtained for values of r_s that grow larger (density becomes smaller) as d/a_B increases meaning that the Wigner solid-liquid transition is very much affected by the variation of the separation distance.

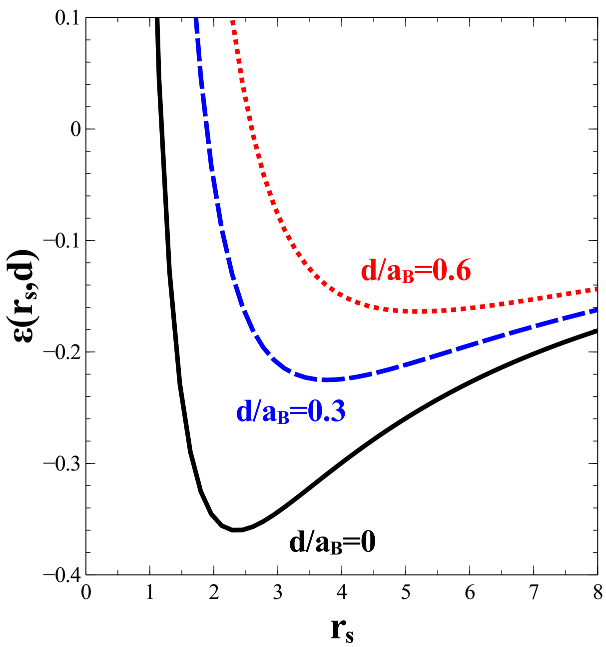

Fig. 1. Energy per particle, $\epsilon(r_s, d)$ as a function of r_s for separation distance parameters, $d/a_B = 0$, 0.3 and 0.6 for a fully spin-polarized 2DEG system in which the 2D system of electrons has a separation distance, d from the 2D neutralizing layer. The energy per particle is given in units of $k_e \, e^2/(2 \, a_B)$.

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