

A two-dimensional electron gas suspended above a neutralizing background

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(Dated: April 5, 2021)

We consider a two-dimensional electron gas system consisting of a layer of electrons suspended above its jellium neutralizing background counterpart. We investigate the energy of the system in the Hartree-Fock approximation as a function of separation distance between the layer of electrons and the background. We find that the energy of the system is influenced by the separation distance in such a way that the new energy contribution originating from such a separation behaves as an effective kinetic energy term. The increase of the overall energy with increase of the separation distance adversely affects the stability of electron liquid states at high density. The results are derived for a fully spin-polarized (spinless) system of electrons but can easily be generalized to a spin unpolarized state.

PACS numbers: 73.43.Cd, 73.20.Dx, 73.21.La.

Keywords: Two-dimensional electron gas, Quantum Hall effects, Jellium model.

I. INTRODUCTION

Experimental progress in fabrication techniques has stimulated a renewed interest to study the properties of two-dimensional electron gas (2DEG) systems. The most commonly manufactured 2DEG system is the 2D layer of electrons found in metal-oxide-semiconductor field-effect transistors (MOSFETs) and related systems^{1–4}. The electrons underneath the gate oxide are confined to the semiconductor-oxide interface when the transistor is in inversion mode and, thus, occupy well defined energy levels. The potential well in the direction transverse to the interface is then tuned in such a way that only the lowest energy quantum level is occupied. Under these conditions, the motion of the electrons transverse to the interface is frozen and, hence, the system can be considered essentially two-dimensional (2D). For simplicity, it is assumed from now on, that we are dealing only with 2DEG systems at absolute zero temperature.

Another very common method to fabricate a 2DEG system relies on confining electrons at the interface between two semiconducting materials at a heterojunction^{5–9}. This is the preferred method to fabricate 2DEG systems for quantum Hall studies^{10–16} by confining the electrons to a triangular quantum well that freezes the motion in the direction perpendicular to the interface. Electrons confined to the interface of such heterojunctions (for example, GaAs/AlGaAs) exhibit much higher mobilities than those in MOSFETs. One can also confine electrons to the surface of a material as done decades ago for free electrons on the surface of liquid helium. The new twist of present-day fabrication techniques is that one can now create atomically thin solid 2D materials (the most famous example is graphene) where the electrons are confined to a quasi-ideal 2D space.

The standard model in condensed matter physics used

to study a 2DEG system is that of an electron gas in a jellium neutralizing positive background. In the uniform jellium model, the electrons interact via a Coulomb interaction while immersed in a uniform, positive neutralizing background^{17–19}. It is assumed that the system of electrons is in the same layer as the 2D jellium background. Despite its simplicity, such a model provides a sound theoretical approach to describe the most important properties of the system and has been used to study a 2DEG under various approximations^{20,21}.

This model has been very useful in the understanding of possible quantum phase transitions that occur in a 2DEG system when density is varied from high to low values. The system of electrons is typically in a liquid state at high density, but crystallization to a 2D Wigner solid state occurs at low densities^{22,23}. Note that an infinite 2DEG is uniquely characterized by its electron number density which is a single constant number in the thermodynamic limit²⁴. The precise value of the density at which the transition from a liquid state to a Wigner solid happens is still the object of many current numerical studies^{25–30} given the miniscule differences in energy between these two quantum phases. The simplest treatment of a 2DEG system involves use of an anti-symmetrized Slater determinant wave function³¹ as in the Hartree-Fock (HF) approximation^{32,33}. This approach allows one to obtain an analytical result for the total energy of the system in the form of two competing terms represented by the kinetic and the potential (exchange) energy term. Other energy terms collectively referred to as the correlation energy are ignored^{34–37}.

Minor modifications of any quantum model may have a huge influence on the properties and energy stability of the system. Based on this observation, in this work, we consider the properties of a 2DEG system in which the 2D layer of electrons is parallel and separated by a finite

distance from the plane of the 2D jellium background. Assuming that the (effective) mass of electrons is constant and isotropic, one expects that all the properties of the system in the thermodynamic limit depend on two single parameters, the average interparticle distance and the separation distance between the layer of electrons and 2D jellium background. The key objective of this study is to see how the overall energy of the 2DEG system is affected by the separation distance between the electrons and the 2D jellium background and whether there are any subtle effects originating from this newly added element. The results are derived for a fully spin-polarized (spinless) 2DEG system of electrons. The generalization of the model to a spin unpolarized state is straightforward.

II. MODEL

We consider a 2DEG system of N electrons, namely, a single 2D layer of electrons separated by an arbitrary distance, d from a neutralizing 2D jellium background occupying an area, A . Any theoretical model for a 2DEG assumes overall charge neutrality of the system. The simplest way to ensure that the total system is charge neutral is to place the 2DEG in presence of a uniformly distributed positive background of equal, but opposite charge^{38,39}. The separation distance, d enters as a new parameter in this model in addition to the electron number density that is written as:

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

where r_s is the dimensionless Wigner-Seitz parameter and a_B is the Bohr radius. For an infinite 2DEG system in the thermodynamic limit, ρ_0 is constant as $N \rightarrow \infty$ and $A \rightarrow \infty$. A schematic view of the system under consideration is shown in Fig. 1.

We assume that we are dealing with a fully spin-polarized (spinless) system of electrons described by the Hamiltonian:

$$\hat{H} = \hat{T} + \hat{V}, \quad (2)$$

where

$$\hat{T} = \sum_{i=1}^N \frac{\hat{p}_i^2}{2m}, \quad (3)$$

is the kinetic energy operator and

$$\hat{V} = \hat{V}_{ee} + \hat{V}_{eb} + \hat{V}_{bb}, \quad (4)$$

is the potential energy operator that represents, respectively, the electron-electron (ee), electron-background (eb) and background-background (bb) interaction potential energy operators.

The ee potential energy operator is written as:

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

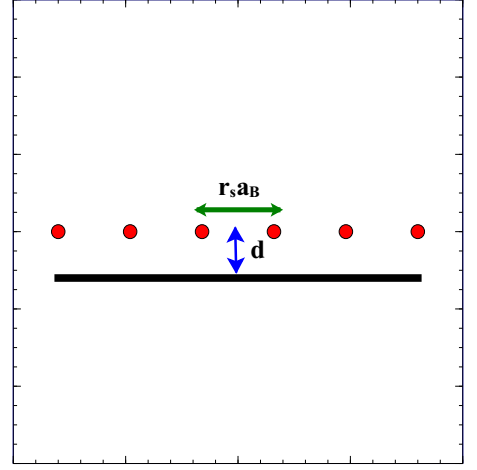


FIG. 1: Schematic view of a 2DEG system (filled circles) separated by a distance d from the neutralizing 2D jellium background layer.

where

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

is the Coulomb interaction potential between two electrons with charge $-e$ ($e > 0$) and k_e is Coulomb's electric constant. Note that $\vec{r}_{i,j}$ are 2D vectors. The eb potential energy operator is written as:

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

where

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

with $d \geq 0$ being the separation distance between the layer of electrons and the 2D jellium background layer. The 2D vector $\vec{r}'$ in Eq.(7) represents the continuous background coordinate while vectors $\vec{r}_i$ are position vectors of electrons. The bb energy term is written as:

$$\begin{aligned} \hat{V}_{bb} &= \frac{\rho_0^2}{2} \int_A d^2 r \int_A d^2 r' v(|\vec{r} - \vec{r}'|) = \\ &= \frac{\rho_0^2}{2} \int_A d^2 r_1 \int_A d^2 r_2 v(|\vec{r}_1 - \vec{r}_2|), \end{aligned} \quad (9)$$

where the background dummy variables, $\vec{r}$ and $\vec{r}'$ have been replaced by $\vec{r}_1$ and $\vec{r}_2$ under the sign of the integral.

A normalized N -particle wave function that is properly antisymmetric and is an eigenstate of the many-particle free Hamiltonian is constructed as a Slater determinant of

the ortho-normalized single-particle space-spin orbitals:

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

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 imposed. In a short-hand notation, $\langle \hat{O} \rangle = \langle \Psi | \hat{O} | \Psi \rangle / \langle \Psi | \Psi \rangle$ represents the quantum expectation value of operator $\hat{O}$ with respect to wave function, $|\Psi\rangle$.

The expectation value of the total kinetic energy operator can be written as:

$$\langle \hat{T} \rangle = \frac{N}{2} \epsilon_F, \quad (11)$$

where $\epsilon_F = \frac{\hbar^2}{2m} k_F^2$ is the Fermi energy and $k_F^2 = 4\pi\rho_0$ for the case of a fully spin-polarized (spinless) 2DEG.

It is a standard calculation to prove that the expectation value of $\hat{V}_{ee}$ can be expressed as:

$$\langle \hat{V}_{ee} \rangle = \frac{1}{2} \int_A d^2r_1 \rho(\vec{r}_1) \int_A d^2r_2 \rho(\vec{r}_2) v(r_{12}) - \frac{1}{2} \int_A d^2r_1 \int_A d^2r_2 |\rho(\vec{r}_1, \vec{r}_2)|^2 v(r_{12}), \quad (12)$$

where $\rho(\vec{r}) = \sum_{j=1}^N |\phi_{\vec{k}_j}(\vec{r})|^2$ is the one-particle density function, $\rho(\vec{r}_1, \vec{r}_2) = \sum_{j=1}^N \phi_{\vec{k}_j}(\vec{r}_1)^* \phi_{\vec{k}_j}(\vec{r}_2)$ is the so-called one-particle density matrix and $r_{ij} = |\vec{r}_i - \vec{r}_j| \geq 0$ is the separation distance between particles i and j .

One can prove that the expectation value of $\hat{V}_{eb}$ can be written as:

$$\langle \hat{V}_{eb} \rangle = -\rho_0 \int_A d^2r_1 \rho(\vec{r}_1) \int_A d^2r_2 v_d(r_{12}), \quad (13)$$

where we substituted the dummy variable $\vec{r}'$ in Eq.(7) by $\vec{r}_2$. Obviously, the expectation value of $\hat{V}_{bb}$ is:

$$\langle \hat{V}_{bb} \rangle = \frac{\rho_0^2}{2} \int_A d^2r_1 \int_A d^2r_2 v(r_{12}). \quad (14)$$

Without any lack of generality, let us rewrite the po-

tential $v_d(r_{12})$ in Eq.(13) as $v(r_{12}) + v_d(r_{12}) - v(r_{12})$ which allows us to express: $\langle \hat{V} \rangle = \langle \hat{V}_{ee} \rangle + \langle \hat{V}_{eb} \rangle + \langle \hat{V}_{bb} \rangle$ as:

$$\begin{aligned} \langle \hat{V} \rangle &= \frac{1}{2} \int_A d^2r_1 \int_A d^2r_2 \left[\rho(\vec{r}_1) - \rho_0 \right] v(r_{12}) \left[\rho(\vec{r}_2) - \rho_0 \right] \\ &\quad - \frac{1}{2} \int_A d^2r_1 \int_A d^2r_2 |\rho(\vec{r}_1, \vec{r}_2)|^2 v(r_{12}) \\ &\quad - \rho_0 \int_A d^2r_1 \rho(\vec{r}_1) \int_A d^2r_2 \left[v_d(r_{12}) - v(r_{12}) \right] \end{aligned} \quad (15)$$

For the present case scenario, we have:

$$\rho(\vec{r}_1) = \rho(\vec{r}_2) = \rho_0. \quad (16)$$

As a result, the quantity in Eq.(15) becomes:

$$\langle \hat{V} \rangle = -\frac{1}{2} \int_A d^2r_1 \int_A d^2r_2 |\rho(\vec{r}_1, \vec{r}_2)|^2 v(r_{12}) - \rho_0^2 \int_A d^2r_1 \int_A d^2r_2 \left[v_d(r_{12}) - v(r_{12}) \right]. \quad (17)$$

The total energy of the system is obtained from:

$$\langle \hat{H} \rangle = \langle \hat{T} \rangle + \langle \hat{V} \rangle. \quad (18)$$

The energy per particle in the thermodynamic limit is calculated from $\epsilon(d) = \langle \hat{H} \rangle / N$ and can be expressed as:

$$\epsilon(d) = \epsilon(d=0) + \Delta\epsilon(d) \quad ; \quad \Delta\epsilon(d) = \frac{\Delta V(d)}{N}, \quad (19)$$

where $\epsilon(d=0)$ corresponds to the standard HF energy per particle (kinetic and exchange) for a fully spin-polarized 2DEG system in the thermodynamic limit with the understanding that the electrons and the background

are on the same 2D plane and

$$\Delta V(d) = \rho_0^2 \int_A d^2r_1 \int_A d^2r_2 \left[v(r_{12}) - v_d(r_{12}) \right], \quad (20)$$

is a new energy term due to the separation distance between the layer of electrons and the neutralizing 2D jellium background. As stated earlier, all the results above apply to a fully spin-polarized (spinless) 2DEG system. Extension of such results to a spin unpolarized state or, in general, to a partially spin-polarized state in which N_α electrons have spin " α " ("up") and N_β electrons have spin " β " ("down") values is straightforward. The

methodology and the main features of the formalism are discussed in the Appendix.

III. RESULTS AND DISCUSSION

It is widespread in the literature to express the energies of a 2DEG system in units of Rydbergs (Ry):

$$1 \text{ Ry} = \frac{\hbar^2}{2m a_B^2} = \frac{k_e e^2}{2a_B}, \quad (21)$$

where $a_B = \hbar^2/(m k_e e^2)$ is the Bohr radius. The density of a 2DEG is typically expressed in terms the Wigner-

Seitz dimensionless parameter, r_s defined in Eq.(1). The expression of $\epsilon(d=0)$ for a fully spin polarized 2DEG is known⁴⁰ and reads:

$$\epsilon(d=0) = \left(\frac{2}{r_s^2} - \frac{16}{3\pi} \frac{1}{r_s} \right) \frac{k_e e^2}{2a_B}, \quad (22)$$

where the first term represents the kinetic energy per particle while the second term is the (exchange) potential energy per particle.

In order to calculate the second energy contribution to the total energy per particle in Eq.(19), let us rewrite the quantity $\Delta V(d)$ in Eq.(20) more explicitly as:

$$\Delta V(d) = k_e e^2 \rho_0^2 \int_A d^2 r_1 \int_A d^2 r_2 \left(\frac{1}{|\vec{r}_1 - \vec{r}_2|} - \frac{1}{\sqrt{|\vec{r}_1 - \vec{r}_2|^2 + d^2}} \right). \quad (23)$$

To obtain correctly the result in the thermodynamic limit ($N \rightarrow \infty$; $A \rightarrow \infty$ but $\rho_0 = N/A$ constant), we initially assume that the surface area is very large (but finite) and has circular disk symmetry, $A = \pi R^2$. It is only at the end of the calculations that we take the explicit limit of $R \rightarrow \infty$ (when necessary). One can facilitate an analytic calculation of the four-dimensional integral in Eq.(23) by using the 2D Fourier transform⁴¹ method:

$$\begin{cases} F(\vec{k}) = \int d^2 r e^{i\vec{k}\vec{r}} f(\vec{r}), \\ f(\vec{r}) = \int \frac{d^2 k}{(2\pi)^2} e^{-i\vec{k}\vec{r}} F(\vec{k}), \end{cases} \quad (24)$$

where $F(\vec{k})$ is the 2D Fourier transform of $f(\vec{r})$, $\vec{k}$ and $\vec{r}$ are 2D vectors, $i = \sqrt{-1}$ is the imaginary unit and the integration extends over all space. It is a simple exercise

to calculate that:

$$\int d^2 r e^{i\vec{k}\vec{r}} \frac{1}{\sqrt{r^2 + d^2}} = \frac{2\pi}{|\vec{k}|} e^{-d|\vec{k}|}. \quad (25)$$

Based on this result, one uses the second expression in Eq.(24) to write:

$$\frac{1}{\sqrt{|\vec{r}_1 - \vec{r}_2|^2 + d^2}} = \int \frac{d^2 k}{(2\pi)^2} e^{-i\vec{k}(\vec{r}_1 - \vec{r}_2)} \frac{2\pi}{|\vec{k}|} e^{-d|\vec{k}|}. \quad (26)$$

Note that the result in Eq.(26) is also valid for $d=0$. After substituting the expression from Eq.(26) (for $d \neq 0$ and $d=0$) into Eq.(23) and rearranging the dependencies we obtain:

$$\Delta V(d) = k_e e^2 \rho_0^2 \int \frac{d^2 k}{(2\pi)^2} \frac{2\pi}{|\vec{k}|} \left(1 - e^{-d|\vec{k}|} \right) \int_{A=\pi R^2} d^2 r_1 e^{-i\vec{k}\vec{r}_1} \int_{A=\pi R^2} d^2 r_2 e^{+i\vec{k}\vec{r}_2}. \quad (27)$$

It is a well-known result in analysis that either integral of the last two ones in Eq.(27) results in $2\pi R^2 \frac{J_1(kR)}{(kR)}$, where $J_1(x)$ is a Bessel function of the first kind and $k = |\vec{k}| \geq 0$.

After casting the integral in polar coordinates and noting that $\rho_0 \pi R^2 = N$, we arrive at the expression:

$$\Delta \epsilon(d) = \frac{\Delta V(d)}{N} = k_e e^2 4 \rho_0 (\pi R^2) \int_0^\infty dk \left(1 - e^{-dk} \right) \left[\frac{J_1(kR)}{kR} \right]^2. \quad (28)$$

At this juncture, we rewrite the quantity shown above as:

$$\Delta\epsilon(d) = k_e e^2 4 \rho_0 (\pi R) \int_0^\infty dx \left(1 - e^{-\frac{d}{R}x}\right) \left[\frac{J_1(x)}{x}\right]^2. \quad (29)$$

One knows that:

$$\int_0^\infty dx \left[\frac{J_1(x)}{x}\right]^2 = \frac{4}{3\pi}. \quad (30)$$

However, there is work to be done to calculate the second integral of the form:

$$f(a) = \int_0^\infty dx e^{-ax} \left[\frac{J_1(x)}{x}\right]^2, \quad (31)$$

where $a = d/R \geq 0$ and $f(a)$ denotes an auxiliary function. The integral in Eq.(31) can be calculated analytically and may be written as:

$$f(a) = -\frac{a}{2} + \frac{a}{6\pi} \left[(4-a^2) E\left(-\frac{4}{a^2}\right) + (4+a^2) K\left(-\frac{4}{a^2}\right) \right], \quad (32)$$

where $K(m)$ and $E(m)$ are, respectively, complete elliptic integrals of the first and second kind:

$$K(m) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1-m\sin^2(\theta)}}, \quad (33)$$

and

$$E(m) = \int_0^{\pi/2} d\theta \sqrt{1-m\sin^2(\theta)}. \quad (34)$$

Recall that, until now, we have not yet taken the thermodynamic limit. This means that the expressions above are very general. One has $R \rightarrow \infty$ in the thermodynamic limit. Since we know that $\Delta\epsilon(d)$ is zero for the case $d = 0$, let us consider $d \neq 0$ (and finite) which implies $a = d/R \rightarrow 0$ in the thermodynamic limit. One can verify that in this limit:

$$f(a \approx 0) \approx \frac{4}{3\pi} - \frac{a}{2} + 0(a^2). \quad (35)$$

Therefore, one can easily deduce from the result in Eq.(35) that the value of $\Delta\epsilon(d)$ in the thermodynamic limit reads:

$$\Delta\epsilon(d) = k_e e^2 \rho_0 (2\pi) d. \quad (36)$$

The expression above can be rewritten as:

$$\Delta\epsilon(d) = \frac{4}{r_s^2} \frac{d}{a_B} \frac{k_e e^2}{2 a_B}. \quad (37)$$

By looking at the expression in Eq.(37) one notices that the separation distance d affects more the high density states (small r_s) in the sense that, for the same value of

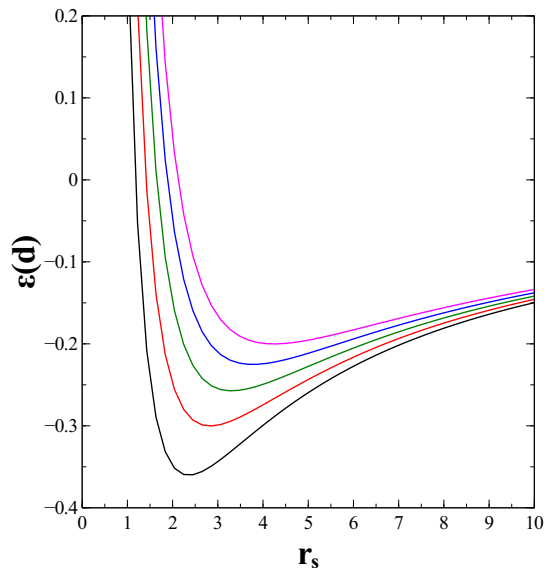


FIG. 2: Energy per particle, $\epsilon(d)$ as a function of r_s for five values of the separation distance parameter, $d/a_B = 0, 0.1, 0.2, 0.3$ and 0.4 (from left to right) corresponding to a fully spin-polarized 2DEG system in which the layer of electrons is separated from the background layer by a distance, d . Note how the minimum of energy shifts to larger values of r_s as d/a_B increases from $d/a_B = 0$ (first left curve) to 0.4 (last right curve). The energy per particle is given in units of $k_e e^2 / (2 a_B)$.

d/a_B , the overall energy of a state with small r_s is raised more than the energy of its counterpart with larger r_s . We know that liquid electronic states are typically stable at high density, while Wigner solid states stabilize at low density. This means that we expect that separation would adversely affect the energy stability of the liquid states and should likely enhance the Wigner crystallization process. We knew that the energy term $\Delta\epsilon(d)$ would act as an upward positive correction to the overall energy. However, we are somehow surprised to see that such a term acts as an effective kinetic energy by being proportional to $1/r_s^2$ exactly as $\langle \hat{T} \rangle / N \propto 1/r_s^2$.

By combining the result in Eq.(22) with that in Eq.(37) and substituting in Eq.(19) one writes the total energy per particle in this model as:

$$\epsilon(d) = \left[\left(2 + 4 \frac{d}{a_B} \right) \frac{1}{r_s^2} - \frac{16}{3\pi} \frac{1}{r_s} \right] \frac{k_e e^2}{2 a_B}. \quad (38)$$

In Fig. 2 we show the dependence of the energy per particle, $\epsilon(d)$ as a function of r_s for values of $d/a_B = 0, 0.1, 0.2, 0.3$ and 0.4 . While the overall energy per particle increases, one also notices that the minimum of energy is obtained for values of r_s that grow larger as d/a_B increases.

IV. CONCLUSIONS

To conclude, we considered a modified 2DEG model in which the 2D layer of electrons is suspended and separated by an arbitrary distance from the neutralizing 2D jellium background layer. We found that the separation of the layer of electrons from the 2D jellium background acts as an effective kinetic energy that increases the overall energy of the system. The effective increase of kinetic energy by the separation effect is more pronounced at high density (small r_s) values.

It is known that typical electronic liquid states are energetically favored at high density as compared to Wigner solid states. Therefore, one would tend to expect that such an effective increase of the kinetic energy would adversely affect the energetic stability of the liquid electronic states in such a way as to further enhance the Wigner crystallization process. Given the well known limitations of the HF method, future studies employing more elaborate Jastrow-Slater wave functions and relying in accurate quantum Monte Carlo calculations would be most welcomed to estimate the magnitude of the effects assessed in this work.

Acknowledgments

The research of O. Ciftja was supported in part by National Science Foundation (NSF) grant no. DMR-2001980. J. Batle acknowledges fruitful discussions with J. Rosselló, Maria del Mar Batle and Regina Batle. J. Batle received no funding for the present research.

APPENDIX: FORMALISM FOR ARBITRARY SPIN POLARIZATION

Consider N_α electrons with spin "α" ("up") and N_β electrons with spin "β" ("down"). Obviously,

$$N_\alpha + N_\beta = N, \quad (\text{A.1})$$

where N is the total number of electrons. One defines the spin-resolved number densities, $\rho_\alpha = N_\alpha/A$ and $\rho_\beta = N_\beta/A$ where A is the area of the system. One writes:

$$\rho_\alpha + \rho_\beta = \rho_0, \quad (\text{A.2})$$

where $\rho_0 = N/A$ is the total number density. One has N_α electrons filling a 2D Fermi disk up to the state with

wave vector $k_{F\alpha}$ and N_β electrons filling a 2D Fermi disk up to the state with wave vector $k_{F\beta}$. For the case of an arbitrary spin polarization of the system, one considers a normalized wave function of the form:

$$|\Psi\rangle = |\Psi_\alpha\rangle |\Psi_\beta\rangle, \quad (\text{A.3})$$

where $|\Psi_{\alpha,\beta}\rangle$ are the spin-resolved Slater determinant wave functions for each species of spin. It is easy to prove that:

$$k_{F\alpha}^2 = 4\pi\rho_\alpha \quad ; \quad k_{F\beta}^2 = 4\pi\rho_\beta. \quad (\text{A.4})$$

From Eq.(A.2) and Eq.(A.4) one concludes that:

$$k_{F\alpha}^2 + k_{F\beta}^2 = 4\pi(\rho_\alpha + \rho_\beta) = 4\pi\rho_0. \quad (\text{A.5})$$

The spin-resolved one-particle density functions are defined as:

$$\rho_\alpha(\vec{r}) = \sum_{j=1}^{N_\alpha} |\phi_{\vec{k}_j\alpha}(\vec{r})|^2 \quad ; \quad \rho_\beta(\vec{r}) = \sum_{j=1}^{N_\beta} |\phi_{\vec{k}_j\beta}(\vec{r})|^2, \quad (\text{A.6})$$

where $\phi_{\vec{k}_j\alpha}(\vec{r})$ are plane-wave state for spin "α" electrons and $\phi_{\vec{k}_j\beta}(\vec{r})$ correspond to the spin "β" counterpart. Note that:

$$\rho_\alpha(\vec{r}) + \rho_\beta(\vec{r}) = \rho(\vec{r}) = \rho_0, \quad (\text{A.7})$$

where $\rho(\vec{r})$ is the total one-particle density function. One can, similarly, define the spin-resolved one-particle density matrices:

$$\begin{aligned} \rho_\alpha(\vec{r}_1, \vec{r}_2) &= \sum_{j=1}^{N_\alpha} \phi_{\vec{k}_j\alpha}(\vec{r}_1)^* \phi_{\vec{k}_j\alpha}(\vec{r}_2) \quad ; \\ \rho_\beta(\vec{r}_1, \vec{r}_2) &= \sum_{j=1}^{N_\beta} \phi_{\vec{k}_j\beta}(\vec{r}_1)^* \phi_{\vec{k}_j\beta}(\vec{r}_2). \end{aligned} \quad (\text{A.8})$$

At this juncture, we have defined all the key elements that allow us to derive general expressions that apply to a 2DEG system with arbitrary spin polarization.

It is easy to calculate that the expectation value of the total kinetic energy operator for the spin-resolved system is:

$$\langle \hat{T} \rangle = \frac{N_\alpha}{2} \epsilon_{F\alpha} + \frac{N_\beta}{2} \epsilon_{F\beta}, \quad (\text{A.9})$$

where $\epsilon_{F\alpha} = \frac{\hbar^2}{2m} k_{F\alpha}^2$ and $\epsilon_{F\beta} = \frac{\hbar^2}{2m} k_{F\beta}^2$.

One can verify that:

$$\begin{aligned}
\langle \hat{V}_{ee} \rangle = & \frac{1}{2} \int_A d^2 r_1 \left[\rho_\alpha(\vec{r}_1) + \rho_\beta(\vec{r}_1) \right] \int_A d^2 r_2 \left[\rho_\alpha(\vec{r}_2) + \rho_\beta(\vec{r}_2) \right] v(r_{12}) \\
& - \frac{1}{2} \int_A d^2 r_1 \int_A d^2 r_2 |\rho_\alpha(\vec{r}_1, \vec{r}_2)|^2 v(r_{12}) \\
& - \frac{1}{2} \int_A d^2 r_1 \int_A d^2 r_2 |\rho_\beta(\vec{r}_1, \vec{r}_2)|^2 v(r_{12}) ,
\end{aligned} \tag{A.10}$$

where $\rho_{\alpha,\beta}(\vec{r})$ are defined in Eq.(A.6) and $\rho_{\alpha,\beta}(\vec{r}_1, \vec{r}_2)$ are defined in Eq.(A.8). The expression for $\langle \hat{V}_{eb} \rangle$ can be written as:

$$\langle \hat{V}_{eb} \rangle = -\rho_0 \int_A d^2 r_1 \left[\rho_\alpha(\vec{r}_1) + \rho_\beta(\vec{r}_1) \right] \int_A d^2 r_2 v_d(r_{12}) . \tag{A.11}$$

Although the quantity $\langle \hat{V}_{bb} \rangle$ is the same as that in Eq.(14), we rewrite it below for the sake of completeness:

$$\langle \hat{V}_{bb} \rangle = \frac{\rho_0^2}{2} \int_A d^2 r_1 \int_A d^2 r_2 v(r_{12}) . \tag{A.12}$$

For a fully spin-polarized state, for instance, one with all electrons having spin "α" values:

$$N_\alpha = N \quad ; \quad N_\beta = 0 , \tag{A.13}$$

$$\rho_\alpha(\vec{r}) = \rho(\vec{r}) = \rho_0 \quad ; \quad \rho_\beta(\vec{r}) = 0 , \tag{A.14}$$

$$\rho_\alpha(\vec{r}_1, \vec{r}_2) = \rho(\vec{r}_1, \vec{r}_2) \neq 0 \quad ; \quad \rho_\beta(\vec{r}_1, \vec{r}_2) = 0 , \tag{A.15}$$

$$k_{F\alpha}^2 = 4\pi\rho_0 \quad ; \quad k_{F\beta}^2 = 0 , \tag{A.16}$$

and likewise.

On the other hand, for a spin unpolarized state, one has:

$$N_\alpha = N_\beta = \frac{N}{2} , \tag{A.17}$$

$$\rho_\alpha(\vec{r}) = \rho_\beta(\vec{r}) = \frac{\rho(\vec{r})}{2} = \frac{\rho_0}{2} , \tag{A.18}$$

$$\rho_\alpha(\vec{r}_1, \vec{r}_2) = \rho_\beta(\vec{r}_1, \vec{r}_2) \neq 0 , \tag{A.19}$$

$$k_{F\alpha}^2 = k_{F\beta}^2 = 2\pi\rho_0 , \tag{A.20}$$

and one can continue this way in a similar fashion.

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