Variation of the elliptical Fermi surface for a two-dimensional electron gas with anisotropic mass

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Abstract. We consider a two-dimensional electron gas in the thermodynamic (bulk) limit. It is assumed that the system consists of fully spin-polarized (spinless) electrons with anisotropic mass. We study the variation of the shape of the expected elliptical Fermi surface as a function of the density of the system in presence of such form of internal anisotropy. To this effect, we calculate the energy of the system as well as the optimum ellipticity of the Fermi surface for two possible liquid states. One corresponds to the standard system with circular Fermi surface while the second one represents a liquid anisotropic phase with a tunable elliptical deformation of the Fermi surface that includes the state that minimizes the kinetic energy. The results obtained shed light on several possible scenarios that may arise in such a system. The competition between opposing tendencies of the kinetic energy and potential energy may lead to the stabilization of liquid phases where the optimal elliptical deformation of the Fermi surface is non-obvious and depends on the density as well as an array of other factors related to the specific values of various parameters that characterize the system.

1. Introduction

The model of a two-dimensional electron gas (2DEG) of electrons with constant isotropic (effective) mass is one of the most studied models in condensed matter physics [1, 2, 3, 4, 5, 6, 7]. At absolute zero temperature and in absence of interactions, the electrons occupy all the quantum states inside a circular Fermi disk in reciprocal space [8]. These quantum states are typically associated with plane wave states that arise when we solve the quantum problem for a two-dimensional (2D) box after imposing periodic boundary conditions. In the common jellium approximation one guarantees the overall charge neutrality of the system by filling the 2D box with uniformly distributed positive charge that represents the neutralizing background.

On the other hand, the 2DEG model for electrons possessing an anisotropic (effective) mass [9] is much less studied. For such a case, based on naive considerations, one expects that an (effective) anisotropic mass will lead to a specific elliptical deformation of the Fermi surface in order to minimize the kinetic energy. However, the role of the potential energy term is overlooked in this discussion. It turns out that kinetic energy and potential energy terms have opposing tendencies under an elliptical deformation of the Fermi surface. This fact calls for a more detailed study of the interplay between these two terms in presence of such form of internal anisotropy of the system as represented by the (effective) mass anisotropy of the electrons.

In our work we study a 2DEG in the thermodynamic (bulk) limit. For simplicity, we assume that the system consists of fully spin-polarized (spinless) electrons with anisotropic mass. The jellium approximation is used and the quantum state of the electrons is described

by an anti-symmetrized Slater determinant wave function of plane waves [10] as required by Pauli's exclusion principle. Two distinct liquid states of electrons are considered: (i) A standard isotropic liquid phase with circular Fermi surface; and (ii) A liquid anisotropic phase with a tunable elliptical deformation of the Fermi surface that includes the state that minimizes the kinetic energy. It is shown that the competition between opposing tendencies of the kinetic energy and potential energy may lead to the stabilization of liquid phases where the optimal elliptical deformation of the Fermi surface is non-obvious and depends on several factors.

2. Theory and model

Let us consider a 2DEG system of N electrons with anisotropic mass, m_x and $m_y(\neq m_x)$ immersed in a 2D region, $\Omega : \left\{-\frac{L}{2} \leq x, y \leq +\frac{L}{2}\right\}$. We assume a spin-polarized (spinless) system of electrons. The electron number density of the system reads:

$$\rho_0 = \frac{N}{L^2} \ . \tag{1}$$

Density remains constant in the $N \to \infty$, $L \to \infty$ limit. We must remember that, differently from other conventional 2DEG systems treated in the literature [11, 12], the current model assumes an anisotropic (effective) mass for the electrons. The Hamiltonian is:

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

where

$$\hat{T} = \sum_{i=1}^{N} \left[\frac{\hat{p}_{ix}^2}{2\, m_x} + \frac{\hat{p}_{iy}^2}{2\, m_y} \right] \ , \tag{3}$$

is the kinetic energy operator and

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

is the potential energy operator. The potential energy operator in Eq.(4) includes the electron-electron (ee), electron-background (eb) and background-background (bb) interaction energy terms written as:

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

$$\hat{U}_{eb} = -\rho_0 \sum_{i=1}^{N} \int_{\Omega} d^2 r' \, v(|\vec{r}_i - \vec{r}\,'|) \ , \tag{6}$$

and

$$\hat{U}_{bb} = \frac{\rho_0^2}{2} \int_{\Omega} d^2 r \int_{\Omega} d^2 r' \ v(|\vec{r} - \vec{r}\,'|) \ , \tag{7}$$

where $v(|\vec{r}_i - \vec{r}_j|) = k_e \, e^2 / |\vec{r}_i - \vec{r}_j|$ represent the Coulomb interaction energy between two electrons with charge, $-e$ $(e > 0)$ at a distance $r_{ij} = |\vec{r}_i - \vec{r}_j|$ and k_e is Coulomb's electric constant.

If electrons fill a circular Fermi surface, all vectors, $\vec{k}$ would be in the region $|\vec{k}| \leq k_F$ where:

$$k_F^2 = 4\, \pi \, \rho_0 \ . \tag{8}$$

where k_F represents the value of the Fermi wave number for a circular Fermi surface. However, if the electrons fill an elliptically deformed Fermi surface, all the vectors, $\vec{k}$ would be in the reciprocal space domain, $D_{\vec{k}}$ written as:

$$\vec{k} \in D_{\vec{k}} : \left\{ \frac{k_x^2}{k_a^2} + \frac{k_y^2}{k_b^2} \leq 1 \right\} \quad ; \quad k_a = \alpha \, k_F \quad ; \quad k_b = \frac{k_F}{\alpha} \ , \tag{9}$$

where we introduced a real positive parameter, $\alpha > 0$ in Eq.(9) consistent with the constraint: $k_a\, k_b = k_F^2$. We describe the ground state of the 2DEG by a normalized Slater determinant wave function of ortho-normalized plane waves

$$\Psi(\alpha) = \frac{1}{\sqrt{N!}}\, Det\left\{\phi_{\vec{k}_1}(\vec{r}_1), \ldots, \phi_{\vec{k}_N}(\vec{r}_N)\right\} \quad ; \quad \vec{k} \in D_{\vec{k}}\ , \tag{10}$$

where the parameter α is shown as argument of the wave function in order to draw asttention to the fact that we are dealing, in general, with an elliptically deformed Fermi surface. The state $\Psi(\alpha = 1)$ would represent the case of an isotropic liquid phase with circular Fermi surface. However, any $\Psi(\alpha \neq 1)$ state represents an anisotropic one with elliptical Fermi surface. The plane wave states are written as: $\phi_{\vec{k}_j}(\vec{r}_i) = \frac{1}{\sqrt{A}}\, e^{i\,\vec{k}_j\,\vec{r}_i}$ where $A = L^2$ is the area of the 2D box.

The total energy of the system, which is the expectation value of the Hamiltonian with respect to the Slater determinant wave function for a system with an elliptical Fermi surface can be calculated through well-established procedures. The total kinetic energy is:

$$T(\alpha) = \frac{\langle\Psi(\alpha)|\hat{T}|\Psi(\alpha)\rangle}{\langle\Psi(\alpha)|\Psi(\alpha)\rangle} = \sum_{\{\vec{k}\in D_{\vec{k}}\}}\left[\frac{\hbar^2\, k_x^2}{2\, m_x} + \frac{\hbar^2\, k_y^2}{2\, m_y}\right]\ . \tag{11}$$

The total potential energy is written as:

$$U(\alpha) = \frac{\langle\Psi(\alpha)|\hat{U}|\Psi(\alpha)\rangle}{\langle\Psi(\alpha)|\Psi(\alpha)\rangle} = -\frac{1}{2}\int_\Omega d^2r_1 \int_\Omega d^2r_2\, |\rho(\alpha, \vec{r}_1, \vec{r}_2)|^2\, v(r_{21})\ , \tag{12}$$

where Ω is the 2D square box region with area, $A = L^2$ in the thermodynamic limit of $L \to \infty$, $v(r_{21})$ is the pair Coulomb interaction potential and $\rho(\alpha, \vec{r}_1, \vec{r}_2) = \sum_{j=1}^{N} \phi_{\vec{k}_j}(\vec{r}_1)^*\, \phi_{\vec{k}_j}(\vec{r}_2) = \frac{1}{A}\sum_{\{\vec{k}\in D_{\vec{k}}\}} e^{i\,\vec{k}\,(\vec{r}_2 - \vec{r}_1)}$ is the so-called one-particle density matrix. Note the negative sign of the (exchange) potential energy in Eq.(12).

3. Results and conclusions

The kinetic energy per particle denoted as $t(\alpha, \beta)$ is calculated to be:

$$t(\alpha,\beta) = \frac{T(\alpha)}{N} = \frac{1}{4}\frac{\hbar^2\, k_F^2}{2\, m_0}\left(\frac{\alpha^2}{\beta} + \frac{\beta}{\alpha^2}\right) \quad ; \quad \beta = \sqrt{\frac{m_x}{m_y}} \quad ; \quad m_0 = \sqrt{m_x\, m_y}\ , \tag{13}$$

where $\beta > 0$ is a dimensionless parameter that measures the mass anisotropy and has a given value. Calculation of the potential energy per particle gives:

$$u(\alpha) = \frac{U(\alpha)}{N} = -\frac{8}{3\pi^2}\, k_F\, k_e\, e^2\, F(\alpha)\ , \tag{14}$$

where

$$F(\alpha) = \frac{1}{\alpha} K\left(m = 1 - \frac{1}{\alpha^4}\right)\ , \tag{15}$$

is an auxiliary function that is expressed in terms of $K(m)$, a complete elliptic integral of the first kind with parameter, m [13]. Note that $F(\alpha = 1) = \pi/2$ represents the largest possible value for this function. This means that the minimum potential energy per particle is always obtained for $\alpha = 1$ and has the value:

$$u_{min} = u(\alpha = 1) = -\frac{4}{3\pi}\, k_F\, k_e\, e^2\ . \tag{16}$$

The key point that we make here is that, for a given mass anisotropy parameter β, the value of kinetic energy depends on it, but the potential energy does not. This means the value of ellipticity that optimizes the kinetic energy depends on β but that value may not be the optimal one for the potential energy. In fact, it can be proved that kinetic energy has its minimum for the specific value: $\alpha_0 = \sqrt{\beta}$, resulting in:

$$t_{min} = t(\alpha = \sqrt{\beta}, \beta) = \frac{1}{2}\frac{\hbar^2 k_F^2}{2\, m_0} \ . \tag{17}$$

On the flip side, the potential energy has its minimum for $\alpha = 1$ (irrespective of the value β) and, thus, favors a circular Fermi surface. In short, an elliptical deformation of the Fermi surface for $\beta \neq 1$ decreases the kinetic energy, but increases the potential energy. This means that a sizeable elliptical deformation is not at all obvious or expected to happen in those instances where the dominant energy term is the potential energy. This is precisely the situation that happens when the density of the 2DEG system is relatively low. Density enters in the expressions for both kinetic and potential energy via the Fermi wave number, k_F. After writing the electron number density as $\rho_0 = 1/[\pi\,(r_s\, a_B)^2]$ where r_s is the Wigner-Seitz radius parameter and $a_B = \hbar^2/(k_e\, m_0\, e^2)$ is some "effective" Bohr radius (related to mass, $m_0 = \sqrt{m_x\, m_y}$) one can prove that $(k_F\, r_s\, a_B)^2 = 4$. Therefore, one concludes that kinetic energy ($\propto 1/r_s^2$) and potential energy ($\propto -1/r_s$) dominate, respectively, at high density (small r_s) and low density (large r_s).

Thus, for $\beta \neq 1$, at relatively low density, the isotropic liquid state, $\Psi(\alpha = 1)$ may have a total energy per particle, $\epsilon(\alpha = 1, \beta) = t(\alpha = 1, \beta) + u(\alpha = 1)$ lower than the total energy per particle, $\epsilon(\alpha = \sqrt{\beta}, \beta) = t(\alpha = \sqrt{\beta}, \beta) + u(\alpha = \sqrt{\beta})$ of its anisotropic counterpart, $\Psi(\alpha_0)$. At all other higher densities, a 2DEG with elliptical Fermi surface might be favored although it is very likely that $\Psi(\alpha_0)$ is not necessarily the optimum state with the lowest global energy.

In conclusion, the results obtained shed light on interesting scenarios that may arise in a 2DEG system with mass anisotropy. The competition between opposing tendencies of the kinetic energy and potential energy may lead to the stabilization of liquid phases where the optimal elliptical deformation of the Fermi surface is non-obvious and may depend on the density of the system. It is also possible that very little deformation of the Fermi surface may happen at small density where the potential energy term dominates over the kinetic energy.

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