Spontaneous Magnetization of a Two-Dimensional Electron Gas

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Abstract. Spontaneous magnetization of a two-dimensional electron gas (2DEG) is discussed. It takes place for sufficiently high electron density (i.e. for a quantum fluid state) with \( r_s < 10 \) which is quite beyond the condition of Wigner crystallization \( (r_s > 37) \) obtained by Tanatar and Ceperley. The effect essentially depends upon screening and disorder. The energy interval under the Fermi level where a spin polarization occurs as a function of electron density is computed. The spontaneous magnetic moment and a decrease of electron density of states (pseudo-gap) at the Fermi level are found.

The investigation of a 2DEG are still in focus of modern physics. Here we discuss a possibility of spontaneous magnetization of a 2DEG due to exchange interaction. The entirely magnetized state of a 2DEG is a Wigner crystal. Tanatar and Ceperley in their earlier paper [1] computed the condition for a two-dimensional electron fluid to cross over to the Wigner crystal state [2] at zero temperature. They obtained that the Wigner crystal melts at \( r_s = 37 \pm 5 \) where \( r_s \) is the Brueckner parameter \( r_s = \alpha_W/\alpha_0, \alpha_0 = \hbar^2\kappa/me^2 \) being an effective Bohr radius (here \( \kappa \) is a permittivity) and \( \alpha_W \) is the Wigner-Seitz radius connected with an electron sheet density \( \sigma \) by a relation \( \alpha_W = 1/\sqrt{\pi \sigma} \). Recently Yoon, et. al. [3] have observed some phase transition at which they attributed to the melting of a Wigner crystal.

Here we deal with a comparatively high electron density \( (r_s \text{ less than } \approx 37) \) corresponding to a homogeneous quantum fluid. The authors of Ref.[1] investigated only the transition between ferromagnetic Wigner crystal and unpolarized quantum fluid state. Thus they have not put into account a partially polarized state which is just the goal of the present consideration.

Firstly, it was pointed out to an exchange interaction as a reason of spontaneous spin polarization in quantum wires by Wang and Berggren [4] with the aim to explain anomalies in quantum wire conductance. Their approach was based on Kohn-Sham local density description of the exchange interaction. Further, this approach was developed in Ref. [5,6]. However, in spite of simplicity, this method is insufficient to reveal subtle details of spin configuration of electron system, for instance, to derive density of states at the Fermi level essential for any transport phenomena.

In our model of a quantum fluid a great number of electrons are confined in a square region. At the very beginning, the problem of two-particle interaction is preliminary considered with Hartree-Fock equations similar to the case of a quantum wire [7-9]. It allows to introduce an exchange interaction in a many-particle Hamiltonian.
The exchange energy of two electrons is assumed to be small compared with kinetic one. Therefore, the Hartree-Fock (HF) approach is employed to describe exchange interaction. In this approach the energy of spin-less Coulomb interaction for two electrons in the region is as follows

\[ V_c(\vec{k}_1, \vec{k}_2) = \frac{e^2}{\kappa} \int \int \frac{|\psi_1(\vec{k}_1, \vec{r}_1)|^2 |\psi_2(\vec{k}_2, \vec{r}_2)|^2}{|\vec{r}_1 - \vec{r}_2|} d\vec{r}_1 d\vec{r}_2 \]  

(1)

The exchange energy magnitude is

\[ V_{ex}(\vec{k}_1, \vec{k}_2) = \pm \left( \frac{e^2}{2\kappa} \int \int \frac{\psi_1^*(\vec{k}_1, \vec{r}_1)\psi_1(\vec{k}_1, \vec{r}_2)\psi_2^*(\vec{k}_2, \vec{r}_2)\psi_2(\vec{k}_2, \vec{r}_1)}{|\vec{r}_1 - \vec{r}_2|} d\vec{r}_1 d\vec{r}_2 + c.c. \right) \]  

(2)

where \( \psi_1, \psi_2 \) are wave functions of the first and second electron normalized per one electron in the area. The sign of exchange energy depends upon spin state of the electron pair. The unperturbed one-particle wave function is

\[ \psi(\vec{k}, \vec{r}) = \frac{1}{L} e^{i\vec{k}\vec{r}} \]  

(3)

where \( L \) is a normalization length, \( \vec{r} = (x, y) \) is a position.

Two electrons with sufficiently small momentum discrepancy \( \hbar \Delta k < \hbar/\lambda \) so that

\[ h\Delta k < h/\lambda \]  

(4)

where \( \lambda \) is an effective screening length (\( \lambda << L \)) possess an exchange energy (2) almost as large as Coulomb one (1). In particular, screening might be caused by mirror charges in adjacent electrodes. In this case for rough estimations \( \lambda \) could be evaluated as a distance from a 2DEG to the nearest electrode.

In further calculations with equ.s (1) and (2) the Coulomb potential was cut off for distances \( x \) larger than effective screening length \( \lambda \).

For greater momentum mismatch than that given by the inequality (4) the exchange integrals (2) involve fast oscillating functions and tend to zero. Worth mentioning that a similar effect could be caused by disorder or scattering which break a wave function phase and thus diminish an overlap integral (2). For approximate evaluations in the case a screening length could be replaced by a coherence length \( \lambda_{\phi} \).

A sign of exchange energy in the exp.(2) depends upon spin configuration. If electrons have an antisymmetric spin configuration (total spin equals unity) then their space wave function is symmetric and the sign of exchange energy is positive, i.e. the same as that of a Coulomb energy. Otherwise, when a total spin equals zero, the exchange energy is negative and reduces total energy of electron system. For the sake of simplicity in further calculations we suppose the exchange energy to be equal to the Coulomb one (1) when the condition (4) is true. Otherwise, it is supposed to equal zero.

The above model of exchange interaction was employed to solve a many-electron problem. It was assumed that electrons with one spin orientation occupy the states
in the momentum $\vec{k} - space$ up to $|\vec{k}| = k^\uparrow$. At the same moment, electrons with the opposite spin orientation occupy the states up to $|\vec{k}| = k^\downarrow$. To characterize this spin configuration we introduce an energy $\delta \epsilon = (\hbar^2/2m)(k^\uparrow)^2 - (k^\downarrow)^2$. In absence of spin polarization (magnetization) $k^\uparrow = k^\downarrow$ and $\delta \epsilon = 0$. The value of $\delta \epsilon$ corresponds to the energy interval under the Fermi level where a spin polarization arises.

The exchange energy is calculated from the equation (2) and the supposition (4). The latter defines a circle of nearby electrons in $\vec{k} - space$ where an exchange interaction is strong. The sign of this interaction much matters, for example, it results in full compensation of exchange energy for deep states in $\vec{k} - space$. Moreover, the exchang energy of any electron in unpolarized fluid is fully compensated too (equals zero). It readily contradicts with the Kohn-Sham description.

The total energy of the electron system reduced per one electron $E_{tot}$ as a function of a parameter $\delta = \delta \epsilon/\epsilon_F$ ($\epsilon_F$ is the Fermi energy) was estimated. Evidently, the value of $E_{tot}$ includes the kinetic, Coulomb and exchange energy. In Rydberg units $R_y = \hbar^2/(2ma_0^2)$ $E_{tot}$ reads

$$E_{tot}(\delta) \approx (4\pi^2/r_s^2)R_y(1 + \delta^2/4 - 1/2\pi^3(L/a_0)R_yE_{ex}f(\delta)) + E_c$$

where

$$f(\delta) = \int_{\sqrt{1-\frac{\lambda}{L}}}^{\sqrt{1+\frac{\lambda}{L}}} \int_{\sqrt{1-\frac{\lambda}{L}}}^{\sqrt{1+\frac{\lambda}{L}}} \int_{0}^{2\pi} \int_{0}^{2\pi} \left(1 - 2\pi \frac{\lambda}{\epsilon_F} \sqrt{t_1^2 + t_2^2} \cos(\alpha_1 - \alpha_2)\right) d\alpha_1 d\alpha_2$$

is a dimensionless function arising from the exp. (2) and inequality (4), $E_{ex}$ is a value of the integral (2) in the limit $|\vec{k}_1 - \vec{k}_2| \to 0$, the Coulomb energy $E_c$ does not depend upon spin configuration, i.e. on the parameter $\delta$.

If the condition $\lambda << L$ is true the value of $E_{ex}x$ can be estimated $E_{ex} \approx 6.1(L/\lambda)$. The expression (5) may be thus written in more explicit form

$$E_{tot}(\delta) \approx (4\pi^2/r_s^2)R_y(1 + \delta^2/4 - 0.01(\lambda/a_0)10 f(\delta)) + E_c$$

The integral (6) was calculated numerically by the Monte Carlo method for typical values of screening length $\lambda$. It was found out that the ground state (i.e. for zero sample temperature $T=0$) corresponding to the minimum of the total energy (7) can be that of spin-polarized electrons near the Fermi level when $r_s > 2$. The dependence of the parameter $\delta = \delta \epsilon/\epsilon_F$ characterizing spin-polarisation degree against the Bruekner parameter $r_s$ is depicted in the Fig.1. In contrast to 1DEG (Ref. [7-9]) a smooth transition to spin-polarized state has been obtained for 2DEG.

On obtaining $\delta$ one can easily evaluate the spontaneous magnetic moment per unit area from the relation

$$M = \mu_B \frac{\delta}(r_s)$$

where $\mu_B$ is the Bohr magneton.
Figure 1: The parameter $\delta = \delta \epsilon / \epsilon_F$ characterizing spin-polarisation degree vs the Bruekner parameter $r_s$ for two typical values of screening length $\lambda$: $\lambda/a_0 = 12.5$ (dotted line) and $\lambda/a_0 = 50$ (solid line).

To estimate the relative decrease of density of states for electrons adjacent to the Fermi level (in a layer $\hbar |k_F - k| \leq \hbar / \lambda$) we have considered an expression for exchange energy as a function of electron momentum. According to the model we have obtained:

$$
\epsilon_{ex}(k) \approx \frac{e^2}{\kappa L} V_{ex} \left( \frac{L}{2\pi} \right)^2 \int_{k_F - 1/\lambda}^{k_F} k_1 dk_1 \int_0^{2\pi} \theta \left( \frac{1}{\lambda} - \sqrt{k_1^2 + k^2 - 2k_1 k \cos(\alpha)} \right) d\alpha \quad (9)
$$

The relation (9) originates from a dependence of an electron exchange energy upon spin configuration of near-by electrons in k-space. The total energy equals $\epsilon_{tot}(k) + \hbar^2 k^2/2m + \epsilon_c$ (the kinetic energy and spin-independent Coulomb energy are added here).

From exp. (9) the relative decrease of electron density of states $\rho$ in this energy interval under the Fermi level was deduced as

$$
\Delta \rho / \rho \approx 0.12 r_s \delta \quad (10)
$$

This decrease of density of states (pseudo-gap) is substantial for transport phenomena in 2DEG.

In conclusion, the criterion of a 2DEG to transit to a spin-polarized (magnetized) state was numerically derived. The exchange interaction in a many-electron system is modeled by the Hartree-Fock description of a pair electron interaction. Spontaneous magnetic moment and a decrease of density of states (pseudo-gap) at the Fermi level were also evaluated. The effect essentially depends on screening
and disorder (dephasing).

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