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Compressibility of a two-dimensional electron gas in a parallel magnetic field

A.L. Subaşı, B. Tanatar*

Department of Physics, Bilkent University, 06800, Bilkent, Ankara, Turkey

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Abstract

The thermodynamic compressibility of a two-dimensional electron system in the presence of an in-plane magnetic field is calculated. We use accurate correlation energy results from quantum Monte Carlo simulations to construct the ground state energy and obtain the critical magnetic field B_c required to fully spin polarize the system. Inverse compressibility as a function of density shows a kink-like behavior in the presence of an applied magnetic field, which can be identified as B_c. Our calculations suggest an alternative approach to transport measurements of determining full spin polarization.

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There has been a large amount of theoretical and experimental activity on the transport properties of two-dimensional (2D) electron systems in the last few decades [1]. A good part of the current interest comes from the metal–insulator transition observed in Si-MOSFETs and GaAs based structures [2]. In these investigations, mostly transport measurements are performed on low density, high quality samples where the electron–electron interaction effects are dominant. In a complementary way, there are a few thermodynamic measurements on the ground state properties of 2D electron systems such as magnetization (or spin susceptibility) and compressibility. It is of importance to have a consistent picture emerging from these measurements of a different nature.

Experiments with in-plane magnetic field have focused on the spin susceptibility, Landé g-factor, and effective mass of the 2D electron systems present in Si-MOSFETS and GaAs quantum-well structures [3–9]. Thermodynamic measurements of magnetization of a dilute 2D electron system were reported by Prus et al. [8], Shashkin et al. [9], and Kravchenko et al. [10]. While the measurements of Prus et al. [8] have not found any indication toward a ferromagnetic instability, Shashkin et al. [9] observed diverging behavior in spin susceptibility χ_s at a critical density coinciding with the metal–insulator transition determined from transport measurements.

Another thermodynamic quantity, the isothermal compressibility κ, has also been measured [11–14] using the capacitance technique originated by Eisenstein et al. [15]. The initial results [11,12] suggested that $1/\kappa$ has a minimum at the metal–insulator transition density. More recent measurements [14] revealed the importance of the role played by charged impurities in leading to a minimum in $1/\kappa$.

In this work, we consider the compressibility of a clean 2D electron gas in the presence of an in-plane magnetic field. Based on our results, we propose that compressibility measurements may allow us to discern the critical field and density at which the full spin polarization occurs. Our calculations, making use of the accurate exchange-correlation energy provided by quantum Monte Carlo (QMC) simulations, suggest that the thermodynamic compressibility will exhibit a distinguishing signature of the full spin polarization. Such experiments should be amenable to current technology and could offer an independent way of probing the magnetic properties of 2D systems.

* Corresponding author. Tel.: +90 312 290 1591; fax: +90 312 266 4579.
E-mail address: tanatar@fen.bilkent.edu.tr (B. Tanatar).

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We consider a 2D electron gas interacting via the $1/r$ Coulomb potential, embedded in a neutralizing background. At zero temperature, the system is characterized by two dimensionless quantities, r_s and ζ. Here, $r_s = 1/\sqrt{\pi n a_B^{*2}}$ is the average distance between electrons in units of effective Bohr radius $a_B^* = \hbar^2 \epsilon/(m^* e^2)$ (where m^* is the effective band mass and ϵ is the dielectric constant) and n is the 2D electron density. $\zeta = |n_\uparrow - n_\downarrow|/n$ is the degree of spin polarization. We envisage a constant magnetic field B applied parallel to the 2D electron system. The total energy of the 2D electron gas is given by

$$E(r_s, \zeta, B) = \frac{1+\zeta^2}{r_s^2} - \frac{4\sqrt{2}}{3\pi r_s}\left[(1+\zeta)^{3/2} + (1-\zeta)^{3/2}\right] + E_c(r_s, \zeta) - \frac{g\mu_B}{E_F}\frac{\zeta B}{r_s^2} \quad (1)$$

in units of effective Rydbergs (i.e. $\mathrm{Ry} = \hbar^2/(2m^* a_B^{*2}) = E_F r_s^2/2$, where E_F is the Fermi energy). In Eq. (1), the first and second terms are the kinetic and exhange energies, respectively, which constitute the Hartree–Fock approximation. The third term is the correlation energy, which has been the subject of many theoretical calculations. The most accurate results for $E_c(r_s, \zeta)$ are provided by QMC simulations [16, 17]. In this work, we adopt the recent parametrized expression given by Attaccalite et al. [17]. Finally, the last term is the Zeeman energy, where g is the Landé g-factor and μ_B is the Bohr magneton. In our numerical calculations, we use material parameters approppriate for GaAs semiconductor structures.

To find the spin polarization of the 2D electron system $\zeta^*(r_s, B)$ at a given magnetic field and density, we minimize the total energy $E(r_s, \zeta, B)$ in Eq. (1), with respect to ζ. Setting $\zeta^* = 1$ allows us to determine the critical magnetic field B_c (r_s) necessary to fully spin polarize the system. In Fig. 1, we show the critical magnetic field B_c in units of B_{c0} as a function of r_s. $B_{c0} = 2E_F/g\mu_B$ is the critical field for a noninteracting system. For the ground state energy we use as the result given by Eq. (1); B_c vanishes around $r_s \approx 25.5$, indicating the fact that the system spontaneously magnetizes at this density according to the QMC results [17]. Other theoretical approaches such as Hartree–Fock (HF) and random-phase approximation (RPA) yield qualitatively similar, but quantitatively very different results. For instance, B_c vanishes around $r_s \approx 2$ and $r_s \approx 5.5$ in HF and RPA, respectively [18].

The spin polarization $\zeta^*(r_s, B)$ for a given density and magnetic field can be related to the spin susceptibility. Another thermodynamic quantity of interest is the isothermal compressibility, whose magnetic field dependence attracted less attention. Using the ground state energy in Eq. (1) we calculate the density dependence of thermodynamic compressibility

$$\frac{1}{\kappa} = -\frac{n r_s}{4}\left[\frac{\partial E}{\partial r_s} - r_s \frac{\partial^2 E}{\partial r_s^2}\right], \quad (2)$$

which is shown in Fig. 2. More specifically, we plot the inverse compressibility scaled by the noninteracting value of the unpolarized system, κ_0/κ, as a function of r_s, for a 2D electron system under an in-plane magnetic field. Here, $1/\kappa_0 = 2n/r_s^2$. We chose two values of the external field, B_c $(r_s = 5)$ and B_c $(r_s = 10)$, namely the critical fields to fully spin polarize the system at $r_s = 5$ and $r_s = 10$. We observe that the inverse compressibility at a constant magnetic field switches to its fully polarized system value with a kink-like behavior. This suggests that in the compressibility measurements similar to those performed recently [11–14], the effects of the polarizing magnetic field could be discerned. Thus, an alternative thermodynamic method to the transport measurements of determining B_c may be provided by

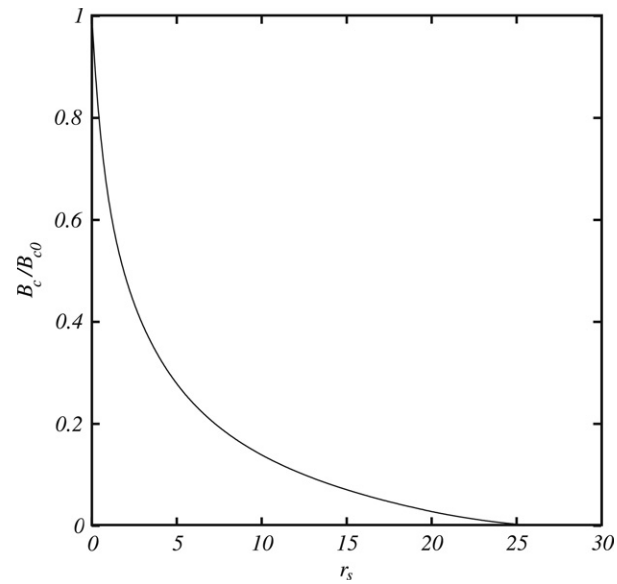

Fig. 1. The critical magnetic field B_c necessary to fully spin polarize a 2D electron gas as a function of r_s.

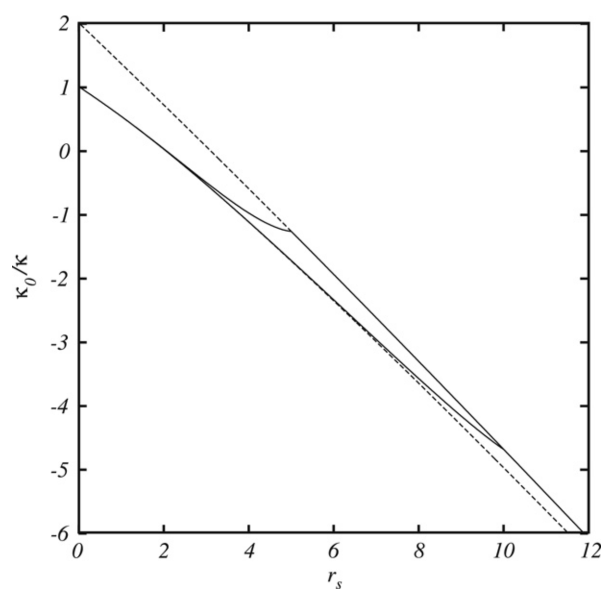

Fig. 2. The scaled inverse compressibility κ_0/κ as a function of r_s. The upper and lower dotted lines indicate unpolarized and fully polarized results, respectively, in the absence of magnetic field. The upper and lower solid lines are at B_c $(r_s = 5)$ and B_c $(r_s = 10)$, respectively.

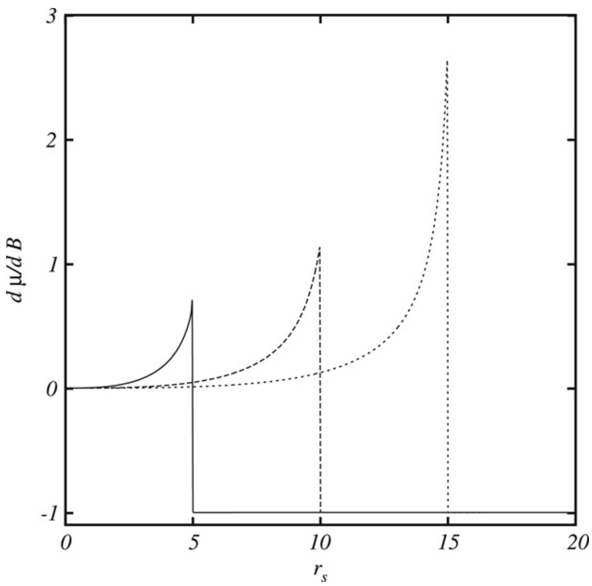

Fig. 3. $\partial\mu/\partial B$ in units of $g\mu_B/2$ as a function of r_s. The three curves from left to right are for the magnetic field values, B_c ($r_s = 5$), B_c ($r_s = 10$), and B_c ($r_s = 15$), respectively.

compressibility measurements with an in-plane magnetic field. Interestingly, the kink-like behavior in compressibility is more visible at smaller r_s, since the difference between the ground-state energies of the polarized and unpolarized phases decrease with increasing r_s.

Another quantity of interest indicating the full spin polarization is provided by the thermodynamic relation $\partial M/\partial n = -\partial\mu/\partial B$. We show in Fig. 3 $\partial\mu/\partial B$ as a function of r_s at three different magnetic field values. The onset of full spin polarization is readily identified as a sharp peak in the critical r_s value for the respective magnetic fields. This quantity has already been measured by Kravchenko et al. [10] for Si-MOSFETS. Our calculations, which are more appropriate for single-valley systems such GaAs, suggest that qualitatively similar results should follow.

We remark that the inverse compressibility exhibits a minimum and an upturn at a larger r_s value due to electron-impurity interactions [12,14]. Therefore the kink-like behavior in κ_0/κ predicted by our calculations could be smeared depending on the level of disorder present in the experimental samples. The experimental samples are of quasi-two-dimensional character, so that for any realistic comparison with experiments, the finite width of the quantum wells should be taken into account.

In conclusion, we have provided a simple calculation for the in-plane magnetic field dependence of the compressibility of a strongly interacting 2D electron gas. The inverse compressibility as a function of r_s exhibits a crossover from the partially polarized to fully polarized state, which should be identifiable experimentally.

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