Quantum nematic as ground state of a two-dimensional electron gas in a magnetic field

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\begin{abstract}
We study the ground state of a nematic phase of the two-dimensional electron gas at filling fraction
\( \nu = 1/2 \) using a variational wavefunction having Jastrow pair-correlations of the form \( \Pi_{i<j}(z_i - z_j)^2 \)
and an elliptical Fermi sea. Using the Fermi hypernetted chain approximation we find that below
a critical value of the layer "thickness" parameter \( \lambda \) and in the actual materials the quantum
nematic is energetically favorable relative to the stripe ordered Wigner crystal phase.
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During the past two decades, the quantum Hall effect (QHE) has been one of the most intriguing research
topics in condensed matter. More recently, the measurements of Lilly et al\textsuperscript{2} and Du et al\textsuperscript{2}
reveal a strong anisotropic behavior of transport properties of electrons for the half-filled Landau level (LL) system
under strong magnetic field and at very low temperature. The anisotropy commences at the second excited LL and
persists up to the sixth excited LL. The sudden exhibition of large anisotropies of resistivities in clean two-
dimensional electron gas (2DEG) suggests that there is an unknown underlying microscopic origin for this kind
of spontaneously symmetry breaking.

These experimental findings prompted several interesting theoretical proposals which attempt to explain the observed anisotropic behavior of the half-filled LL system. First of all, these anisotropic transport properties are consistent with already predicted stripe
and bubble charge-density-wave phases found\textsuperscript{1} by means of Hartree-Fock calculations of the 2DEG. However, Fradkin
and Kivelson\textsuperscript{6} suggested that the anisotropic transport might be due to a stripe nematic phase of the 2DEG in a high magnetic field. This point of view was investigated further by Fradkin et al\textsuperscript{2} where a model for the nematic phase in a symmetry breaking field was studied using Monte Carlo simulation. The results of the Monte Carlo simulation provide a good fit of the experimental data of Lilly et al\textsuperscript{2}. This simulation suggests that the nematic phase might be a good candidate to explain the anisotropic behavior observed in Ref.\textsuperscript{2} and Ref.\textsuperscript{6}. Furthermore, by deriving a long-wavelength elastic theory of the quantum Hall smectic state, Wexler and Dorsey\textsuperscript{13} have estimated the transition temperature from an isotropic to nematic phase to be of the order of 200mK. Later, Cooper et al\textsuperscript{13} by applying an in-plane magnetic field in 2DEG samples which show the above anisotropy in transport, give further support for the possible presence of such a quantum nematic phase.

In the composite fermion theory given by Jain\textsuperscript{14}, the fractional quantum Hall effect (FQHE) is interpreted as
the integer quantum Hall effect of composite Fermions. Furthermore, Halperin et al\textsuperscript{14} developed a theory of half-
filled LL system, which is the case of our interest, as a compressible Fermi liquid. Rezayi and Read\textsuperscript{15} proposed a ground state wave function for the half-filled LL system having the Jastrow-Slater form as follows:

\[
\Psi (\vec{r}_1, \vec{r}_2, ..., \vec{r}_N) = \hat{P} \prod_{j<k}^{N} (z_j - z_k)^2 e^{-1/4 \sum_{k=1}^{N} |z_k|^2} \times \det \left| \varphi_k (\vec{r}_i) \right|, \quad (1)
\]

where \( \varphi_k (\vec{r}_i) \) are two-dimensional (2D) plane-wave states, and \( \hat{P} \) is the LL projector operator. Here \( z_j = x_j + iy_j \) is the complex 2D coordinate of the \( j \) electron. This wavefunction is a Jastrow correlated Slater determinant with Jastrow part similar to the Laughlin state.

Ciftja and Wexler\textsuperscript{13} used the Fermi-hypernetted-chain (FHNC) approximation to study a broken rotational
state of the half-filled LL where the symmetry breaking parameter was introduced in the correlation part of the wavefunction and the single particle determinant of the wavefunction was characterized by a circular Fermi sea.

The ground state wavefunction for the nematic state proposed in Ref.\textsuperscript{11} has the same form as the wavefunction given by Eq.\textsuperscript{1} however, the single particle momenta form an elliptical Fermi sea as opposed to the circular Fermi sea. In this paper we will use this wavefunction to study the nematic phase. The broken symmetry parameter in our problem is the ratio \( \alpha = k_1/k_2 \) of the major \( k_1 \) and minor \( k_2 \) axis of the elliptic Fermi sea. We will study the nematic state of the half-filled LL system using the variational approach and we will employ the Fermi hypernetted chain approximation\textsuperscript{16,17,18,19}. We adopt the ansatz for the ground state of the nematic state proposed by Oganesyans et al\textsuperscript{16} as trial wavefunction in our variational calculations. Namely, we investigate whether or not this state, in which the anisotropy is due to an elliptical Fermi sea, can be energetically favorable relative to the isotropic state and the stripe ordered Wigner crystal at high LL. We find that the nematic phase can be stabilized against the isotropic case beyond the second excited LL. In addition, we have compared the energy of the nematic state to that obtained by a self-consistent
We find that there is a transition between the stripe ordered ground state and the nematic phase as a function of the parameter $\lambda$ of the Zhang-Das Sarma interaction, i.e., the layer finite thickness. In particular, for the case of the material $^3$He, we find that the ground state corresponds to the nematic state.

The FHNC formalism for Fermi systems was introduced and developed in Refs. 10,20,21,22. A significant advantage of FHNC over the variational Monte Carlo is that FHNC does not suffer from finite-size effects. In the FHNC technique, each term in the expansion is represented as graphical diagrams with well-defined topological rules. There are nodal, composite and elementary diagrams. In the FHNC/0 approximation, which neglects the elementary diagrams, the pair distribution function is obtained by solving the FHNC integral equations given in Ref. 21 for the case of polarized liquid $^3$He. These equations require as input, (a) the pair correlation (or Jastrow) factor, which in our case is given as $f^2(r) = \exp(u(r))$ with $u(r) = 4\ln(r)$, and (b) the statistical exchange factor $l(r)$, which for a 2D Slater determinant is given by: $l(r) = C(k_F r)$, where $C(x) = 2J_1(x)/x$, $J_1(r)$ is the first order Bessel function, and $k_F$ is the Fermi momentum of the isotropic state. Alternatively for the anisotropic state having an elliptic Fermi surface with major and minor axes $k_1$ and $k_2$, we find $l(r) = C(X)$, with $X = \sqrt{(k_1 x)^2 + (k_2 y)^2}$ where $x$ and $y$ are the coordinates of $r$.

Since the pseudo-potential $u(r)$ has a long-range logarithmic form, we follow the standard procedure used in Ref. 10 and Ref. 1 to separate it into a short-range and a long-range part. This leads to a new set of FHNC equations for the short range nodal and composite functions which are solved iteratively using a combination of momentum space and real space approach.

Our calculation proceeds as follows: First, we will calculate the pair distribution functions for isotropic and nematic states with different values of the anisotropic parameter for the LLL using the FHNC approximation. Second, the interaction energies will be calculated via the pair distribution functions by using the single-LL approximation, i.e., via Eq. 2. Next, the kinetic energy is evaluated for the isotropic and different nematic states. The energy values of the isotropic state are compared with anisotropic states for the lowest, first and second excited LL to find out if the nematic state becomes energetically favorable. Finally, we will carry out a self-consistent Hartree-Fock calculation for the more general case where $\lambda$ can be non-zero and we will compare the energy of the nematic, isotropic and stripe ordered Wigner crystal.

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LL and for small values of $\lambda$ changes rapidly at small distances and oscillates at large distances. We have used an adaptive mesh to incorporate these multi-scale oscillations accurately for up to $L = 2$. For higher Landau levels it becomes increasingly more difficult to carry out an accurate calculation due to the fact that these oscillations become increasingly more rapid.

Our calculated pair distribution function for the isotropic accurately reproduces the pair distribution function reported in Ref. 22. The potential energy difference $\Delta V_L(\alpha, \lambda)$ for various values of $\alpha$ is calculated and is shown in Fig. 1(top), in units of $e^2/l_0$ where $l_0 = \sqrt{\hbar/c/eB}$. Notice that for the case of the LLL and for the first excited LL, $\Delta V_L(\alpha, \lambda) < 0$, i.e., the isotropic state is energetically favorable for all values of $\lambda$ and $\alpha$. However, as it is illustrated in Fig. 1(top), for the case of the second excited LL, $\Delta V_2(\alpha, \lambda) > 0$, for all values of $\alpha$ and for some range of the parameter $\lambda$, the anisotropic state can be energetically favorable provided that the energy loss due to the anisotropy of the Fermi surface is not larger than the potential energy gain.

In the single-LL approximation the kinetic energy of the isotropic state is quenched. We can estimate the kinetic energy difference between the isotropic and the anisotropic case by ignoring the Landau level projection operator and, thus, writing the wave function as $\Psi = F\Phi$ where $\Phi$ is the non-interacting Slater determinant and $F$ the Jastrow part. The kinetic energy contains terms in which the operator $(\nabla - \vec{A})^2$ acts on $F$. This term gives the same contribution of $\hbar\omega_c/2$ in both isotropic and anisotropic case. Therefore, the main difference, coming from the term $|F|^2\Phi^*\nabla^2\Phi$, is due to the difference in shape of the Fermi sea. This leads to the following kinetic energy difference between isotropic and anisotropic Fermi sea: $\Delta K \simeq -\frac{\hbar^2k_F^2}{4m^*} \frac{1 - \alpha^2}{2\epsilon_0}$. In Fig. 1(bottom) we present the total energy difference $\Delta E_2(\alpha, \lambda)$ between the anisotropic and the isotropic state. Notice that the nematic state is energetically favorable relative to the isotropic below $\lambda_c \simeq 0.6$.

Hartree-Fock energies of the stripe and bubble charge-density-wave energy have already been reported in Refs. 23,24, however, they are only available for the case of $\lambda = 0$. In order to compare the energy of the nematic state with that of the ordered stripe and the bubble states for a non-zero value of $\lambda$, we carried out a Hartree-Fock calculation using the method outlined in Refs. 23,24. In Fig. 2 the total energy (apart from a common constant value of $\hbar\omega_c/2$) is compared with the results of our Hartree-Fock calculation for finite values of $\lambda$. In addition, in Fig. 3 the minimum energy with respect to the anisotropy parameter $\alpha$ is compared to the minimum Hartree-Fock energy value with respect to the uniaxial anisotropy parameter $\epsilon$ (the lattice constants of the uniaxial Wigner crystal are given in terms of $\epsilon$ as $a_1 = \sqrt{3a/2\sqrt{1-\epsilon}}$ and $a_2 = \sqrt{1-\epsilon a/2}$). Notice that there is a critical of $\lambda$, namely, $\lambda_c \simeq 0.4$ below which the nematic phase is energetically favored.

A value for the parameter $\lambda$ can be estimated using the calculation presented in Ref. 17. Using the value of the 2D electron density for these materials we find that $\lambda \sim 62\AA$. This corresponds to a value of $\lambda \sim 0.34$ in units of the magnetic length $l_0$ ($l_0 = 181\AA$ for the value of $B \sim 2T$ which corresponds to the second excited LL in the experiments of Refs. 2,3). This value of $\lambda$ is less than the critical value $\lambda_c \simeq 0.4$ below which the nematic phase is energetically favorable as compared to the stripe ordered phase (see Fig. 3). Therefore, we conclude that our calculation suggests that for the case of the 2DEG in the heterojunctions used in Refs. 2,3 the quantum nematic state may be energetically lower than the stripe ordered or bubble phases. Furthermore, it is interesting to probe this transition from the nematic to stripe to isotropic by either experimentally altering the value of $\lambda$ or indirectly by means of an in-plane field.

So far, because the Hartree Fock calculations predict a stripe state, the observed anisotropy in transport was taken as a signature of a stripe ordered state. This state
breaks both translational invariance in one direction and rotational invariance. The results of Haldane and Rezayi and Yang are also usually interpreted as a stripe state. However, the systems which can be done with such an approach are very small, and, in addition, toroidal boundary conditions were used, which break rotational invariance. Therefore, because of these limitations it cannot be discerned if the true ground state is a stripe or a nematic. In our calculation we find that the optimum nematic phase corresponds to an anisotropy of $\alpha \sim 10$ near the physically realized value of the parameter $\lambda$. This implies that a nematic state with such large anisotropy cannot be distinguished from the stripe state in systems with only twelve electrons.

There are two possible sources of systematic error in the present calculation. First, the use of the FHNC/0 approximation to evaluate the distribution function, where the contribution of the elementary diagrams is neglected. This approximation works very well in low-density systems, i.e., where the average interparticle distance is large compared to a hard core diameter. In the present problem such a condition is not clearly fulfilled as there is only a soft core of size $\lambda$. The second source of error is the fact that we have neglected the projection operator and assumed that the unprojected wave function given by Eq. 2 is a good approximation to the lowest LL. In order to address these concerns, in Fig. 4 we compare only the potential energy of the nematic and isotropic states with the results of the Hartree-Fock approximation obtained for the same values of $\lambda$. Notice that for values of $\lambda > 0.6$ the results of the FHNC and the HF calculation are almost identical. Moreover, the results of the FHNC calculation for the isotropic state agree very well with those of the HF calculation for all values of $\lambda > 0.3$. This is an indication that the energy difference between the nematic phase and that of the isotropic state and the stripe state below $\lambda \simeq 0.5$ may not be an artifact of the difference in the treatment of the two states (i.e., the difference between HF and FHNC approximations) but rather due to the fact that the nematic state for long-range interactions is energetically favorable for at least the second excited LL.

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