Variational Monte-Carlo calculation of the nematic state of the two-dimensional electron gas in a magnetic field

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We use a Jastrow-Slater wave function with an elliptical Fermi sea to describe the nematic state of the two-dimensional electron gas in a magnetic field and the Monte Carlo method to calculate a variational energy upper bound. These energy upper bounds are compared with other upper bounds describing stripe-ordered ground states which are obtained from optimized Hartree-Fock calculations and with those which correspond to an isotropic ground state. Our findings support the conclusions drawn in our previous study where the Fermi-hypernetted chain approximation was used instead of the Monte Carlo method. Namely, the nematic state becomes energetically favorable relative to the stripe-ordered Wigner crystal phase for the second excited Landau level and below a critical value of the layer “thickness” parameter which is very close to its value in the actual materials.

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I. INTRODUCTION

The measurements of Lilly et al.1 and Du et al.2 reveal strong anisotropic transport properties of the two-dimensional electron gas (2DEG) for the half-filled Landau-level system for high Landau-levels (LL) and at very low temperature. The anisotropic behavior in the transport properties is consistent with stripe and bubble charge-density-wave phases which were predicted early on in Refs. 3,4,5 by means of Hartree-Fock calculations and with those which correspond to an isotropic ground state. Our findings support the conclusions of a Monte Carlo simulation of the nematic phase of the 2DEG and were confirmed more recently by numerical studies of systems with up to 12 electrons6,7. However, Fradkin et al.8 have challenged this interpretation and suggested that the anisotropic transport might be due to a possible nematic phase of the 2DEG in a magnetic field. This idea finds support in the good comparison between the results of the temperature dependence of the anisotropy of the resistivity obtained by means of a Monte Carlo simulation of the nematic phase with that which has been experimentally observed. In addition, the idea is supported by the experiments of Cooper et al.9 where an in-plane magnetic field was applied in the 2DEG and the results of the experiment were interpreted on the basis of the presence of a nematic state; further support of the idea is provided by the fact that the theoretically estimated transition temperature from an isotropic to nematic phase10 is of similar magnitude as the experimentally determined temperature at which the onset of the anisotropic transport occurs.

Rather recently we have presented11 a variational calculation of the nematic state as ground state of the half-filled Landau-level system in a magnetic field based on an ansatz ground state wavefunction proposed by Oganesyan et al.12 which is of the Jastrow-Slater form and is given by the following expression:

\[ \Psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N) = \hat{P}_0 \prod_{j<k} (z_j - z_k)^2 e^{-\sum_{k=1}^{N} \|z_k\|^2/4} \times \det \left| \varphi_k(\vec{r}_i) \right| \] (1)

where \( \hat{P}_0 \) is the projection operator onto the lowest LL, \( \varphi_k(\vec{r}_i) \) are two-dimensional (2D) plane-wave states. 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.14. This ground-state wavefunction has the same form as the form proposed by Rezayi and Read,15 however, the single-particle momenta form an elliptical Fermi sea as opposed to the circular Fermi sea. There is a broken-symmetry parameter which is the ratio \( \alpha = k_1/k_2 \) of the semi-major \( k_1 \) and semi-minor \( k_2 \) axes of the elliptic Fermi sea. Using this wave function to describe the nematic state we had carried out a variational study of the half-filled system using the so-called Fermi-hypernetted-chain (FHNC) approximation.16

The results of the above mentioned variational calculation indicate that there is a certain value of the parameter \( \lambda \) (\( \lambda \) is proportional to the 2DEG layer thickness) below which the nematic state is energetically favorable as compared to the isotropic and the stripe-ordered ground states for the second excited LL. It is interesting to note that this critical value of \( \lambda \) is very close to the value of \( \lambda \) which can be estimated based on the actual experimental conditions which are applicable for the case of the data by Lilly et al.1 and by Du et al.2. However, one of the weak points of the above described variational study is the fact that the FHNC approximation is plagued by an unknown-size error and the results cannot be improved in a controlled manner. Therefore, there is a need to check the validity of these results and conclusions using the variational Monte Carlo method and this task is undertaken in the present work.

There is a different variational approach to the problem of a broken rotational state of the half-filled LL introduced by Ciftja and Wexler.18 They have 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 as $(z_i - z_j)^2 \to (z_i - z_j - \alpha)(z_i - z_j + \alpha)$, and they used the standard single-particle determinant with a circular Fermi sea.

In this and in the work of Ref. [12] we considered the unprojected wavefunction of the nematic state. The advantage of this simplified version is that it has a Jastrow form with a Slater determinant so it can be applied directly with FHNC and it allows us to study large-size systems using the variational Monte Carlo method. The paper is organized as follows: In the following Section we discuss the formulation and the procedure; in Sec. [III] we present the results and we compare them with those obtained for the case of a stripe-ordered state and the isotropic state. In Sec. [IV] we summarize the conclusions of the present calculation.

II. METHOD

We have adopted the toroidal geometry of a square with periodic boundary conditions. This geometry has the advantage of naturally adapting to the nematic and isotropic state wavefunction. There are several steps in applying the MC approach for this problem. First, as part of the wavefunction of nematic state we construct a Slater determinant of plane waves characterized by momentum vectors which lie inside an elliptical Fermi sea. Second, since the pseudo-potential is $ln(r)$, which is a long-range interaction, we need to take into account all periodic image charge interactions. One of the methods to do this is the Ewald summation technique. In subsection [V] of the appendix we describe the Ewald summation technique for the case of toroidal boundary conditions and the $ln(r)$ interaction. In the present section we will discuss our implementation of the MC to study the nematic state.

Given a value of $\alpha$ there are definite values of the number of particles $N$ which correspond to a closed shell. These definite values of $N$ are calculated as follows. The occupied states characterized by $k_x, k_y$ must satisfy the following condition:

$$\frac{k_x^2}{k_1} + \frac{k_y^2}{k_2} \leq 1,$$

where $k_1$ and $k_2$ are the major and minor axis of the Fermi sea and given by:

$$k_1 = \sqrt{\frac{4\pi \rho}{\alpha}},$$

$$k_2 = \sqrt{\frac{4\pi \rho \alpha}{\alpha}}.$$

where $\rho$ is the uniform particle density of the system. For a finite system of size $L \times L$, $k_x = n_x \Delta k$ and $k_y = n_y \Delta k$ where $\Delta k = 2\pi/L$ and $n_x, n_y \in \mathbb{Z}$. So one can deduce the conditions for $n_x, n_y$ such that:

$$\frac{\pi}{N} \left( \alpha n_x^2 + \frac{n_y^2}{\alpha} \right) \leq 1.$$

For a value of $N$ to be acceptable the number of states, i.e., the number of pairs $(n_x, n_y)$ satisfying the above inequality should be equal to $N$. For example, for $\alpha = 1$, $N$ can be $1, 5, 9, 13, 21, 25, 29, 37, 45, \ldots$; for $\alpha = 2$, they can be $1, 3, 7, 11, 15, 17, 21, \ldots$

![FIG. 1: Occupied states for the nematic state with $\alpha = 2$ (top) and $\alpha = 4$ (bottom) for the case of 89 particles.](image)

In Figs. [1] we present two examples of closed shell which correspond to $\alpha = 2$ and 4 for $N = 89$. Notice that with anisotropy parameter $\alpha = k_x/k_y > 1$, the occupied states (i.e those satisfying equation [5]) are anisotropically distributed along the preferred $k_x$ axis. In our MC calculation we will use these cases as well as larger size systems up to 145 particles.

We follow the Metropolis MC scheme for sampling the wavefunction where the ratio needed between the new and the old wavefunction is:

$$\left| \frac{\psi(\vec{r}_{\text{new}})}{\psi(\vec{r}_{\text{old}})} \right|^2 = e^{\exp(u(\vec{r}_{\text{new}}) - u(\vec{r}_{\text{old}})) \frac{\text{Det}(e^{i\vec{k} \cdot \vec{r}_{\text{new}}})}{\text{Det}(e^{i\vec{k} \cdot \vec{r}_{\text{old}}})}},$$

where $u(\vec{r})$ is the periodic pseudo-potential which is derived in the subsection [VII] of the appendix. To carry out the calculation of the ratio between the Slater determinant of the new configuration and the old configuration efficiently, we use the inverse updating technique developed by Ceperley et al. [10]. We found that the number of MC steps needed for “thermalization” is of the order of $10^5$ and we use of the order of $2 \times 10^6$ MC steps to calculate averages of the distribution function.
The potential energy of the high LL can be expressed via the pair distribution function of the LLL using the single mode approximation discussed in Ref. [20], namely,

$$V_L = \frac{\rho}{2} \int \left[ g(r) - 1 \right] V^L_{\text{eff}}(r) d^2r$$  \hspace{1cm} (7)

where the effective potential $V^L_{\text{eff}}(r)$ for Landau level L is the convolution of the effective interaction

$$V(r) = e^2 / \epsilon \sqrt{r^2 + \lambda^2}$$  \hspace{1cm} (8)

with the $L$-order Laguerre polynomial; namely, it is the Fourier transform of:

$$\tilde{V}^L_{\text{eff}}(q) = \frac{2\pi e^2}{eq} e^{-\lambda q} \left[ \lambda_L(q^2/2) \right]^2$$  \hspace{1cm} (9)

In the above formula, $\lambda$ is a length scale which characterizes the confinement of the electron wave function in the direction perpendicular to the heterojunction.

We use the single mode approximation to calculate the interaction energy at high LL (equation 7) and we are only interested in obtaining the pair distribution function $g(r)$. The kinetic energy advantage of the isotropic phase over the nematic phase is calculated in the subsection $\mathtt{V \ B}$ of the appendix. The approach can be divided into the following steps:

- The pair distribution function for the LLL for different anisotropic parameters $\alpha$ is calculated.
- The single mode approximation $\mathtt{20}$ is used to calculate the interaction energies at a high LL.
- The kinetic energy for different anisotropic parameters is evaluated (see appendix $\mathtt{V \ B}$).
- We compare total energies of the isotropic and nematic state to determine at what LL the nematic becomes energetically favorable.
- The optimum value of $\alpha$ is determined by minimizing the total energy.

- The HF results which have been reported so far $\mathtt{21, 22, 23}$ correspond to the case of $\lambda = 0$. Therefore, we needed to carry out Hartree-Fock calculations following Refs $\mathtt{21, 22, 23}$ for the case of the interaction given by Eq. 8 for $\lambda \neq 0$. The optimum total energies of the nematic states will be compared with those of the stripe states at different values of $\lambda$ for the 2nd excited LL to determine a critical value of $\lambda$ below which the nematic state may be energetically favorable.
- The above mentioned critical value of $\lambda$ is compared with the value which corresponds to those samples used in the experiment $\mathtt{1}$.
- A comparison of the MC results to the ones obtained by FHNC will also be presented.

### III. RESULTS

The pair distribution function $g(r)$ obtained using MC integration has important differences when compared to $g(r)$ obtained by FHNC $\mathtt{12}$ as illustrated in Fig. 2. Thus, it is important to obtain the energies of the nematic state at high LL by MC and to compare them with those obtained by FHNC.

We first compare the interaction energies obtained for different values of $\alpha > 1$ with the potential energy of the isotropic state ($\alpha = 1$) (Figs. 3 and 4). Notice from Figs. $\mathtt{3}$ and $\mathtt{4}$ that the potential energy of the isotropic state is lower than the potential energy of the nematic state for the 1st excited LL and LLL for all values of the parameter $\lambda$. The potential energy is calculated with the pseudo-potential obtained using the Ewald sum as discussed in subsection $\mathtt{V \ A}$ of the appendix. Essentially the same result is also found with a pseudo-potential obtained using the Lekner summation technique $\mathtt{24}$. Furthermore, as shown in appendix $\mathtt{V \ B}$ the kinetic energy of the isotropic state is below that of the nematic state, and, thus, the total energy of the isotropic state is always lower than that of the nematic state. Hence, our MC calculation shows that the isotropic state is energetically favorable as compared to the nematic state for the LLL and the 1st excited LL for all values of the parameter $\lambda$. Also note that the same conclusion was reached using the FHNC technique $\mathtt{12}$ with the same wavefunction. These findings solidify the conclusion that for the LLL and the 1st excited LL, the isotropic state is more stable than the nematic state, which is also in agreement with the experimental findings of Refs. $\mathtt{3}$ and $\mathtt{2}$.

![Fig. 2: Comparison of the pair distribution function obtained by FHNC and MC.](image)

For the 2nd excited LL, however, the situation changes as illustrated in Fig. 5. The conclusion which can be drawn from the comparison of Fig. 5 is that the interac-
The isotropic state

FIG. 3: Comparison of the potential energy of the nematic state calculated for various values of $\alpha \neq 1$ as function of $\lambda$ with the isotropic state ($\alpha = 1$) for LLL.

The isotropic state

FIG. 4: Comparison of the potential energy of the nematic state calculated for various values of $\alpha \neq 1$ as function of $\lambda$ with the isotropic state ($\alpha = 1$) for the 1st excited LL.

The isotropic state

FIG. 5: Comparison between the potential energy of the nematic state calculated for various values of the anisotropic parameter $\alpha \neq 1$ as a function of $\lambda$ and the potential energy of the isotropic state ($\alpha = 1$) at the 2nd excited LL.

The isotropic state

FIG. 6: Comparison of total energy of the nematic state calculated for various values of the anisotropic parameter $\alpha \neq 1$ as functions of $\lambda$ with the isotropic state ($\alpha = 1$) at the 2nd excited LL.

The isotropic state

In Refs. 3, 4, 5 the stripe-ordered phase was predicted based on HF calculations and this ordering can also explain the anisotropy observed in the transport properties of the 2DEG at low temperature. Therefore, we need to investigate the stability of the nematic state against the stripe-ordered state as follows. First, we find the optimum energies of the nematic state with respect to the...
anisotropic parameter $\alpha$ for various values of $\lambda$. Next, we compare these with the optimum energies of the stripe state obtained by the HF approximation\textsuperscript{21,22,23}. Calculations for the case where $\lambda = 0$ have been carried out in Refs. 21,22 and 23. For making a comparison with the optimum energy of the nematic state at various values of $\lambda$, we carried out detailed HF calculations for the case where $\lambda \neq 0$. For the stripe-ordered state, the optimum energy is obtained by minimizing the energy with respect to the uniaxial anisotropy parameter $\varepsilon$ defined in Ref. 23. Fig. 7 shows the comparison of the optimal energies obtained by MC for the nematic state with the optimum (with respect to $\varepsilon$) energy for the stripe state obtained by HF. Note that, for $\lambda \geq 0.5$, the optimum nematic state is obtained for $\alpha = 1$, i.e., it is the isotropic state. Furthermore, Fig. 7 demonstrates that the nematic state is energetically lower than the stripe state for the values of $\lambda \leq \lambda_c = 0.37$. As discussed earlier the pseudo-potential can be obtained by using either the Ewald or the Lekner summation technique\textsuperscript{24}. We have also carried out the same calculation using the Lekner summation technique and the results obtained are in good agreement with those obtained using the Ewald summation method. Thus, we can conclude that with MC calculation, for $\lambda \leq \lambda_c = 0.37$, the energy of the nematic state is lower than the stripe-ordered state.

### IV. CONCLUSIONS

In Fig. 8 the results for the optimum total energy of the nematic state obtained with the variational MC method is compared with that obtained by FHNC in Ref. 12 and with the optimum energy of the stripe-ordered state. The critical value of $\lambda_c$ we found from FHNC\textsuperscript{22} is 0.4 which is close to the value of 0.37 obtained above by MC. The critical value of $\lambda$ corresponding to the sample used in experiment\textsuperscript{1}, which was calculated in Ref. 12, using the conditions of the experiment and sample characteristics, is approximately 0.34, which can be below the critical value found above. Thus, both MC and FHNC calculations indicate that the nematic state might be the state observed experimentally for the 2DEG at the heterojunction in the samples used in experiment described in Ref. 1. There is still a remaining question about the validity of our approximation to neglect the projection operator in the wavefunction (1). However, in both FHNC treatments of the problem\textsuperscript{12,18}, where, in addition to neglecting the projection operator for arguments presented there, there was a second rather annoying question (and rather straightforward to answer) of the validity of the FHNC approximation in evaluating the energy expectation value. In the present paper the latter question is answered by employing the Monte Carlo method. Therefore, we conclude that the present calculations eliminates the suspicion that the conclusions drawn in Ref. 12 might be due to an artifact of the FHNC approximation employed in Ref. 12.

### V. APPENDIX

#### A. Ewald summation technique for the logarithmic potential

The long-range nature of the pseudo-potential $\ln(r)$ which appears in the exponent of the wavefunction of the Jastrow factor in the case of periodic boundary conditions requires a summation over all periodic images.
charges. Specifically, the “charge” distribution required to give rise to a logarithmic interaction is given as:

$$\rho(\vec{r}) = \sum_{\vec{R}} \delta(\vec{r} - \vec{R}) + \rho_{\text{background}}$$  \hspace{1cm} (10)

The two-dimensional (2D) Poisson equation is given by:

$$\nabla^2 \Phi(\vec{r}) = -2\pi \rho(\vec{r})$$  \hspace{1cm} (11)

and its solution in 2D is the logarithmic interaction. We need to solve the above equation for a periodic square $L \times L$. The idea of Ewald summation is to add around each charge an opposite Gaussian charge distribution of an appropriately chosen width $\mu$, and, in addition, to subtract the same Gaussian charge distribution. Let us split $\rho$ into long-range and short-range portions in the following manner:

$$\rho(\vec{r}) = \rho_1(\vec{r}) + \rho_2(\vec{r})$$  \hspace{1cm} (12)

$$\rho_1(\vec{r}) = \sum_{\vec{R}} e^{-\frac{(\vec{r} - \vec{R})^2}{\mu^2}} + \rho_{\text{background}}$$  \hspace{1cm} (13)

$$\rho_2(\vec{r}) = \sum_{\vec{R}} \left[ \delta(\vec{r} - \vec{R}) - e^{-\frac{(\vec{r} - \vec{R})^2}{\mu^2}} \right]$$  \hspace{1cm} (14)

$\phi_1$, which corresponds to $\rho_1$ is a short-range potential, and, thus, we can calculate $\phi_1$ in real space since it converges very quickly. The other combined charge configuration, i.e., $\rho_2$, consisting of the Gaussian and the background charge and the corresponding potential is denoted by $\phi_2$. Since $\phi_2$ is a long-range potential it will be calculated in Fourier space. The solution to each of the Poisson’s equations for the two charge distributions and the corresponding potential is straightforward. We note that for our case the “charge” of the particle is $e^2 = 2m$. We find

$$\phi_1(\vec{r}) = \frac{4m\pi}{A} \sum_{k \neq 0} \frac{e^{-\mu^2k^2/4}}{k^2} e^{i\vec{k} \cdot \vec{r}},$$  \hspace{1cm} (15)

$$\phi_2(\vec{r}) = -m \sum_{\vec{R}} E_i \left[ -\frac{(\vec{r} - \vec{R})^2}{\mu^2} \right].$$  \hspace{1cm} (16)

where $\vec{k} = 2\pi/L\vec{n}$ with $\vec{n} \in Z^2$ and $E_i(t)$ is the Exponential integral function and is defined by: $E_i(t) = -\int_t^{\infty} e^{-x}/x \, dx$.

For the Ewald summation, the convergence of (15) and (16) is achieved choosing the width of the Gaussian charge distribution $\mu = 1$, the number of cells for the sum in (16) to be 10 and by carrying out the sum in momentum space in (15) over 200 k-states.

In order to check the validity of this approach for the case of our use of toroidal boundary conditions we calculated the distribution function and the energy for the 1/3 ($m = 3$) case using the expressions (15) and (16) and our results for the energy and distribution function are identical to the results of Morf and Halperin, who used the disk geometry.

B. Evaluation of kinetic energy of the nematic state

In this subsection of the appendix, we compute the kinetic energy difference between the nematic and the isotropic state. In the single-LL approximation, the kinetic energy is quenched. In addition, the same is true in the HF treatment of the stripe, namely, there is no kinetic energy due to any correlation factors or operators. While this approximation gives a significant difference between the potential energy of the isotropic state and the nematic state, it gives no difference between their kinetic energy which is unacceptable because of the difference in the geometry of the Fermi sea. We want to estimate this difference. We can start with:

$$\left(\nabla - \vec{A}\right)^2 F\Phi = \left(\nabla - \vec{A}\right)^2 2F\Phi$$  \hspace{1cm} (17)

The first term in the above equation yields:

$$\left(\nabla - \vec{A}\right)^2 F\Phi = \frac{\hbar \omega_c}{2} F\Phi,$$  \hspace{1cm} (19)

which is common for all states under our consideration so for simplicity we can drop it. The last term is:

$$F\nabla^2 \Phi = F \sum_{\vec{k} \in FFS} \frac{\hbar^2 k^2}{2m^*}$$  \hspace{1cm} (20)

So the contribution of the last term is:

$$\sum_{\vec{k} \in FFS} \frac{\hbar^2 k^2}{2m^*}$$  \hspace{1cm} (21)

where $\vec{k} \in FFS$ stands for a summation over all vectors $\vec{k}$ in the corresponding filled Fermi sea. The summation over the circular Fermi sea in the isotropic case is given by:

$$\frac{1}{N} \sum_{\vec{k}} \frac{\hbar^2 k^2}{2m^*} = \frac{h^2 k_F^2}{4m^*}.$$  \hspace{1cm} (22)

and the in the case of the elliptic Fermi sea in the anisotropic case the summation is given by

$$\frac{1}{N} \sum_{\vec{k}} \frac{\hbar^2 k^2}{2m^*} = \frac{h^2 k_1^2 + k_2^2}{4m^*}.$$  \hspace{1cm} (23)

Using the facts that $k_F^2 = k_1 \cdot k_2$ and $k_1/k_2 = \alpha$, the kinetic energy difference between the isotropic state and the nematic state is given as follows:

$$\Delta(KE) = \frac{\hbar^2 k_F^2 (1 - \alpha)^2}{4m^*} - \frac{2\alpha}{2\alpha}.$$  \hspace{1cm} (24)

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