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Finite-size Monte Carlo results for anisotropic quantum Hall liquids

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At low temperatures, two-dimensional electron systems in a perpendicular magnetic field exhibit remarkable quantum phenomena. In these extreme conditions, strongly correlated electron systems stabilize in different quantum phases as the filling factor of Landau levels is varied. In this Brief Report we present finite-size Monte Carlo simulation results for anisotropic quantum Hall liquid states observed at certain even-denominator filling factors. The anisotropic electronic liquid phases are described by a broken rotational symmetry wave function. Our investigations of systems of few electrons in disk geometry indicate that an anisotropic liquid crystalline quantum Hall phase with broken rotational symmetry is energetically favored relative to an isotropic liquid one.

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Discovery of extreme magneto-transport anisotropy in the longitudinal resistivity[1,2] of a two-dimensional electron system (2DES) in the quantum Hall effect (QHE) regime around filling factors $\nu = 2\,n + \nu^*$ ($n \geq 2$; $\nu^* = 1/2$) seemed consistent with earlier theoretical predictions for the appearance of charge density wave (CDW) states[3]. This earlier work was based on the Hartree-Fock (HF) approximation and the main conclusions were that electrons in a partially occupied n-th Landau level (LL) form domains (stripes) with filling factors equal to 1 and 0 that alternate with a spatial period of the order of the cyclotron radius. A CDW corresponds to a state with broken rotational symmetry and density modulation, therefore, it can be viewed as a quantum Hall *smectic* (QHS) state. The HF-based CDW theory implies that stripes should form at a temperature in the order of few Kelvins[4,5]. Such a high critical temperature contrasts with the experimental observation that anisotropy only sets in at much lower temperatures of the order of $100 - 150\ mK$[1,2]. Even though factors not included in the HF approximation of the CDW theory may account for some of the discrepancies with the experiment, other scenarios are possible.

An alternative approach that would be consistent with observed experimental facts would view the onset of anisotropy as signature of a phase transition from an isotropic to an anisotropic liquid phase. In fact, it has been suggested[4] that the appearance of anisotropy reflects the orientational ordering of local regions having pre-existing order, in analogy with what happens in an isotropic-to-nematic liquid transition. This way, it is perfectly logical to interpret the onset of anisotropy as a transition to a quantum Hall nematic (QHN) state, rather than the first signal of the creation of a CDW modulation. Monte Carlo simulation results[6] based on a model of a classical nematic in a symmetry breaking field appear to support the view that anisotropic transport occurs when the 2DES is in a QHN phase[7]. In the above approach, the prevailing view is that the underlying physics involves the existence of Fermi liquid states and the Pomeranchuk instability (PI) effect[8]. Through the PI mechanism, a Fermi liquid state (presumably the half-filled states in high LLs) may "spontaneously" enter an anisotropic "nematic" state characterized by a deformed elliptical Fermi suface[9,10]. The idea and the possibility that a Fermi liquid may enter a "nematic" phase by deforming the Fermi surface (in this scenario anisotropy emerges at one-particle level) is plausible. However, it is also plausible that anisotropy may emerge at a two-particle level (in our case, because of the non-monotonic effective interaction potential, $v_{n=2}(r)$, as seen in the discussion below). This study favors this second scenario which assumes that electrons stabilize in a liquid crystalline phase with no rotational invariance[11–13] that can be described by a ground state wave function that contains a suitable symmetry breaking term in the two-particle correlation factor and a Slater determinant of one-particle plane wave states characterized by a circular Fermi sea.

In this work, we present finite-size Monte Carlo simulation results for anisotropic quantum Hall liquid states seen at filling factor $\nu = 9/2$. When more than one LL is filled (as in the $\nu = 9/2$ case), a common assumption is to consider the completely filled underlying spin-resolved LL-s as inert. We consider the spin of N electrons in the uppermost half-filled LL to be fully polarized. We describe the anisotropic liquid crystalline state for $\nu = 9/2$ ($n = 2$; $\nu^* = 1/2$) by means of a broken rotational symmetry (BRS) Fermi liquid wave function of the form:

$$\Psi_\alpha = \hat{P}_{n=2} \left[det \left| e^{i\,\vec{k}_\beta\,\vec{r}_j} \right| \Psi_{B\,\alpha} \right] \ , \tag{1}$$

where

$$\Psi_{B\,\alpha} = \prod_{i>j}^{N} (z_i - z_j + \alpha)(z_i - z_j - \alpha) \exp\left(-\sum_{j=1}^{N} \frac{|z_j|^2}{4\,l_0^2} \right) , \tag{2}$$

represents a phase with broken rotational invariance. Above, one sets up a Fermi liquid state by having N electrons occupy the N lowest-lying plane wave states, $\{\vec{k}_\beta\}$ corresponding to an ideal spin-polarized 2D Fermi gas, $z_j = x_j + i\,y_j$ is the position coordinate in complex notation, l_0 is the electronic magnetic length, $\hat{P}_n$ is a n-

th LL projection operator and α is a (real) parameter (a nematic director) that introduces directional anisotropy.

Differently from a CDW (smectic) state that does not possess neither translational, nor rotational invariance, a nematic state would break rotational symmetry while preserving translational symmetry. Thus, a translationally invariant wave function with no rotational symmetry would represent a nematic liquid state. A quantum description of BRS liquid crystalline states would at least require that: *(i)* the states obey Fermi statistics; *(ii)* the states be translationally invariant (at least far away from the boundaries for finite systems); *(iii)* the states have broken rotational symmetry induced by an anisotropic parameter; *(iv)* the states belong to the appropriate Hilbert space for the problem under consideration. The above BRS Fermi liquid wave function satisfies all the above requirements. It is constructed by splitting the zeroe-s of the isotropic Bose Laughlin liquid state in a way that conserves the anti-symmetry (Fermi statistics) and translational invariance, but breaks the rotational invariance of the wave function (note that the Gaussian factors are innocuous). For $\alpha \neq 0$ the rotational symmetry is broken while the state still posseses translational invariance. Thus, as explained earlier this state has nematic order and α can be interpreted as a nematic director. If we consider α to be real the system will have a stronger modulation in the x-direction, and therefore likely have larger conductance in the perpendicular direction, $\sigma_{yy} > \sigma_{xx}$.

For $\alpha = 0$ the above wave funtion reduces to the isotropic Rezayi-Read (RR) wave function[14] since $\Psi_{B\,\alpha}$ becomes a Bose Laughlin wave function in such a limit[15]. The RR wave function is written as a product of a Jastrow factor with a Slater determinant (of plane waves) even though all electronic states are quantized into LLs. The justification behind this choice lies in the Halperin-Lee-Read (HLR) theory[16] for half-filled states. Such theory argues that a 2DES subject to a perpendicular magnetic field at which a LL is half-filled is mathematically equivalent with a system of fermions interacting with a Chern-Simons gauge field such that the average effective magnetic field acting on the fermions is zero. At precisely half-filling the fermions do not see a net magnetic field. Therefore, in absence of correlations, they would form a 2D Fermi sea of uniform density much like an ideal 2D Fermi gas. Obviously, inclusion of correlations among these "free" fermions inspires the RR choice for the microscopic wave function. The action of the n-th LL projection operator, is reflected on the modification of the interaction potential, $\hat{P}_n\,\hat{V}_{ee}\,\hat{P}_n$, where $\hat{V}_{ee} = \sum_{i>j}^{N} e^2/r_{ij}$ is the bare electron-electron Coulomb interaction potential. By following standard procedures[17] one derives a fully n-th LL projected effective interaction potential:

$$v_n(r) = \frac{e^2}{l_0}\int_0^\infty dq\, J_0\left(q\,r\right)\left[L_n\left(\frac{q^2}{2}\right)\right]^2 \exp\left(-\frac{q^2}{2}\right)\ , \tag{3}$$

where $J_0(x)$ and $L_n(x)$ are, respectively, Bessel and Laguerre functions. Note that r and q are dimensionless quantities (given in terms of the magnetic length, l_0). This effective interaction potential for $n = 2$ is non-monotonic[18].

TABLE I: Energies per particle for various BRS liquid crystalline states at filling factor $\nu = 9/2$ where α is the anisotropy parameter and N is the number of electrons in the $n = 2$ LL. Energies are in units of e^2/l_0. The statistical uncertainty of the computed QMC values is in the last digit.

N	$\alpha = 0$	$\alpha = 1$	$\alpha = 2$	$\alpha = 3$	$\alpha = 4$
5	-0.395987	-0.396171	-0.397252	-0.401383	-0.406501
9	-0.375311	-0.375376	-0.376905	-0.377485	-0.303281
13	-0.359823	-0.359907	-0.360263	-0.360269	-0.301946
21	-0.342097	-0.342086	-0.342650	-0.338028	-0.306805
25	-0.337674	-0.337681	-0.338179	-0.334828	-0.280462
29	-0.331773	-0.331734	-0.332940	-0.328880	-0.251877
37	-0.322153	-0.322140	-0.323392	-0.318271	-0.234691
49	-0.314131	-0.314101	-0.315207	-0.310208	-0.262212

For our calculations, we consider small finite-size systems of N electrons and perform a systematic quantum Monte Carlo (QMC) study of the stabilization mechanism of anisotropic liquid crystalline phases relative to their isotropic liquid counterparts. In a disk geometry, N electrons are immersed in a finite neutralizing background disk of radius, $R_N = l_0\sqrt{2N/\nu^*}$ and uniform charge density $\rho^* = \nu^*/(2\pi l_0^2)$. Since we are looking at the $\nu = 9/2$ case, we take $v_{n=2}(r)$ as interaction potential between electrons. The total interaction energy of the system, $\hat{V} = \hat{V}_{ee} + \hat{V}_{eb} + \hat{V}_{bb}$ is the usual sum of electron-electron (ee), electron-background (eb) and background-background (bb) terms. The ground state interaction energy per particle is: $\epsilon = \epsilon_{ee} + \epsilon_{eb} + \epsilon_{bb}$ where $\epsilon = \langle\hat{V}\rangle/N$ is the total interaction energy per particle. We choose systems of electrons with N to correspond to a completely filled shell in the 2D $\vec{k}$-space for fully spin-polarized electrons. Implementation of QMC calculations is straightforward and we rely on the Metropolis algorithm[19] to calculate the expectation value of various quantities. To reduce the statistical error, we discard the initial QMC runs and then use the next few million (between 2 to 4 million) runs to carry out the statistical average[20]. We perform a systematic study of all closed-shell systems with $N = 5, 9, 13$ leading to $N = 49$ electrons and thus extend a preliminary work[21] in which we very briefly reported only $N = 25$ energy results. Given a finite-size system of N electrons, we were able to calculate the energies of various states (isotropic versus anisotropic BRS) by varying the value of the parameter α. Energies per particle for selected systems are shown in Table. I. The results are rounded in the last digit. Such results indicate that there is always some value of $\alpha \neq 0$ for which an anisotropic liquid state has a lower energy than the

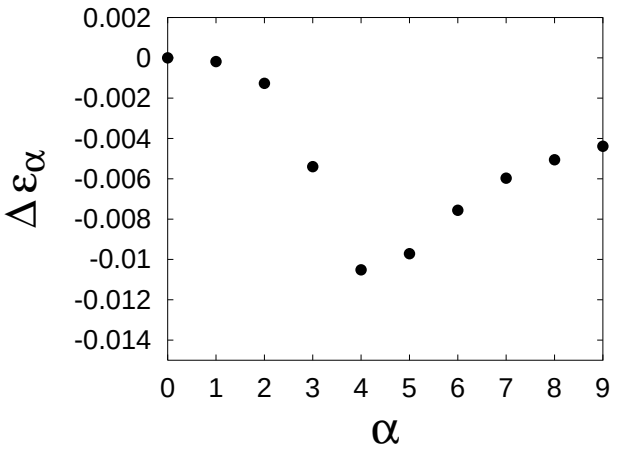

FIG. 1: Difference of energy per electron, $\Delta\epsilon_\alpha = \epsilon_\alpha - \epsilon_0$ between the anisotropic BRS states, ϵ_α and the corresponding isotropic state, ϵ_0 for the quantum Hall state at filling factor $\nu = 9/2$ as a function of the anisotropy parameter, α. The results were obtained after QMC simulations in a disk geometry for systems of $N = 5$ electrons in the $n = 2$ LL. Energies are in units of e^2/l_0.

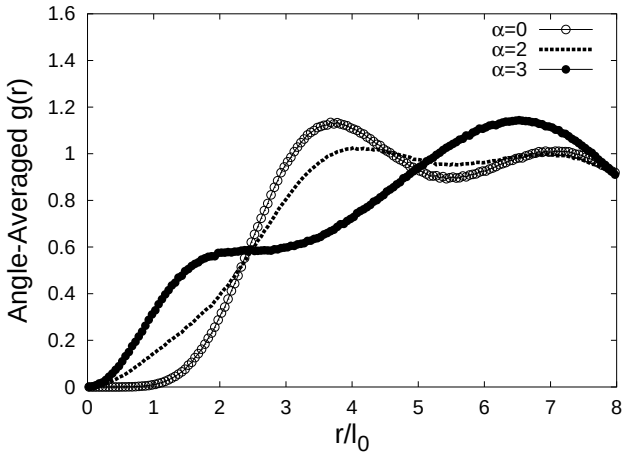

FIG. 2: Angle-averaged pair distribution function, $g(r)$ as a function of dimensionless distance, r/l_0 for a system of $N = 25$ electrons with anisotropy parameter values of $\alpha = 0$ (Solid line - Empty circle), $\alpha = 2$ (Dashed line) and $\alpha = 3$ (Solid line - Filled circle). Note that the $\alpha = 0$ value represents an isotropic liquid phase.

isotropic counterpart.

The optimal value, α_0 (in units of l_0) for which a minimum energy is obtained initially decreases when the system size increases. For instance, $\alpha_0 \approx 4$ for $N = 5$, then it goes from 3 (for $N = 9, 13$) to 2 when system size increases to $N = 21$. Additional calculations for larger systems (from $N = 21$ to $N = 49$) indicate that the value of α_0 does not decrease further with increasing N. For larger systems ($N \geq 21$), we always found $\alpha_0 \approx 2$. We attribute the sizeable variations of α_0 for $5 \leq N \leq 13$ to the small size of the system and "edge" effects. Clearly, for larger N the behavior of the system becomes more "bulk-like" with a clear pattern suggesting something special about the value $\alpha_0 = 2$. At closer inspection, one notices that this value approximately corresponds to the length where the dominant cusp of the non-monotonic potential, $v_{n=2}(r)$ occurs[18]. An exact calculation of $v_{n\to\infty}(r)$ using Eq.(3) indicates that the dominant cusp occurs at precisely, $r_c/l_0 = 2$ (while for finite n we see a cascade of n plateaus/cusps). On these premises, we conjecture that the value $\alpha_0 = 2$ mimicks this fact. Energy results for $N = 5$ electrons are shown in Fig. 1. We verified that such results are typical and pretty much apply to all systems of electrons under consideration. The implication is that a degree of anisotropy is always favoured as observed by looking at how the energy difference, $\Delta\epsilon_\alpha = \epsilon_\alpha - \epsilon_0$, between the anisotropic BRS state, ϵ_α and the corresponding isotropic state, ϵ_0 becomes negative for certain $\alpha \neq 0$ values. This indicates tendency towards liquid crystalline order.

To get a more reasonable bulk estimate of the energy for different states one needs to perform a careful finite-size analysis of the available results. In order to obtain a more meaningful comparison between the energies of isotropic ($\alpha = 0$) and anisotropic BRS states (those with lowest energy for a value $\alpha_0 \neq 0$), we performed a more detailed size-dependence of the data. To this effect, we followed the procedure of Morf and Halperin[22] and fitted the available energies in Table I to a polynomial function (of $1/\sqrt{N}$). As found earlier[22], a quadratic polynomial provides quite a good fit: $\epsilon_0 = \left(-0.247512 - \frac{0.533301}{\sqrt{N}} + \frac{0.450617}{N}\right) e^2/l_0$ and $\epsilon_{\alpha_0} = \left(-0.258734 - \frac{0.436851}{\sqrt{N}} + \frac{0.239319}{N}\right) e^2/l_0$. Extrapolation of the results (for $N \to \infty$) provides a useful estimate to the energy in the thermodynamic limit (the first term in each of the parentheses). Even though the convergence of the results (as a function of N) is quite slow (typical for such systems), the $N \to \infty$ extrapolation seems unambiguous suggesting that the negative energy difference (while being size-dependent), $(\epsilon_{\alpha_0} - \epsilon_0)$ favours a BRS liquid crystalline state even in the complete bulk limit. In Fig. 2 we plot the angle-averaged pair distribution function, $g(r) = \int_0^{2\pi} \frac{d\theta}{2\pi} g(r, \theta)$ for $\alpha = 0, 2$ and 3 and systems of $N = 25$ electrons. One can immediately note the noticeable impact of parameter $\alpha \neq 0$ on the pair distribution function. Firstly, the short-range behavior of $g(r)$ changes from $\propto r^6$ ($\alpha = 0$) to $\propto r^2$ ($\alpha \neq 0$). Secondly, one notices that as α increases, the major peak of $g(r)$ becomes less pronounced and shifts to larger values of r. At the same time with this shifting, a shoulder develops as can be clearly seen around $r = 2$ for $\alpha = 3$.

As in any MC approach, the statistical uncertainty of the results can be easily calculated. We estimate such uncertainty to affect the last digit of our results which has been rounded. On the other hand, given the trial wave function, there is some uncertainty while determin-

ing the optimal value of the parameter, α_0. Since our main point was to prove whether there is an anisotropic state (with $\alpha_0 \neq 0$) lower in energy than an isotropic one (with $\alpha = 0$), we found satisfactory to select a given set of α-s and calculate corresponding energies. A careful determination of the optimal α_0 for selected cases indicates no qualitative impact on the results with only negligible quantitative adjustments. Thus, while our Monte Carlo scheme is essentially a variational procedure, the only (insignificant) uncertainty affects the determination of the optimal value of α. Other than that, in the realm of QHE studies, the choice of a wave function is one imposed by physical constraints. Routinely, a microscopic description of QHE states involves trial wave functions that despite the "trial" label, have no parameters to fit. In this sense, our trial wave function mirrors the same logic (despite the presence of an additional trial parameter) and can be seen as a generalization of the RR wave function to describe not only isotropic, but also anisotropic Fermi liquid states at half-filling. So far, the RR wave function is considered the best starting microscopic choice at half-filling. Other wave functions that, for example, do not use plane waves, but rely on LL states appear unsatisfactory[23]. Clearly, this study was focused on the $\nu = 9/2$ state, however it worthy to note that anisotropy is quite sizeable in a $\Delta\nu_n$ range around half-filling. Based on the HLR theory, states away from half-filling are not supposed to be Fermi liquids and, thus, it is unlikely that anisotropy can originate from the PI effect. Away from half-filling (for instance at $\nu = 2n + 1/3$), one might argue that the non-monotonic features of the interaction potential may favor a BRS liquid crystalline phase. Such phase may have a similar nature as the state discussed here, with the difference that it is built by breaking the rotational symmetry of a 1/3 Laughlin's wave function[24].

In summary, we obtained accurate QMC results for anisotropic quantum Hall liquid crystalline phases at filling factor $\nu = 9/2$ in the second excited LL. We considered a series of finite-size systems with N electrons in the $n = 2$ LL and employed fully LL projected states to investigate whether the anisotropic liquid crystalline phases are more energetically favorable than the isotropic ones. Our energy investigations of finite-size systems of few electrons in a disk geometry indicate that a BRS anisotropic quantum Hall phase is energetically favored relative to an isotropic liquid one at filling factor $\nu = 9/2$. This study seems to be consistent with some of our earlier findings[11] based on the Fermi hypernetted-chain (FHNC) method[25,26], albeit without projection and with different unprojected interaction potentials.

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