Transition between Compressible and Incompressible States in Infinite-Layer Fractional Quantum Hall Systems

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Possible phase transitions between incompressible quantum Hall states and compressible three-dimensional states are discussed for infinite-layer electron systems in strong magnetic field. By variational Monte Carlo calculation, relative stability of some trial states is studied. If the inter-layer distance is large enough, the Laughlin state is stabilized for the Landau-level filling \( \nu = 1/3 \) of each layer. When the inter-layer distance is comparable to the magnetic length, the Laughlin state becomes unstable against a different fractional quantum Hall state with inter-layer correlation, and/or against a three-dimensional compressible state. It is discussed how the quantum phase transition between them can be controlled in actual systems.

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I. INTRODUCTION

Although the fractional quantum Hall effect is originally a two-dimensional phenomenon [1–4], multi-layer systems have been studied as natural development [4–8]. Multi-layer systems show some unusual effects because of new additional degrees of freedom, namely the inter-layer Coulomb interaction and the inter-layer electron tunneling. For example, in the case of the simplest double-layer system, the "even denominator" fractional quantum Hall effect with the Landau level filling \( \nu = 1/2 = 1/4 + 1/4 \) has been observed [9], and is interpreted in terms of Halperin’s \( \Psi_{331} \) state [5].

One may then naturally ask what happens in infinite multi-layer systems. Experimentally, the integer quantum Hall effect is observed in a 30-layer GaAs/AlGaAs superlattice system [10] and also in organic conductors (TMTSF)$_2$X [11–14] and BEDT-TTF salts [15]. Motivated by these works we study the ground state of the infinite-layer system under a strong magnetic field and discuss quantum phase transitions between incompressible and compressible states.

We can have the following naive expectation in advance of quantitative analysis: In the limit of infinite inter-layer distance \( d_s \), layers are completely independent of each other and the Laughlin state is realized for appropriate fillings, e.g., \( \nu = 1/q \) where \( q \) is an odd integer. However for \( d_s \sim l_B \) where \( l_B \) is the magnetic length, other fractional quantum Hall states can be realized because of the inter-layer Coulomb interaction. Furthermore three-dimensional states are also realizable with increasing electron tunnelings between layers. The fractional quantum Hall states are incompressible, but the last three-dimensional state is compressible because the Bloch states are formed perpendicular to layers and the Fermi surface should appear. Therefore a transition between incompressible and compressible states is expected at a certain value of \( d_s \), provided that \( d_s \) is a variable parameter.

Based on the above expectation we introduce three typical trial states for the ground state with the lowest Landau level filling \( \nu = 1/3 \) and compute energies of them in order to find which one is the ground state. Under a strong magnetic field we restrict the single-particle states within the lowest Landau level, and consider only the Coulomb energy and tunneling energy. We calculate the Coulomb energy by the variational Monte Carlo (VMC) method for the two-dimensional trial states [14,17], while the Hartree-Fock approximation is used for the three-dimensional trial state.

II. MODEL

We consider a system with the area \( S \) of each layer and the height \( L_z \) as shown in Fig. 1. The total number \( N_z \) of layers is given by \( N_z = L_z/d_s \). Then, with the total number \( N \) of electrons in the system, we define the electron number per layer \( N_\perp \) by \( N_\perp = N/N_z \). Taking into account the layer structure of the system, we assume the positive charge distribution

\[
n_0(r) = \sum_{z=1}^{N_z} \frac{N_\perp}{S} \delta(z - ld_s).
\]
This positive charge density corresponds to the uniform distribution in each layer and the discrete distribution along the layer. Under a magnetic field \( \mathbf{B} = B\mathbf{e}_z \), the Landau level degeneracy \( m_D \) is given by \( m_D = S/2\pi l_B^2 \) where \( l_B = (\hbar/eB)^{1/2} \) is the magnetic length. The average filling factor of each layer \( \nu \) is defined as \( \nu = N_\perp / m_D \). Under the strong magnetic field with \( \nu \leq 1 \) we may deal with only the lowest Landau level (LLL) explicitly and neglect higher levels. We will discuss possible ground states in the subspace of the LLL in the following.

Now we write down the Hamiltonian of the system with \( N \to \infty \) as

\[
H = \sum_{i=1}^{\infty} H_{0i} + \sum_{i<j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} - \sum_{i=1}^{N} \int d\mathbf{r} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}|} n_b(\mathbf{r}) + \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} n_b(\mathbf{r}) n_b(\mathbf{r}').
\]

(2.2)

Here the one-body part is given by

\[
H_{0i} = \frac{1}{2m_\perp} \left( \mathbf{p}_\perp + \frac{e}{c} \mathbf{A}_\perp(\mathbf{r}_i) \right)^2 + \frac{1}{2m_\parallel} \mathbf{p}_\parallel^2 + V_0(z_i),
\]

(2.3)

where \( m_\perp^* \) and \( m_\parallel^* \) are the effective masses in the layer and along the \( z \)-direction respectively. The squared effective charge \( e^* \) is defined by use of the dielectric constant \( \varepsilon \) as \( e^* = e^2/\varepsilon \). \( V_0(z) \) is the binding potential of electrons to layers (like a multi square well potential). We choose two types of configuration as follows: one is the circular shape and the other is the rectangular shape. These shapes are chosen for convenience of calculations.

### A. Circular Geometry

Let us consider a pile of infinitely large layers (\( S = \infty \)) with the circular symmetry and take the symmetric gauge. For the \((x, y)\)-space this geometry is the same as the one that Laughlin chose [3]. We adopt for this geometry the periodic boundary condition in the \( z \)-direction. This geometry is convenient for description of two-dimensional states and also convenient for the VMC calculation [17]. If we assume that electrons do not transfer between layers, then the one-particle state is written as

\[
\psi_{lm}(\mathbf{r}) = (2^{m+1} \pi m l_B^{2m+2})^{-1/2} \xi^m \exp \left[ -\frac{|\xi|^2}{4l_B^2} \right] \phi_0(z - ld_s),
\]

(2.4)

where \( \xi = x - i y \) is the complex coordinate in the \((x, y)\)-space and \( \phi_0(z - ld_s) \) defined by (2.14) is the normalized wave function localized at the layer \( l \). Since the uniform positive charge is inconvenient for finite particles which we actually study numerically, we take an alternative positive charge density \( \tilde{n}_b(\mathbf{r}) \) which has the same distribution as that of electrons. Namely with \( P(\{\mathbf{r}_i\}) = \left| \psi(\{\mathbf{r}_i\}) \right| ^2 \) being the probability distribution function of electrons, we require

\[
\tilde{n}_b(\mathbf{r}) = \sum_{j=1}^{N} \int \left( \prod_{i} d\mathbf{r}_i \right) \delta(\mathbf{r} - \mathbf{r}_j) P(\{\mathbf{r}_i\}).
\]

(2.5)

This positive charge distribution tends to the uniform one in the infinite-size limit.

We now discuss the Coulomb potential with periodic boundary condition along the \( z \)-axis. Taking account of mirror images we obtain the potential as

\[
V(\mathbf{r}, \mathbf{r}') = \frac{e^*}{\left[ (\mathbf{r}_\perp - \mathbf{r}'_\perp) + (z - z' + n L_z) \right]^{1/2}}.
\]

(2.6)

The summation over \( n \) is divergent logarithmically. This divergence should be canceled by the attractive part in the final result. In this paper we replace it by the following one:

\[
V(\mathbf{r} - \mathbf{r}') = \frac{e^*}{\left[ (\mathbf{r}_\perp - \mathbf{r}'_\perp)^2 + \left( \frac{2\pi}{L_z} \sin \left( \frac{2\pi z'}{L_z} \right) \right)^2 \right]^{1/2}}.
\]

(2.7)

This potential has the right periodicity along the \( z \)-axis and becomes equivalent to the Coulomb potential in the limit of \( L_z \to \infty \). The Hamiltonian with finite \( N \) is represented as follows:
\[ H = \sum_{i=1}^{N} H_{0i} + \sum_{i<j} V(\mathbf{r}_i - \mathbf{r}_j) - \sum_{i=1}^{N} \int d\mathbf{r} V(\mathbf{r}_i - \mathbf{r}) \tilde{n}_b(\mathbf{r}) + \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' V(\mathbf{r} - \mathbf{r}') \tilde{n}_b(\mathbf{r}) \tilde{n}_b(\mathbf{r}') \tag{2.8} \]

The expectation value is given by

\[ \langle H \rangle = N\Omega + \sum_{i<j} \int \left( \prod_{i=1}^{N} d\mathbf{r}_i \right) V(\mathbf{r}_i - \mathbf{r}_j) P(\{r_i\}) \]

\[ -\frac{1}{2} \sum_{i,j} \int \left( \prod_{i=1}^{N} d\mathbf{r}_i d\mathbf{r}_j' \right) V(\mathbf{r}_i - \mathbf{r}_j') P(\{r_i\}) P(\{r_j'\}) \tag{2.9} \]

where \( \Omega \) is a constant representing the single-particle energy. It is given by

\[ \Omega = \frac{1}{2} \sum_{n=-\infty}^{\infty} \int dz \phi_0^* (z) \left( \frac{r_x^2}{2m_\|} + V_0(z) \right) \phi_0(z), \tag{2.10} \]

where we have assumed that the tunneling along the \( z \)-direction is suppressed.

### B. Rectangular Geometry

Next we consider a pile of rectangular \( (S = L_x \times L_y) \) layers. We impose the periodic boundary condition in each \( (x, y) \) and \( z \) direction and choose the Landau gauge. We obtain \( m_D = L_x L_y / 2\pi l_B^2 \). In the case of three-dimensional states, this geometry is convenient. When there are tunnelings, the one electron state is written as

\[ \phi_{jk}(\mathbf{r}) = \phi_{\perp j}(\mathbf{r}_\perp) \phi_{\parallel k}(z), \tag{2.11} \]

where \( j = (1, 2, \ldots, m_D) \) indicates the degree of freedom in the LLL, and \( k = 2\pi n_L / L_z \) \((n = -N_z / 2, -N_z / 2 + 1, \ldots, N_z / 2 - 1)\) is the wave number along the \( z \)-direction. The \((\mathbf{r}_\perp)\)-dependent part \( \phi_{\perp j}(\mathbf{r}_\perp) \) is the Landau wave function [3]:

\[ \phi_{\perp j}(\mathbf{r}_\perp) = \left( \frac{1}{L y B \sqrt{\pi}} \right)^{1/2} \sum_{n=-\infty}^{\infty} \exp \left[ -i\kappa_j + m_D n y - \frac{(x - X_j + m_D n)^2}{2l_B^2} \right], \tag{2.12} \]

where \( \kappa_j = 2\pi j / L_y \) and \( X_j = l_B^2 \kappa_j \). For the \( z \)-dependent part \( \phi_{\parallel k}(z) \) we make the Bloch function by use of \( \phi_0 \) as

\[ \phi_{\parallel k}(z) = \frac{1}{\sqrt{N_z}} \sum_{n=-\infty}^{\infty} \sum_{n=1}^{N_z} e^{iknd_x} \phi_0 (z - nd_x - n_z L_z), \tag{2.13} \]

where we take the following localized function:

\[ \phi_0(z) = \left( \frac{1}{e^{2d_x^2\pi}} \right)^{1/4} e^{-z^2/2e^2d_x^2}, \tag{2.14} \]

with \( e \) being positive infinitesimal. Under the tight-binding approximation \( \phi_{jk}(\mathbf{r}) \) becomes the eigenstate of the one-particle Hamiltonian \( H_0 \). We introduce the creation and annihilation operators, \( a^\dagger_{jk} \) and \( a_{jk} \), corresponding to \( \phi_{jk}(\mathbf{r}) \). Then the total Hamiltonian of this system is given in second quantized form by

\[ \mathcal{H} = \sum_j \sum_k \left( E_k - \frac{N}{2V} \varepsilon_j^2 \right) a^\dagger_{jk} a_{jk} \]

\[ + \frac{1}{2V} \sum_{\mathbf{q} \neq 0} v(\mathbf{q}) \left[ \rho(\mathbf{q}) \rho(-\mathbf{q}) - \rho(0) \exp \left[ -\frac{\mathbf{q}^2}{4l_B^2} - \frac{e^2d_x^2\pi}{2} \right] \right]. \tag{2.15} \]

Here \( E_k = \Omega - 2t \cos kd_s \) is the eigenvalue of the one-electron state with the inter-layer transfer \( -t \), \( \zeta(n) \) is the Riemann’s zeta function, \( v(\mathbf{q}) = 4\pi e^2 / q^2 \) is the Fourier coefficient of the Coulomb potential, and \( \rho(\mathbf{q}) \) is the density operator defined by

\[ \rho(\mathbf{q}) = \int d\mathbf{r} \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}) e^{-i\mathbf{q} \cdot \mathbf{r}}, \tag{2.16} \]

where \( \psi(\mathbf{r}) = \sum_{jk} a_{jk} \phi_{jk}(\mathbf{r}) \) is the electron field operator projected onto the LLL.
III. TRIAL STATES

We introduce three trial states for the ground states with $\nu = 1/3$ of the Hamiltonians \(2.8\) and \(2.15\). As mentioned in the previous section, we take \(2.8\) for states without the tunneling (two-dimensional states) and \(2.15\) for states with the tunneling (three-dimensional states). Here we remark on the index of position coordinates. The position coordinates in the Hamiltonian \(2.8\) have the index \(i = 1, 2, \cdots, N\) of electrons. However when we refer to two-dimensional states, we make the position coordinates have the layer index additionally because electrons belonging to different layers are distinguishable. Hence the position coordinates have the two indices \(l = 0, 1, \cdots, N - 1\) is the layer index and \(p = 1, 2, \cdots, N_l\) is the particle index in a layer. Indices \(i\) and \(l, p\) are related to each other by \(i = N_l l + p\).

The first trial state is a two-dimensional one without the tunneling represented by

\[
\Psi_{\nu=1/3}^{(1)} = \prod_{l=1}^{N_z} \chi_{\nu=1/3}^{(l)}(\{\xi_{lp}\}) \Phi(\{\{z_{lp}\}\}),
\]

where $\chi$ and $\Phi$ describe the motion in the \((x, y)\)-space and along the $z$-direction respectively. They are given by

\[
\chi_{\nu=1/3}^{(l)}(\{\xi_{lp}\}) = \prod_{p<p'}(\xi_{lp} - \xi_{lp'})^3 \exp \left[ -\frac{1}{4l_B} \sum_{p=1}^{N_z} |\xi_{lp}|^2 \right],
\]

\[
\Phi(\{\{z_{lp}\}\}) = \prod_{l=1}^{N_z} \prod_{p=1}^{N_l} \phi_0(z_{lp} - l d).
\]

Here \(\{\{z_{lp}\}\}\) denotes \((z_{11}, \cdots, z_{1N_l}; \cdots; z_{N_l1}, \cdots, z_{N_lN_l})\) and \(\{\xi_{lp}\}\) does \((\xi_{11}, \cdots, \xi_{1N_l}; \cdots; \xi_{N_l1}, \cdots, \xi_{N_lN_l})\). We call the state \(\{\{z_{lp}\}\}\) the "multi-Laughlin state". It is the direct product of the Laughlin state with \(\nu = 1/3, 2\) in each layer and is expected to be stable for a large inter-layer distance: \(d_s \gg l_B\).

The second trial state is also a two-dimensional one without the tunneling. It is represented by

\[
\Psi_{\nu=1/3}^{(111)} = \chi_{\nu=1/3}^{(111)} \Phi(\{\{z_{lp}\}\}),
\]

where

\[
\chi_{\nu=1/3}^{(111)} = \prod_{l=1}^{N_z} \prod_{p<p'}(\xi_{lp} - \xi_{lp'}) \prod_{p,p'}(\xi_{lp} - \xi_{l+1p}) \exp \left[ -\frac{1}{4l_B} \sum_{p=1}^{N_z} |\xi_{lp}|^2 \right].
\]

We call this state the "(111) state" \([3]\). This state is expected to be stable for \(d_s \sim l_B\) where the inter-layer Coulomb interaction becomes comparable to the intra-layer one. The numbers \((111)\) indicate the exponents of the Jastrow factor which controls the strength of the electron correlation. The first "1" is the exponent of the Jastrow factor between a given layer and the nearest lower layer, the second "1" is that within the layer, and the last "1" is that between the layer and the nearest upper layer. Generally we can define \((\lambda\mu\lambda)\) state for our system. For example \((131)\) state is possible for \(\nu = 1/5\), and \((212)\) state is also possible for the same \(\nu\). Physically \((212)\) state should be unstable because the inter-layer correlation becomes larger than the intra-layer one in this state. In the case of \(\nu = 1/3\) only the \((111)\) state is allowed within the subspace of Halperin-type states.

The third state is expected to be stable at \(d \ll l_B\) when electrons transfer between layers. We call such a state the "itinerant state" and define it as follows. With the tunneling, Bloch waves are formed along the $z$-direction. Then the simplest candidate for the ground state is the one with the smallest kinetic (tunneling) energy. Namely the cosine band in the $z$-direction is filled up to the Fermi level \([19]\) with the filling of the Landau level for each wave number being unity below the Fermi level and zero above it. We can write it by use of electron creation operators as

\[
|\text{itinerant}\rangle = \prod_{j=1}^{m_D} \prod_{k|k| \leq k_F} a_{jk}^\dagger |0\rangle,
\]

where $k_F$ is the Fermi wave number given by $k_F = \nu \pi / d_s$. Although we assume $\nu = 1/3$ in this paper, the itinerant state can be defined for all $\nu \in [0, 1]$. 

4
IV. GROUND-STATE ENERGIES

A. Multi-Laughlin State and (111) State

We use the VMC method to calculate the expectation value of the Coulomb energy numerically for the multi-Laughlin state and the (111) state. Technical details are explained in Appendix. In the case of the multi-Laughlin state, \( \langle H \rangle \) are reduced to the sum of the two-dimensional result simply because all layers are independent of each other, and the inter-layer Coulomb energy is exactly canceled. We obtain

\[
N\varepsilon_L = \langle H \rangle_L - N\Omega = N_{\perp} \sum_{p \neq p'} \left( \prod_p d\rho_{\perp lp} \right) \frac{e^2}{|\mathbf{r}_{\perp lp} - \mathbf{r}_{\perp lp'}|} |\chi_L^{L} \{ \{ \xi_{lp} \} \}|^2
\]

\[
- \frac{1}{2} N_{\perp} \sum_{p \neq p'} \left( \prod_p d\rho_{\perp lp} \right) \frac{e^2}{|\mathbf{r}_{\perp lp} - \mathbf{r}_{\perp lp'}|} |\chi_L^{L} \{ \{ \xi_{lp} \} \}|^2 |\chi_L^{L} \{ \{ \xi_{lp'} \} \}|^2.
\]

(4.1)

On the other hand such cancellations do not occur for the (111) state, and the calculation becomes more complicated because of the inter-layer correlation. The energy is given by

\[
N\varepsilon_{(111)} = \langle H \rangle_{(111)} - N\Omega
\]

\[
= \left( \sum_{l \neq l'} \sum_{l \neq l'} + \sum_{l \neq l'} \sum_{l \neq l'} \right) \left( \prod_l \prod_p d\rho_{lp} \right) V(\mathbf{r}_{lp} - \mathbf{r}_{l'p'}) |\Psi^{(111)}_{\nu = 1/3}(\{ \{ \mathbf{r}_{lp} \} \})| |\Psi^{(111)}_{\nu = 1/3}(\{ \{ \mathbf{r}_{l'p} \} \})|
\]

\[
- \frac{1}{2} \sum_{l \neq l'} \sum_{l \neq l'} \left( \prod_l \prod_p d\rho_{lp} d\rho_{l'p} \right) V(\mathbf{r}_{lp} - \mathbf{r}_{l'p'}) |\Psi^{(111)}_{\nu = 1/3}(\{ \{ \mathbf{r}_{lp} \} \})|^2 |\Psi^{(111)}_{\nu = 1/3}(\{ \{ \mathbf{r}_{l'p} \} \})|^2.
\]

(4.2)

Figure 3 shows the size dependence of the Coulomb energy of the multi-Laughlin state. The extrapolated value is in good agreement with that in the literature [17]. The dependence of the Coulomb energy for the (111) state on the inter-layer distance is shown in Fig. 4. The calculation was performed for three cases of finite size systems: \( N_{\perp} = 20, 30 \) and 42 with \( N_z = 5 \). We find that the energy decreases with decreasing inter-layer distance. The dependence on \( N_{\perp} \) is small in the region of small inter-layer distance.

B. Itinerant State

We calculate the energy of the itinerant state for the Hamiltonian (2.13) with use of the Hartree-Fock approximation. Since we take the homogeneous trial state, the mean field is given by

\[
\Delta(jk; j'k') = \langle a_j^\dagger a_{j'k'} \rangle = \langle \text{itinerant}|a_j^\dagger a_{j'k'}|\text{itinerant}\rangle = \delta_{jj'} \delta_{kk'} \theta(k_F - |k|).
\]

(4.3)

The mean field for the interaction part of the Hamiltonian (2.13) consists of the direct and the exchange interactions. Of these the energy due to the direct term is written as

\[
\frac{1}{2V} \sum_{q \neq 0} v(q) \langle \rho(q) \rangle_{\rho(-q)} = \frac{N^2}{2V} \sum_{q \neq 0} v(q) \delta_{q-LG} \delta_{q_z, h} = \frac{N^2 e^2}{2V} \frac{d^2}{\pi} 2\zeta(2),
\]

(4.4)

where we used the relation \( \langle \rho(q) \rangle = N \delta_{q-LG} \delta_{q_z, h} \) valid in the macroscopic limit. Here we have \( \mathbf{g} = \left( \frac{2\pi}{L_x} n_D n_x, \frac{2\pi}{L_y} n_D n_y \right) \) and \( h = \frac{2\pi}{d_z} n_z \) with \( n_x, n_y, n_z \) integers. The direct term cancels exactly with the Coulomb energy of the positive charge because of homogeneity of the itinerant state within each layer. Therefore the Hartree-Fock Hamiltonian is given by
\[ \mathcal{H}^{HF} = \sum_{j} \sum_{k} E_k a_j^\dagger a_{jk} \]
\[-\frac{1}{2V} \sum_{j_1,j_2,k_1,k_2} a_{j_1k_1}^\dagger a_{j_2k_2} \theta (k_F - |k_2|) \sum_{q \neq 0} v(q) M(j_1k_1,j_2k_2;q) M(j_2k_2,j_1k_1;-q), \] (4.5)

where the matrix element for the exchange mean-field is given by

\[ M(jk,j'k';q) = \int d\mathbf{r} \Phi_{jk}^*(\mathbf{r}) \Phi_{j'k'}(\mathbf{r}) e^{i\mathbf{q} \cdot \mathbf{r}} \]
\[ = \sum_{h} \sum_{n=-\infty}^{\infty} \delta_{\mathbf{q}',\mathbf{k}-\mathbf{q}+\mathbf{h}\delta_{j-j'+m_Dn,-\frac{\mathbf{L}}{2\pi}q_h}} \exp \left[ -\frac{t_B^2 q_h^2}{4} - \frac{\epsilon^2 d_s^2 q_h^2}{2} \right]. \] (4.6)

The energy of the itinerant state is obtained as

\[ E = m_D \sum_{|k| \leq k_F} E_k \]
\[-\frac{m_D}{2V} \sum_{q \neq 0} v(q) \sum_{k} \theta (k_F - |k|) \theta (k_F - |k - q_z + h|) \exp \left[ -\frac{t_B^2 q_h^2}{2} - \frac{\epsilon^2 d_s^2 q_h^2}{2} \right]. \] (4.7)

The region of summation over \( k \) in the above formula is shown in Fig. 4. In order to derive the sum \( S \) we analyze the cases as follows: (1) \( S = 0 \) for \( q_z - h > 2k_F \), (2) \( S = \frac{L_z}{2\pi}(k_F - (q_z - h - k_F)) \) for \( 0 < q_z - h \leq 2k_F \), (3) \( S = \frac{L_z}{2\pi}(q_z - h + k_F - (-k_F)) \) for \(-2k_F < q_z - h \leq 0 \), and (4) \( S = 0 \) for \( q_z - h \leq -k_F \). As a result we summarize the four cases into a single expression given by

\[ S = \frac{L_z}{2\pi}2k_F \left( 1 - \frac{|q_z - h|}{2k_F} \right) \theta (2k_F - |q_z - h|). \] (4.8)

Therefore the energy per particle which contains the kinetic term is given in the thermodynamic limit by

\[ \epsilon^{HF} = \alpha - \frac{2t}{\sqrt{\pi}} \sin (\nu \pi) \]
\[-\frac{1}{2(2\pi)} \sum_{h} \int_{0+}^{\infty} 2\pi q_\perp dq_\perp \int_{-2k_F}^{h+2k_F} dq_z v(q) \left( 1 - \frac{|q_z - h|}{2k_F} \right) \exp \left[ -\frac{t_B^2 q_h^2}{2} - \frac{\epsilon^2 d_s^2 q_h^2}{2} \right]. \] (4.9)

At this stage we let \( \epsilon \to 0 \). It can be shown that the contribution of large \( q_z \) (\( \sim 1/\epsilon d_s \)) to the integration is negligible. To see this we observe that \( v(q) = \frac{1}{q_\perp^2 + q_\parallel^2} \) becomes \( \mathcal{O}(\epsilon^2) \) and summation over \( h \) converges in the limit of \( \epsilon \to 0 \). Therefore, \( \epsilon^{HF}_{\text{int}} \) becomes

\[ \epsilon^{HF}_{\text{int}} = -\frac{1}{2(2\pi)^2} \int_{0+}^{\infty} q_\perp dq_\perp \int_{-2k_F}^{2k_F} dq_z \sum_{h} \frac{4\pi \epsilon^2}{q_\perp^2 + (q_z + h)^2} \left( 1 - \frac{|q_z|}{2k_F} \right) \exp \left( -\frac{t_B^2 q_h^2}{2} \right). \] (4.10)

With use of the following formula:

\[ \sum_{n=-\infty}^{\infty} \frac{1}{x^2 + (y + 2\pi n)^2} = \frac{\sinh x}{2x (\cosh x - \cos y)}, \] (4.11)

we can accomplish the summation over \( h \) as

\[ \sum_{h} \frac{1}{q_\perp^2 + (q_z + h)^2} = \frac{d_s^2 \sinh d_s q_\perp}{2d_s q_\perp (\cosh d_s q_\perp - \cos d_s q_z)}. \] (4.12)

Consequently we obtain the following result:

\[ \epsilon^{HF}_{\text{int}} = \frac{\epsilon^2}{t_B} \frac{1}{2\pi d_s} \int_{0}^{\infty} ds \int_{0}^{2\pi/3} dt \left( 1 - \frac{t}{2\pi \nu} \right) \sinh s \frac{\sinh s}{\cosh s - \cos t} \exp \left( -\frac{s^2}{2d_s^2} \right). \] (4.13)

where \( d_s = d_s/l_B \) denotes the inter-layer distance in units of the magnetic length. Figure 4 shows \( \epsilon^{HF}_{\text{int}} \) as a function of the inter-layer distance. We remark that \( \epsilon^{HF}_{\text{int}} \) decreases with decreasing \( d_s \). This result originates from the fact that the inter-layer Coulomb interaction becomes more effective as layers get closer.
C. Comparison of Ground-State Energies

We first compare the Coulomb energy per particle of the three states. Figure 3 shows the results. The energy of the (111) state is obtained by the VMC calculation for 5 layers with 42 particles in each layer. For the multi-Laughlin and the itinerant states the result is shown for the infinite-size system. We remark the energy of the multi-Laughlin state does not depend on the inter-layer distance since all layers are independent of each other and electrons feel other layers neutral. In the region of $d_s \gtrsim l_B$ the Coulomb energy of the multi-Laughlin state is the lowest. This is evident because the system becomes a pile of almost independent two-dimensional layers in such a region. In the region of $d_s \lesssim l_B$ the (111) state has the lowest Coulomb energy. This result originates from the fact that the (111) state gains the inter-layer Coulomb energy at the cost of the intra-layer one in the region where intra- and inter-layer interactions are comparable. With respect to the itinerant state, the Coulomb energy decreases in the region of $d_s \lesssim l_B$. There is however no region where it is the lowest.

So far we have considered only the Coulomb energy. We must take into account the tunneling energy of the itinerant state in order to compare the total energies of the three states. Let us assume that the transfer energy $t$ depends on the inter-layer distance as

$$t = A \exp(-\alpha d_s),$$  \hspace{1cm} (4.14)

where $A$ and $\alpha$ are constants. Then as shown in Fig. 4 we find a region of $d_s$ where the itinerant state has the lowest total energy. Here we put appropriate values into $A$ and $\alpha$, namely $A = 0.2 e^{+2}/l_B$, $\alpha = 1.0/l_B$ for a case shown as $t_1$, and $A = 0.3 e^{+2}/l_B$, $\alpha = 0.6795/l_B$ for another case shown as $t_2$. The parameters for $t_2$ with $B = 10 T$ are chosen to reproduce the band width of $4t = 2.5$ meV $= 0.179 e^{+2}/l_B$ at $d_s = 0.226 A = 2.8 l_B$ which seems appropriate for a GaAs/AlGaAs superlattice.

On the basis of the comparison we propose a phase diagram as shown in Fig. 8 for the ground state of the present system in the plane of $t$ and $d_s$. If we assume the relation (4.14) between $t$ and $d_s$ in the diagram, possible states follow a curve in Fig. 8 as $d_s$ is varied. Depending on the parameters $A$ and $\alpha$, there are either single transition ($t_1$) or double transitions ($t_2$). Consequently the phase diagram Fig. 8 is interpreted as follows.

(i) In the region $d_s \gg l_B$, the system is a pile of independent two-dimensional layers and the incompressible multi-Laughlin state is stable.

(ii) In the region of $d_s \lesssim l_B$ and the tunneling energy is small ($t \lesssim 0.1 e^{+2}/l_B$), the (111) state which is also incompressible is stabilized instead of the multi-Laughlin state by the inter-layer correlation.

(iii) When the tunneling energy is large, the compressible itinerant state is stabilized by competition of the tunneling energy and the Coulomb energy.

V. DISCUSSION

We compared the result of the (111) state for a finite size system and that of the multi-Laughlin and the itinerant states for the infinite size system. The finite size ($N_1$ and $N_2$) correction should be taken into account in the (111) state for more quantitative discussion. While we have no information with respect to the dependence on $N_2$, the following remark is given from Fig. 3 about the dependence on $N_1$. When one increases $N_1$ the Coulomb energy much increases in the region of $d_s \gg l_B$. While for $d_s \sim l_B$ the Coulomb energy looks almost independent of $N_1$ within the error bars. Since the boundaries of the (111) state occurs with $d_s/l_B < 2$ in Fig. 8, the finite-size correction should not change the results qualitatively.

It should be possible to observe transitions in actual systems by adding a pressure to the system or tilting the magnetic field. Since adding a pressure corresponds to control of $d_s$, a change of parameters along a curve like $t_1$ or $t_2$ in the diagram Fig. 8 is expected. On the other hand tilting the magnetic field corresponds to control of $t$ independent of $d_s$ because the horizontal component of the magnetic field works on electrons to localize in the vertical direction and reduces $t$. Then the parameter change along a vertical straight line at a certain $d_s$ in Fig. 8 is expected.

The transition between incompressible and compressible states is analogous to the Mott transition in the Hubbard model. Namely the incompressible multi-Laughlin and (111) states correspond to an insulator, while the compressible itinerant state corresponds to a metal. The transition between incompressible and compressible states occurs due to competition of the transfer (tunneling) and the on site (intra-layer) Coulomb energy. In our model we estimate that the critical transfer energy is almost $0.1 e^{+2}/l_B$.

Although we discussed only three trial states for $\nu = 1/3$ in the present study, we cannot exclude the possibility of other states. In terms of two-dimensional incompressible states for $\nu = 1/3$, it is difficult to construct states.
more stable than the multi-Laughlin and the (111) states within the simple family of Jastrow-type functions. One may however ask whether other states with three-body correlation or even more correlations are more favorable energetically. For three-dimensional compressible states, the itinerant state is taken to be the simplest homogeneous state. Then inhomogeneous states like CDW [20,21] should also be discussed for more refined argument. Furthermore we have neglected the spin degree of freedom which may be relevant to some systems. For example the SDW state, which accounts for the QHE of (TMTSF)$_2$X [13], can be a relevant state depending on parameters in the system.

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APPENDIX: VMC METHOD FOR THE (111) STATE

We describe the method of numerical calculation for the (111) state in this appendix. The expectation value of the Coulomb energy for the (111) state is represented by

$$\langle \epsilon^{(111)} \rangle = \frac{1}{(2\pi)^2} \int d\mathbf{q}_\perp \tilde{V}_{\mathbf{q}_\perp} (\mathbf{q}_\perp) e^{i\mathbf{q}_\perp \cdot (\mathbf{r}_- - \mathbf{r}_+)}$$

(A1)

We can obtain the numerical value of $\epsilon^{(111)}$ for finite size (finite particles) systems by the VMC method. In evaluating the second term with minimum statistical errors, we separate the variables in it and reduce the expectation value of the quantity between two bodies to that of one body. For this purpose we introduce the Fourier transform of the Coulomb potential $\tilde{V}$, one body distribution function $f$, and its Fourier transform $g$ as follows:

$$\tilde{V}_{\mathbf{q}_\perp} (\mathbf{q}_\perp) = \frac{4\pi e^2}{q_\perp} \exp \left( -q_\perp \frac{L_z}{\pi} \sin \left( \left| \mathbf{z} - \mathbf{z}' \right| \right) \right)$$

(A3)

$$f (\mathbf{r}_\perp) = \frac{1}{(2\pi)^2} \int d\mathbf{q}_\perp \tilde{V}_{\mathbf{q}_\perp} (\mathbf{q}_\perp) e^{i\mathbf{q}_\perp \cdot (\mathbf{r}_- - \mathbf{r}_+)},$$

(A4)

$$g (\mathbf{q}_\perp) = \frac{1}{(2\pi)^2} \int d\mathbf{r}_\perp f (\mathbf{r}_\perp) e^{-i\mathbf{q}_\perp \cdot \mathbf{r}_\perp}$$

(A5)

where we wrote $z/d_s$ as $\mathbf{z}$. Then the second term $V_2$ in (A1) is arranged into

$$V_2 = -\frac{1}{2} \frac{1}{(2\pi)^2} \int_0^\infty N_\perp^2 \sum_{l,l'} 2\pi q_\perp dq_\perp \tilde{V}_{\mathbf{q}_\perp} (\mathbf{q}_\perp) g (\mathbf{q}_\perp)^2$$

(A6)
We use this formula to obtain the numerical value of $V_2$. Figure 3 shows an example of numerical results. The integral with respect to $q_\perp$ is performed by the trapezoidal rule because only discrete values of $q(q_\perp)$ are obtained by the VMC calculation. We cut off the upper region in the integral at a finite value of $q_c (\gg 1/l_B)$ because the integrand converges to zero near $q_\perp \sim q_c$ and its contribution to the integral is negligible in the region $q_c < q_\perp < \infty$.

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FIG. 1. Configuration of the infinite-layer system. Layers are arranged perpendicular to the $z$-axis with the inter-layer distance $d_s$. A magnetic field is applied along the $z$-direction.

FIG. 2. Coulomb energy per particle of the multi-Laughlin state. The four points correspond to the particle number per layer $N_\perp = 20, 30, 42$ and 72. The error bar indicates the Monte Carlo error. We estimate the value in the thermodynamic limit by extrapolating the line which fits the four points with the least squares method. The value is $-0.4089 \pm 0.0002 e^2/l_B$.

FIG. 3. Coulomb energy per particle of the (111) state vs. the inter-layer distance. The calculation is done for five layers with 20, 30 and 42 particles in each layer.

FIG. 4. Common regions where two step functions, $\theta(k_F - |k|)$ and $\theta(k_F - |k - q_z + g|)$, are nonzero. We have common regions in the cases (see text): (2) $0 < q_z - q \leq 2k_F$ and (3) $-2k_F < q_z - g \leq 0$. But we do not have a common region in the cases: (1) $q_z - g > 2k_F$ and (4) $q_z - g \leq -2k_F$.

FIG. 5. Coulomb energy per particle of the itinerant state in the thermodynamic limit.
FIG. 6. Comparison of Coulomb energies $\varepsilon$ per particle for the three states. The result on the (111) state is shown for a finite size system ($N_\perp = 42$ and $N_z = 5$), while the other two results are shown for the infinite size system ($N_\perp = \infty$ and $N_z = \infty$). The (111) state has the lowest energy in the region of small inter-layer distance while the multi-Laughlin state becomes stable for large $d_s$. The crossing of the two states occurs near $d_s \sim l_B$. The itinerant state has no region where its Coulomb energy is the lowest.

FIG. 7. Energy per particle of the itinerant state with the tunneling energy. We assume the dependence of $t$ on the inter-layer distance as $t = A \exp(-\alpha d_s)$ and show two exemplary cases.

FIG. 8. Proposed phase diagram in the plane of $t$ and $d_s$. The solid lines are drawn on the basis of the VMC calculation for the (111) state of the finite size system ($N_\perp = 42$ and $N_z = 5$). The boundary with the itinerant state is determined from comparison with the Hartree-Fock calculation in the thermodynamic limit.

FIG. 9. An example of $g(q)$ calculated by VMC method. Calculation is performed for the system with $N_\perp = 20$ and $N_z = 5$. 

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$\frac{\epsilon_L}{[\epsilon^* / l_B]}$ vs $N^{-1/2}$
\[ \frac{\varepsilon_{(111)}}{[e^*e']/l_B]} \]

- \( \square \) \( N = 42 \)
- \( \bigcirc \) \( N = 30 \)
- \( \bigtriangleup \) \( N = 20 \)
\[ \frac{\varepsilon}{|e^{*2}|/l_B} \]

\[ d_s/l_B \]

- \( t=0 \)
- \( t_1 (A=0.2, \alpha=1.0) \)
- \( t_2 (A=0.3, \alpha=0.6795) \)
Laughlin (111)

\[ t_1 \ (A=0.2, \alpha=1.0) \]

\[ t_2 \ (A=0.3, \alpha=0.6795) \]

itinerant

multi

Laughlin

(111)
