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Numerical Study of Quantum Hall Bilayers at Total Filling $\nu_T = 1$: A New Phase at Intermediate Layer Distances

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We study the phase diagram of quantum Hall bilayer systems with total filling $\nu_T = 1/2 + 1/2$ of the lowest Landau level as a function of layer distances d . Based on numerical exact diagonalization calculations, we obtain three distinct phases, including an exciton superfluid phase with spontaneous interlayer coherence at small d , a composite Fermi liquid at large d , and an intermediate phase for $1.1 < d/l_B < 1.8$ (l_B is the magnetic length). The transition from the exciton superfluid to the intermediate phase is identified by (i) a dramatic change in the Berry curvature of the ground state under twisted boundary conditions on the two layers; (ii) an energy level crossing of the first excited state. The transition from the intermediate phase to the composite Fermi liquid is identified by the vanishing of the exciton superfluid stiffness. Furthermore, from our finite-size study, the energy cost of transferring one electron between the layers shows an even-odd effect and possibly extrapolates to a finite value in the thermodynamic limit, indicating the enhanced intralayer correlation. Our identification of an intermediate phase and its distinctive features shed new light on the theoretical understanding of the quantum Hall bilayer system at total filling $\nu_T = 1$.

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Introduction.—The multilayer quantum Hall systems demonstrate tremendously rich physics when tuning the interlayer interaction by changing layer distance d . One of the prominent examples is the bilayer systems[1–4] at a total filling $\nu_T = 1$ ($\nu = 1/2$ in each layer) with negligible tunneling. Experimentally, the bilayer systems can be realized in single wide quantum wells, double quantum wells or bilayer graphenes [5–9]. Theoretically, the quantum states in small and large d limits have been well understood. When the layer distance is small, the strong interlayer coulomb interaction drives the electron system into a pseudospin (layer) ferromagnetic long range order (FMLRO) state with the spontaneous interlayer phase coherence and interlayer superfluidity [10–14]. The FMLRO can also be described as an exciton condensation state as an electron in an orbit of one layer is always bound to a hole in another layer forming an exciton pair. This excitonic superfluid state can be described by Haldane “111 state” wavefunction [15, 16]. In the limit of infinite layer separation, the bilayer system reduces to two decoupled composite Fermi liquids (CFL)[17–21].

Several theoretical scenarios[22–35] have been proposed for understanding the transition between the exciton superfluid and CFL at intermediate layer distances. Due to its non-perturbative nature, controlled analytical method for this problem is still lacking, and numerical techniques have been playing an important role. Some numerical studies report a single phase transition, or a crossover, between the small and large distance regimes[36–38]. Meanwhile, an intermediate phase is found in ED and variational studies [39–42], where the p -wave paired composite fermions state [40, 41] is proposed. Until now it remains controversial for the phase at intermediate distances.

On the experimental side, transport measurements indicate a transition between an exciton condensed interlayer coherent incompressible quantum Hall effect state and compress-

ible liquid with varying the layer distance[43–46]. At smaller layer distance, the total Hall conductance is quantized to e^2/h . A strong enhancement in the zero-bias interlayer tunneling conductance [47] and the vanishing of the Hall counterflow resistance [46, 48] provide evidence for interlayer coherence [4]. Above a critical distance $d \approx 1.6 \sim 2$ (in units of magnetic length l_B) which depends on the quantum well thickness, a compressible liquid state is found [4, 43–50]. However, the nature of the state at the intermediate distance is unsettled after numerous investigations[4].

Motivated by this unsolved issue, we perform an extensive ED study of $\nu = 1/2 + 1/2$ bilayer system on torus[51–53] up to 20 electrons, the phase diagram is summarized in Fig. 1. We identify signatures of two phase transitions between the exciton superfluid and the CFL at critical distances $d_{c_1} \approx 1.1$ and $d_{c_2} \approx 1.8$, respectively. For layer distance $d < d_{c_1}$, we establish the exciton superfluid state by the existence of Goldstone mode, vanishing of single pseudospin excitation gap and finite exciton superfluid stiffness. Furthermore, the Berry curvature shows strong fluctuation, leading to non-quantized drag Hall conductance which is consistent with the gapless feature. For the intermediate layer distance $d_{c_1} < d < d_{c_2}$, we find the gapped single pseudospin excitation with even-odd effect, which is combined with a finite exciton superfluid stiffness. The drag Hall conductance is quantized to zero with no singularity in the Berry curvature, while the total Hall conductance remains exactly quantized to e^2/h . The quantum phase transition between the exciton condensed state and intermediate phase is identified by a dramatic change in the Berry curvature of the ground state under twisted boundary conditions on the two layers, and the level crossing with a change of the nature of the low-lying excitations at $d = d_{c_1}$. The fact of level crossing near d_{c_1} is consistent with previous studies[37, 39, 42]. The second transition between the intermediate phase and the CFL is characterized by the vanishing of the exciton super-

fluid stiffness. Further discussions of the finite size effect of numerical simulation can be found in supplementary materials.

Model and Method.— We consider bilayer electron systems subject to a magnetic field perpendicular to the two dimensional (2D) planes. We use torus geometry with the length vectors \mathbf{L}_x and \mathbf{L}_y , and an aspect angle θ between them. Here, $L_x = L_y = L$ and $\theta = \pi/2$ for most of calculations. The magnetic length $l_B \equiv \sqrt{\hbar c/eB} \equiv 1$ is set to be the unit of the length and N_ϕ represents the number of magnetic flux quanta determined by $|L_x L_y \sin\theta| = 2\pi N_\phi$. In the presence of strong magnetic field, the Coulomb interaction, projected onto the lowest Landau level, is written as

$$V = \frac{1}{2\pi N_\phi} \sum_{i < j, \alpha, \beta} \sum_{\mathbf{q}, \mathbf{q} \neq 0} V_{\alpha\beta}(q) e^{-q^2/2} e^{i\mathbf{q} \cdot (\mathbf{R}_{\alpha,i} - \mathbf{R}_{\beta,j})}. \quad (1)$$

Here, $\alpha(\beta) = 1, 2$ are indices of two layers (which are the two components of a pseudospin $1/2$), $V_{\alpha,\alpha}(q) = 2\pi e^2/(\varepsilon q)$ and $V_{12}(q) = V_{21}(q) = 2\pi e^2/(\varepsilon q) \cdot e^{-qd}$ are the Fourier transformations of the intralayer and interlayer Coulomb interactions, respectively. d is the distance between two layers and $\mathbf{R}_{\alpha,i}$ is the guiding center coordinate of the i th electron in layer α . In the present work, we consider the physical systems with two identical 2D layers (with zero width) in the absence of electron interlayer tunneling while spins of electrons are fully polarized due to strongly magnetic field.

We use ED algorithm to study the energy spectrum and state information on torus. In order to study the physics of the pseudospin sector, we generalize the periodical boundary condition to twisted boundary condition with phase $0 \leq \theta_\lambda^\alpha \leq 2\pi$ along λ direction in the layer α . By a unitary transformation, one can get the the periodic wave function Ψ on torus with $|\Psi\rangle = \mathbf{exp}[-i \sum_\alpha \sum_i ((\theta_x^\alpha/L_x)x_i^\alpha + (\theta_y^\alpha/L_y)y_i^\alpha)] |\Phi\rangle$. Then the Berry curvature is defined by $F(\theta_x^\alpha, \theta_y^\beta) = \mathbf{Im}(\langle \partial\Psi/\partial\theta_x^\alpha | \partial\Psi/\partial\theta_y^\beta \rangle - \langle \partial\Psi/\partial\theta_y^\beta | \partial\Psi/\partial\theta_x^\alpha \rangle)$. The integral over the boundary phase unit cell leads to the topological Chern number matrix $C_{\alpha,\beta} = 1/2\pi \int d\theta_x^\alpha d\theta_y^\beta F(\theta_x^\alpha, \theta_y^\beta)$, which contains topological information for the bilayer quantum Hall state[38, 55–60]. Numerically, applying common and opposite boundary phases on two layers, one can obtain the Hall conductances in the layer symmetric and anti-symmetric channel, denoted by $C^c(e^2/h)$ and $C^s(e^2/h)$, respectively. The drag Hall conductance, defined by $\sigma_{xy}^d = (C^c - C^s)(e^2/2h) = (C_{1,2} + C_{2,1})(e^2/h)$, can be obtained directly by calculating $C_{1,2}$ (or $C_{2,1}$), corresponding to twisting boundary phases along x direction in one layer and along y direction in another layer. One can also obtain the exciton superfluid stiffness when applying twisted boundary phases[38].

Energy Spectrum and Pseudospin Excitation Gap.—In Fig. 2 (a), we show the lowest energies in each momentum sector for different layer distances d . For smaller layer separations $d \lesssim 1.1$, indeed we find the low energy excitation has the form of linear dispersing Goldstone mode for small momenta[54]. One can also measure the pseudospin excita-

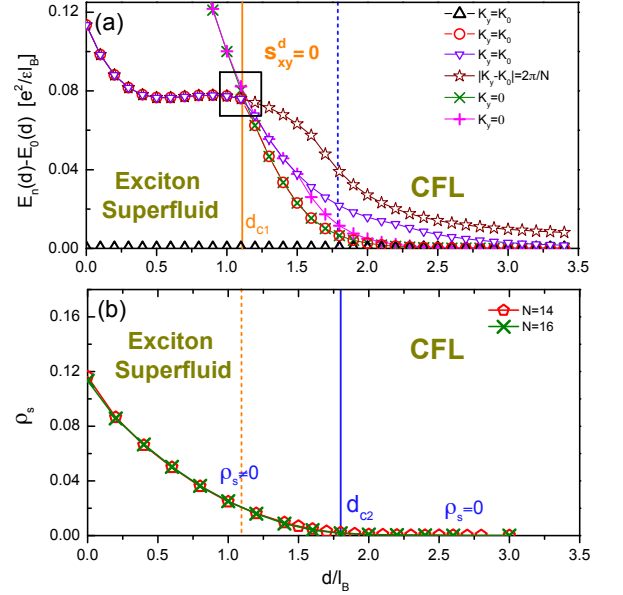


Fig. 1: (Color online) The phase diagram of $\nu = 1/2 + 1/2$ quantum Hall bilayers with varying layer distance d/l_B . We identify three phases: exciton superfluid phase, the intermediate phase and composite Fermi liquid (CFL) phase. (a) The transition from exciton superfluid to intermediate phase near $d_{c1} \approx 1.1$ is identified by the drag Hall conductance σ_{xy}^d and the energy level crossing. Here, the ground state is in the momentum sector $K_0 = \pi$ and $N = 16$. (b) The transition from intermediate phase to CFL phase near $d_{c2} \approx 1.8$ is identified by the exciton superfluid stiffness ρ_s [see Eq. 2].

tion gap directly, which represents the energy cost of moving one electron from one layer to another layer and is defined as $\Delta_{ps}(d) \equiv E_0(N_\uparrow, N_\downarrow, d) - E_0(N/2, N/2, d) + d \cdot S_z^2/N_\phi$. Here, $N_\uparrow = N/2 + \Delta N$ and $N_\downarrow = N/2 - \Delta N$ denote the number of electrons in two layers for $S_z = \Delta N = 1, 2, \dots$ excitation. The energy shift $d \cdot S_z^2/N_\phi$ is the charge energy induced by the imbalance of electron number in two layers with total pseudospin S_z [61]. As shown in Fig. 2 (b), the finite size scaling of $\Delta_{ps}(d)$ for $S_z = 1$ goes to zero in the thermodynamic limit for $d \lesssim 1.1$.

As for layer distance $d \gtrsim 1.1$, the low energy linear dispersion spectrum moves up in energy [see Fig. 2 (a)] with new lower energy excitations appearing at other momenta sectors for $d \gtrsim 1.1$ as shown in Fig. 1 (a). For the layer distance $d \approx 1.1$, the energy spectrum shows the level crossing of the first excited states between the $K_y = \pi$ (or $K_y = 0$) and $|K_y - K_0| = 2\pi/N$ sectors (see Fig. 1(a)). Although the ground state still locates in $K_y = K_0$ sector at $d \approx 1.1$, the level crossing for the first excited state indicates the change of the low-lying energy spectrum for the bilayer systems. Here, level crossing also characterizes a phase transition based on the indications of pseudospin gap.

For $d \gtrsim 1.1$, the $S_z = 1$ pseudospin excitation displays even-odd effect determined by the electron number in each layer [see the inset of Fig. 2 (c)], indicating of the trend of

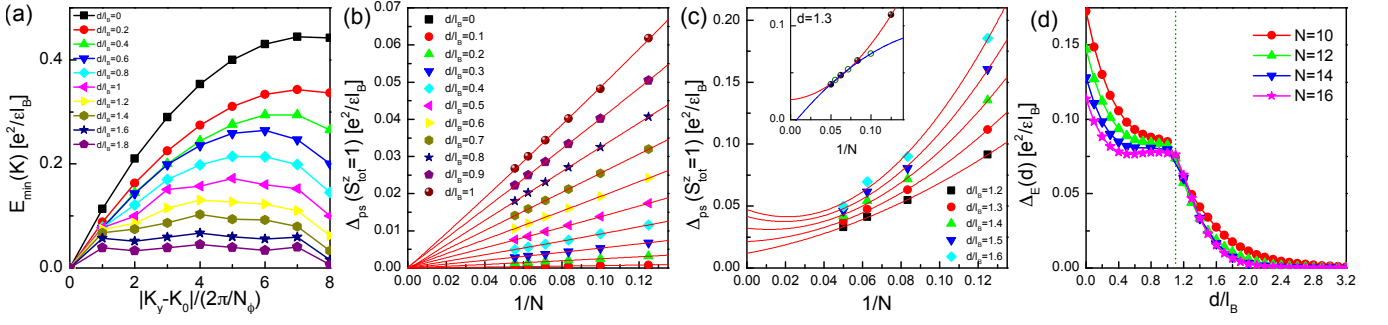


Fig. 2: (Color online) (a) The energy dispersion curves of lowest-energy excitations at each momentum sector. Here, the ground state is in the momentum sector $K_0 = \pi$. (b) and (c) show finite size scaling of the single pseudospin excitation gap Δ_{ps} by using parabolic function for layer distance $d/l_B < 1.1$ (b) and $d/l_B > 1.1$ (c). The inset of (c) indicates the even-odd effect in the intermediate phase up to $N = 20$. (d) The energy spectrum gap $\Delta_E \equiv E_1(d) - E_0(d)$ as a function of d/l_B . The cusp near $d/l_B \approx 1.1$ indicates the level crossing for the excited states.

intralayer pairing. As shown in Fig. 2 (c) with system sizes up to 20 electrons, the finite size scaling indicates gapped pseudospin excitation for even electron number in each layer, while it is gapless when the electron number in each layer is odd. One should be careful in the fitting due to limited number of data points, however, the finite pseudo-spin excitation gap is also implied by the disappearance of linear dispersion mode [see Fig. 2 (a)], the flat Berry curvature, and well-defined spectrum gap when twisting boundary conditions [see Fig. 3 (b) and (d) below].

Fig. 2 (d) shows the energy gap $\Delta_E(d) \equiv E_1(d) - E_0(0)$ between two lowest energy states, one can find that the cusp due to the level crossing for the lowest energy excitations near the transition point $d_{c_1} \approx 1.1$ is robust and independent on the lattice size, indicating the intrinsic property of such a transition. Clearly, we have identified a transition from the gapless pseudospin FMLRO state at smaller distance to the intermediate phase with new low-lying excitation and finite pseudospin gap.

Berry Curvature and Energy Spectrum Under Twisted Boundary Conditions.— The transition near $d_{c_1} \approx 1.1$ can also be identified by the Berry curvature $F(\theta_x^\alpha, \theta_y^\beta)$ and the energy spectrum under twisted boundary conditions. Physically, a gap state has a well-defined smooth Berry curvature, while a gapless state may have singular Berry curvature associated with gapless points in low energy spectrum. Fig. 3 (a) and (b) show the Berry curvatures at the $d < d_{c_1}$ and $d_{c_1} < d < d_{c_2}$ by applying $\theta_x^1 = \theta_x$, $\theta_x^2 = 0$ and $\theta_y^1 = 0$, $\theta_y^2 = \theta_y$ for the lowest energy state in the sector (π, π) . Fig. 3 (a) shows the strong fluctuation of the Berry curvature, suggesting the gapless pseudospin spectrum when $d < d_{c_1}$. The Berry phase is not well defined due to near level crossing (with Berry phase integrated over each singular point only defined up to the fractional part of 2π), which gives rise to the non-quantized drag Hall conductance in this regime[38]. Since the Hall conductance in the symmetric channel is well defined in this regime, the non-quantized drag Hall conductance indicates gapless feature of the antisymmetric channel. On the

other hand, the Berry curvature is near flat without any singularity in $d_{c_1} < d < d_{c_2}$ regime [see Fig. 3 (b)], which is consistent with the well-defined single pseudospin excitation gap in this phase. Furthermore, the integral of the Berry curvature gives us zero drag Hall conductance in the intermediate phase, indicating the well defined Hall conductance in symmetric channel or finite charge gap in the intermediate phase. We also find that Berry curvatures in all four sectors $(0, 0)$, $(0, \pi)$, $(\pi, 0)$, (π, π) always have similar features and twisting boundary phases will connect the ground state (π, π) to the other three states. In Fig. 3 (c) and (d), one can find the energy spectrum of the lowest two states in the same momentum sector $(K_x, K_y) = (\pi, \pi)$ with twisted phases. Here, we map the phase θ_x, θ_y into one-dimensional quantity $\theta \equiv 10\theta_x + \theta_y$ for convenience of plotting. The singularity in the Berry curvature for $d < d_{c_1}$ originates from the energy level crossing as the bilayer relative boundary phase θ_y approaching 2π in contrast to the behavior in the $d > d_{c_1}$ regime, where a small gap opens to separate the lowest two states, indicating the existence of the pseudospin gap. Based on the above analysis, we confirm that the pseudospin Berry curvature also indicates the phase transition taking place near d_{c_1} .

Exciton Superfluid Stiffness.— To study the evolution of exciton superfluidity with the layer distances, we obtain the exciton superfluid stiffness ρ_s by adding a small twisted boundary phase[38], which is proportional to the superfluid density and identifies the energy cost when one rotates the order parameter of the magnetically ordered system by a small angle. In our ED calculation, the exciton superfluid stiffness can be obtained according to

$$E(\theta_t)/A = E(\theta_t = 0)/A + \frac{1}{2}\rho_s\theta_t^2 + O(\theta_t^4), \quad (2)$$

where $E(\theta_t)$ is the ground-state energy with twisted (opposite) boundary phases θ_t between two layers $\theta_t = \theta_x^1 - \theta_x^2$ ($\theta_y^{1,2} = 0$), $A = |\mathbf{L}_x \times \mathbf{L}_y|$ is the area of the torus surface. Fig. 3 (c) to (e) show the energy spectrum as a function of twisted phases for different layer distance. At smaller layer

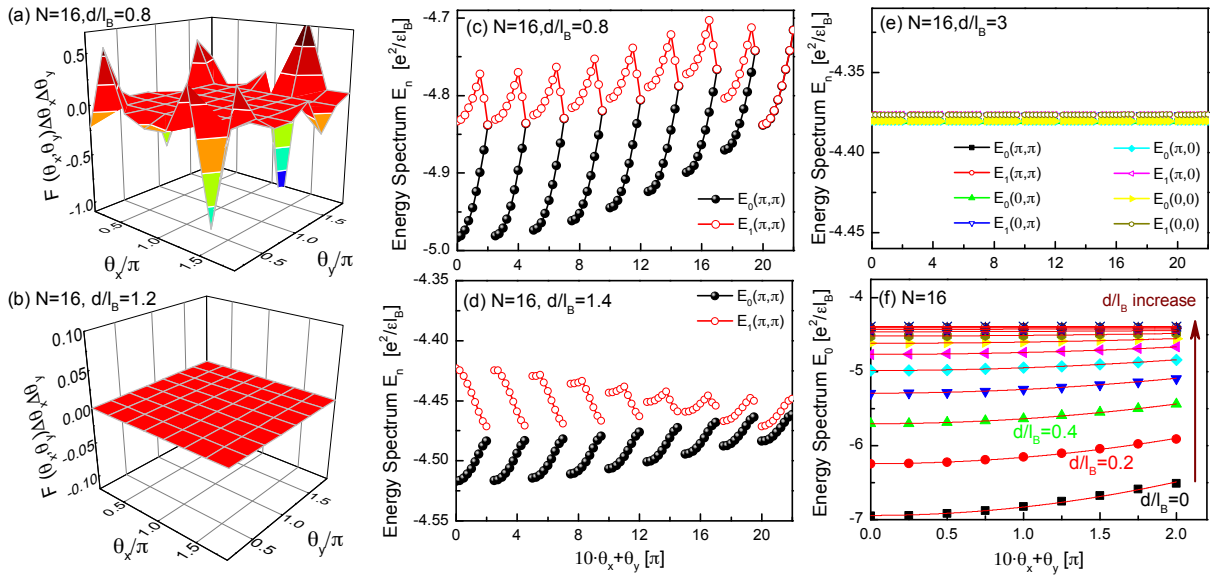


Fig. 3: (Color online) The Berry curvature $F(\theta_x^\alpha, \theta_y^\beta)$ for $d/l_B=0.8$ (a), $d/l_B=1.2$ (b). Here, $\Delta\theta_x$ and $\Delta\theta_y$ are the interval of mesh in phase space. It has strong fluctuation in FMLRO phase (a), while it is smooth in the intermediate phase (b). (c) to (e) are energy spectrum of $N = 16$ system with twisted boundary phases for $d/l_B=0.8$ (c), $d/l_B=1.4$ (d) and $d/l_B=3$ (e). By fitting the energy spectrum with twisted phases, one can get the exciton superfluid stiffness ρ_s [see Eq. 2] (f), which decreases with the layer distance and finally vanishes for $d > d_{c2}$. (f) From bottom to top, d/l_B increases from $d/l_B = 0$ with interval 0.2.

separation, one can find the ground state energy increases with tuning the twisted phases [see Fig. 3 (c) and (d)]. By fitting the energy curve using the quadratic function [see Fig. 3 (f)], we get the exciton superfluid stiffness ρ_s , which decreases with the increase of the layer distance, and finally falls down to a negligible value for $d > d_{c2}$ [see Fig. 1 (b)]. As shown in Fig. 3 (e), the energy almost does not change with the twisted phases for larger distances, indicating the vanish of superfluidity and the decoupling of two layers for $d > d_{c2}$, corresponding to CFL states.

Discussion.— We study the phase diagram of $\nu = 1/2 + 1/2$ quantum Hall bilayers on torus and find that the exciton superfluid phase and CFL phase are separated by an intermediate phase, which exhibits finite exciton superfluid stiffness, flat Berry curvature, zero drag Hall conductance and even-odd effect of pseudospins.

Theoretical interpretation of the intermediate phase may start from two well known limits. Starting from the infinite distance, it is nature to choose composite Fermion (CF) picture[31–34, 63]. Recently, a fully gapped interlayer pairing phase is proposed based on random-phase approximation calculation[33], which is consistent with our numerical findings of flat Berry curvature as well as gapped spin-1 and charge excitations, but the explanation of finite exciton superfluid stiffness is lacking. The other candidate, interlayer coherent CFL (ICCFL)[31] state, has finite pseudospin stiffness due to interlayer $U(1)$ phase fluctuations and possesses quantized Hall conductance in antisymmetric channel, which is consistent with our ED findings on finite pseudospin gap and flat Berry curvature. However, ICCFL indi-

cates compressible property with respect to symmetric current, while our numerical data indicates finite charge gap as well as enhanced intralayer correlation [see supplementary material]. To understand the physics in charge channel better, one may start from the small distance limit in the composite boson (CB) picture[28, 42, 62] and assuming the system is $\nu = 1$ integer quantum Hall state. Based on recent proposed wavefunction[62], the $SU(2)$ symmetry for CBs emerges near d_{c1} , leading to the level crossing of first excited state[see Fig.1(a)]. The low-lying charge excitation is dominated by interlayer bound state of CB merons for $d < d_{c1}$ while it is replaced by intra-layer bound state of CB merons for $d_{c1} < d < d_{c2}$, which explains the finite charge gap or quantized charge Hall conductance and the enhanced intralayer correlations in the intermediate phase.

When taking both limits into account, a mixed-state representation with considering both interlayer and intralayer correlations has been intensively studied[28, 40–42, 64]. Such mixed representation leads to a p -wave interlayer pairing phase[40, 41] or the superfluid disordering phase [42] in the intermediate distance, which are consistent with numerical finding of the incompressibility in charge channel and the disappearance of Goldstone mode as the lowest energy excitation [64]. However, to explain all of numerical data consistently, it seems that one has to take into account the interplay between the interlayer and intralayer correlations, which is still a theoretical challenge and calls for further theoretical study.

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