Quantum Hall bilayer in dipole representation

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The Quantum Hall Bilayers (QHB) at filling factor $\nu = 1$ represents a competition between Bose-Einstein condensation (BEC) at small distances between layers and fermionic condensation, whose influence grows with distance and results in two separate Fermi liquid states for the underlying quasiparticles at very large (or infinite) distances. The question that can be raised is whether, at intermediate distances between layers, a distinct phase exists or if a singular transition occurs, with the possibility that this happens at infinite distances. Here, using a dipole representation for fermionic quasiparticles, we find support for the latter scenario: Within a large and relevant range of distances, BEC condensation, identified as Cooper s-wave pairing of dipole quasiparticles, prevails over both Cooper p-wave pairing and s-wave excitonic pairing of the same quasiparticles.

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I. INTRODUCTION

The QHB [1,2] is a fractional quantum Hall effect (FQHE) system with an additional layer degree of freedom: Two layers of two-dimensional electron gases at distance d from each other are pierced by a strong magnetic field, B, perpendicular to the layers. The total density of the system, n_T, matches the density of available states in the (lowest) Landau level (LL), $(eB)/h$, in which electrons live. Thus the total filling factor is $\nu_T = n_T(2\pi l_B^2) = 1$, with the characteristic length of the system, $l_B = \sqrt{\hbar/(cB)}$, the magnetic length.

Therefore, each layer is half-filled, i.e., it represents a system of electrons that occupy half of the available states in the lowest LL (LLL), and thus $\nu_T = \nu_\uparrow + \nu_\downarrow$, $\nu_\sigma = 1/2$, $\sigma =\uparrow, \downarrow$, where the up and down signs refer to a specific layer. At long distances, $d \gg l_B$, the layers are almost independent, at least much less intertwined, and at $d \lesssim l_B$, they are strongly coupled and an excitonic binding between a hole in one layer and a particle in the opposite one dominates. Thus, a distance, $\bar{d} \sim l_B$, may represent a characteristic distance for the transition from a strong-coupling to a weak-coupling regime for the system of two layers, and a question can be raised: What happens at these intermediate, $d \sim l_B$ distances? A new intermediate phase, a single transition between two phases (connected with two extremes, small and large distances), or a crossover with no phase transition? Various scenarios appeared in the literature and in this work we will address this question using a special formalism.

The first proposals for multicomponent FQHE systems and studies of the QHB in Refs. [3–6] were followed by experiments [7,8] that confirmed the integer QHE for small distances between the layers in the case of the QHB. Further development of the theoretical understanding of the system at $d \lesssim l_B$, as an excitonic condensate or an ordered state of the pseudospin of electrons [9–12], was followed by experiments [13,14] that revealed the new ordered state and phase at small distances. On the other hand, there is an expectation that at large distances ($d \gg l_B$), we have well-separated layers, each in a compresssible state [15] of a single layer at filling factor 1/2 [16,17].

Many theoretical, analytical, and numerical studies have been done [9–12,18–51] in order to understand the evolution of the QHB with distance; in particular with the assumption of the projection of the physics into the LLL in the absence of disorder. The modeling and understanding of the FQHE is based on the composite excitations—particles which are often identified as composite fermions (CFs) [52–54].

In the case of the single-layer at filling factor 1/2, and under assumption that all electrons are in the LLL, composite fermion can be viewed as a composite of electron and its correlation hole, which represents a unit of a positive charge. Thus CF is an overall neutral fermionic object which can make a Fermi sea of CFs (and we may expect a compressible behavior of the system). If we apply a classical analogy, such an overall neutral composite, in an external magnetic field, B, then it must have its momentum proportional to its dipole moment, and at and near Fermi surface we have dipoles [55–57]. This dipole picture is a direct consequence of the projection into a LL [55–57].

Nevertheless, there is an additional feature of the system of electrons that fill half of available states in a LL: The physics should be invariant under exchange of particles and holes, i.e., we have a particle-hole (PH) symmetry and, together with CFs, we should also consider and incorporate composite holes (CHs) in our description to have the PH symmetry manifestly represented. To include the PH symmetry, a two component Dirac-type description was introduced in Ref. [58] for the description of half-filled LL. But, to describe, in a Fermi-liquid (FL) framework, a half-filled LL of electrons, we may also consider a variant of the dipole construction in a one-component fermion formalism, as introduced in Ref. [59]. This construction is a generalization of the dipole, i.e., CF representation in the case of bosons at filling factor $\nu = 1$ in the LLL [60,61], and it is applicable in the low-energy limit (of the effective FL description).

In this work, we applied the variant of the dipole representation that we developed [59], in order to understand the evolution of the QHB with distance. We identified, at all distances between layers, the presence of a single phase that can be described as an s-wave Cooper pairing of dipole quasiparticles. The underlying physics of this pairing is the excitonic attraction between electrons in one layer and holes in the opposite layer, and thus the phase that is well understood at small distances continues to exist at large distances. This scenario was proposed in Ref. [49], on the basis of the Dirac description [58] of the physics in each layer, and was numerically supported in a recent work [50] by modeling the system on a sphere. This work modeled the underlying physics as an attraction (Cooper pairing) between CF in one layer and CH in the other, opposite layer. In our study, using the formalism of Ref. [59], the nature of the dominant phase is further elucidated, as is the competition among other candidates for the ground state of the system as the distance d is varied. The s-wave Cooper pairing of dipoles prevails over a Cooper p-wave pairing and s-wave excitonic pairing of dipole quasiparticles. The excitonic pairing would represent a topological, incompressible phase inside an LLL. Our formalism and the BCS treatment of its setup are more accurate in the weak-coupling regime, and the confirmation at intermediate and large distances of the same phase (that is dominant in the strong-coupling regime at small distances) is, in this sense, reliable and supports the extension to all d's.

In the dipole formalism that we applied, in the case of bilayer, the dipole quasiparticles [which are neither CFs nor CHs but are symmetric objects that are consistent with the PH symmetry] enable a representation that has manifest symmetry under the exchange of particles and holes is done simultaneously in both layers. The dipole representation has additional, artificial degrees of freedom - correlation holes, which are identified with holes in the electron system(s). This unusual constraint, which we have to incorporate into the description, comes from the projection into a single LL of the states of fermionic quasiparticles that reside near the Fermi level (and most significantly influence the physics). To incorporate the constraint and use the mean-field method, we need to deal with effective Hamiltonians which are adapted to the use of the method by explicit inclusion of the constraint (as null operators) in their description. We focus (narrow possibilities) on small number of effective Hamiltonians which explicitly represent, in their forms, physics of potential phases. We solve them (in the mean-field approximation) and compare the energies of different Hamiltonians to find the most stable solution at distance d.

The paper is organized as follows. Section II provides a review of the dipole representation in a single layer. We discuss the key concepts and principles underlying the dipole representation and its relevance to our study. In Sec. III, we investigate the implications of the dipole representation in the QHB case and present results on the competition among phases and the resulting phase diagram. Finally, in Sec. IV, we summarize our findings and provide concluding remarks.

II. DIPOLE REPRESENTATION FOR HALF-FILLED LL

The dipole representation for half-filled LL is an extension of the formalism introduced for the description of the CF quasiparticles for a system of bosons at a filling factor $\nu = 1$ in an isolated LL [60,61]. In an enlarged space the CF annihilation operator, c_{mn}, is introduced as an operator with double indices, where each index corresponds to a state in a LL, $n, m = 1, 2, \ldots, N_\phi$, the left ($L$, physical) index is associated with a state of an elementary boson, and the right (R, artificial) index is associated with the state of the corresponding correlation hole. In the context of FQHE the correlation hole can be defined by a (local) insertion of flux quanta in the system and represents a well-defined object with charge and statistics. In the system of bosons, the many-body hole is fermionic, and the resulting composite object is a fermion, i.e., boson + correlation hole = CF. We may introduce the physical and artificial (of additional degrees of freedom) densities,

$$\rho^L_{nn'} = \sum_m c^\dagger_{mn} c_{n'm}, \tag{1}$$

and

$$\rho^R_{mm'} = \sum_n c^\dagger_{mn} c_{nm'}, \tag{2}$$

and their forms in the inverse space,

$$\rho^L_{\boldsymbol{q}} = \int \frac{d\boldsymbol{k}}{(2\pi)^2} c^\dagger_{\boldsymbol{k}-\boldsymbol{q}} c_{\boldsymbol{k}} \exp\left(i\frac{\boldsymbol{k}\times\boldsymbol{q}}{2}\right), \tag{3}$$

and

$$\rho^R_{\boldsymbol{q}} = \int \frac{d\boldsymbol{k}}{(2\pi)^2} c^\dagger_{\boldsymbol{k}-\boldsymbol{q}} c_{\boldsymbol{k}} \exp\left(-i\frac{\boldsymbol{k}\times\boldsymbol{q}}{2}\right), \tag{4}$$

which have the same form as the projected densities of systems of elementary particles into a single LL; they are nonlocal and obey the Girvin-MacDonald-Platzmann algebra. The collapse from the two-particle to a single-particle index $\boldsymbol{k}$ is physically enabled by the existence of the well-defined dipole object (CF) which momentum ($\boldsymbol{k}$) in the (external) magnetic field is proportional to its dipole moment.

To complete the description of the system we need to impose constraints in order to have as many degrees of freedom as required by the definition of the problem. It is not hard to see (due to the fact that the total number of CFs is equal to the number of bosons and due to their fermionic statistics) that we need to have $\rho^R_{nn} = 1$ for each n, or $\rho^R_{\boldsymbol{q}} = 0$ when $\boldsymbol{q} \neq 0$, in inverse space. In the case of the half-filled LL of electrons, details can be found in Ref. [59], we may formally proceed with the same constructions as in the previous case, but now the correlation holes have bosonic statistics. To have a well-defined description we need to impose $\rho^L_{nn} + \rho^R_{nn} = 1$ for each n or $\rho^L_{\boldsymbol{q}} + \rho^R_{\boldsymbol{q}} = 0$ when $\boldsymbol{q} \neq 0$ (which requires that correlation holes are hard-core bosons). But these constraints include the densities of the physical sector and thus have nontrivial influence on the physical degrees of freedom: The correlation holes are on the positions of the real (fermionic) holes. This is an unexpected constraint that opposes the usual interpretation of the correlation hole as a potential well for an elementary particle. Nevertheless, the constraint corresponds to the physics of the CFs near the Fermi level, i.e., to the most important, effective physics of the problem: The magnitude of the momentum of these CFs is $|\boldsymbol{k}| \sim k_F = 1/l_B$ (l_B is the magnetic length), and due to the projection to a fixed LL [55–57], this implies that the correlation hole is shifted, distanced from the electron for the same amount, $|\boldsymbol{k}|l_B^2 \sim l_B$. Furthermore, we consider the Hamiltonian of the problem in a PH symmetric form, one that is symmetric under exchange of particles and holes, i.e., L and R densities,

$$H = \frac{1}{2}\int \frac{d\boldsymbol{q}}{(2\pi)^2}\tilde{V}(|\boldsymbol{q}|)\frac{[\rho^L(-\boldsymbol{q})-\rho^R(-\boldsymbol{q})]}{2}\frac{[\rho^L(\boldsymbol{q})-\rho^R(\boldsymbol{q})]}{2}. \tag{5}$$

Because of the constraint and the implied PH symmetry, we may refer to the composite object not as a CF but simply as a dipole, i.e., a symmetric object which is neither CF nor CH.

III. THE QUANTUM HALL BILAYER IN DIPOLE REPRESENTATION

We begin with the Hamiltonian for the QHB in the second quantization, with electron density operators, $\rho_\sigma(\boldsymbol{q})$, $\sigma =\uparrow,\downarrow$ ($\uparrow$ and $\downarrow$ refer to the two different layers):

$$\mathcal{H}_e = \int \frac{d\boldsymbol{q}}{(2\pi)^2}\left\{\sum_\sigma \frac{1}{2}V(|\boldsymbol{q}|)\ :\rho_\sigma(\boldsymbol{q})\ \rho_\sigma(-\boldsymbol{q}): + V_{\uparrow\downarrow}(|\boldsymbol{q}|)\ \rho_\uparrow(\boldsymbol{q})\ \rho_\downarrow(-\boldsymbol{q})\right\}. \tag{6}$$

In the enlarged space formalism, the bilinears $\rho_\sigma(\boldsymbol{q})$ become

$$\rho_\sigma^L(\boldsymbol{q}) = \int \frac{d\boldsymbol{k}}{(2\pi)^2}c_\sigma^\dagger(\boldsymbol{k}-\boldsymbol{q})c_\sigma(\boldsymbol{k})\exp\left(i\frac{\boldsymbol{k}\times\boldsymbol{q}}{2}\right), \tag{7}$$

where formally we have, instead of electron annihilation and creation operators, the quasiparticle operators, $c_\sigma(\boldsymbol{k})$ and $c_\sigma^\dagger(\boldsymbol{k})$. Quasiparticles in the long-distance approximation can be interpreted as fermionic dipoles. In the Hamiltonian we recognize the intrainteraction terms with $V(|\boldsymbol{q}|) = (1/|\boldsymbol{q}|)\exp(-|\boldsymbol{q}|^2/2)$ and the interinteraction term with $V_{\uparrow\downarrow}(|\boldsymbol{q}|) = V(|\boldsymbol{q}|)\exp(-d|\boldsymbol{q}|)$, where d denotes the distance between the layers. We then proceed by using the dipole representation, which we find optimal for exploring the influence of the fermionic quasiparticles and physics that grows with distance. This representation allows the inclusion of the PH symmetry of the system (under exchange of all electrons, irrespective of index, and holes) in a manifestly invariant way in the Hamiltonian. We then proceed to utilize the dipole representation, which we find optimal for exploring the influence of the fermionic quasiparticles and the physics that evolves with distance.

By imposing the constraints,

$$\rho_\sigma^L(\boldsymbol{k}) + \rho_\sigma^R(\boldsymbol{k}) = 0 \quad \sigma =\uparrow,\downarrow, \tag{8}$$

that define the dipole representation in each layer, we place correlation holes where holes are, and thus the PH exchange is followed by the density exchange:

$$\rho_\sigma^L(\boldsymbol{k}) \leftrightarrow \rho_\sigma^R(-\boldsymbol{k}) \quad \sigma =\uparrow,\downarrow\ . \tag{9}$$

Therefore, the Hamiltonian can be written (by using the constraints) in an explicitly invariant form under this exchange:

$$\begin{aligned}\mathcal{H}_0 = \int \frac{d\boldsymbol{q}}{(2\pi)^2}\Bigg\{&\sum_\sigma \frac{1}{8}V(|\boldsymbol{q}|)\big[\rho_\sigma^L(-\boldsymbol{q})-\rho_\sigma^R(-\boldsymbol{q})\big]\\ &\times\big[\rho_\sigma^L(\boldsymbol{q})-\rho_\sigma^R(\boldsymbol{q})\big] + \frac{V_{\uparrow\downarrow}(|\boldsymbol{q}|)}{4}\big[\rho_\uparrow^L(-\boldsymbol{q})-\rho_\uparrow^R(-\boldsymbol{q})\big]\\ &\times\big[\rho_\downarrow^L(\boldsymbol{q})-\rho_\downarrow^R(\boldsymbol{q})\big]\Bigg\}.\end{aligned} \tag{10}$$

Note the absence of normal ordering due to the requirement that the constraints commute with the Hamiltonian in the physical space. This induces single particle terms (beside purely interacting) with effective mass M (due to the intralayer interaction) [62,63]. By treating the constraints as null operators (in the physical space), which we can include in the Hamiltonian, we reach forms of the Hamiltonian that are adapted to the mean-field approach, as they offer obvious interpretation which phase in the mean-field approach they support.

In the QHB case we can add and subtract (product of) constraints and define the following (effective) Hamiltonians:

$$\begin{aligned}\mathcal{H}_1 = \int \frac{d\boldsymbol{q}}{(2\pi)^2}\Bigg\{&\sum_\sigma \frac{1}{8}V(|\boldsymbol{q}|)\big[\rho_\sigma^L(-\boldsymbol{q})-\rho_\sigma^R(-\boldsymbol{q})\big]\\ &\times\big[\rho_\sigma^L(\boldsymbol{q})-\rho_\sigma^R(\boldsymbol{q})\big] + \frac{V_{\uparrow\downarrow}(|\boldsymbol{q}|)}{2}\\ &\times\big[-\rho_\uparrow^L(-\boldsymbol{q})\rho_\downarrow^R(\boldsymbol{q})-\rho_\uparrow^R(-\boldsymbol{q})\rho_\downarrow^L(\boldsymbol{q})\big]\Bigg\},\end{aligned} \tag{11}$$

and

$$\begin{aligned}\mathcal{H}_2 = \int \frac{d\boldsymbol{q}}{(2\pi)^2}\Bigg\{&\sum_\sigma \frac{1}{8}V(|\boldsymbol{q}|)\big[\rho_\sigma^L(-\boldsymbol{q})-\rho_\sigma^R(-\boldsymbol{q})\big]\\ &\times\big[\rho_\sigma^L(\boldsymbol{q})-\rho_\sigma^R(\boldsymbol{q})\big] + \frac{V_{\uparrow\downarrow}(|\boldsymbol{q}|)}{2}\\ &\times\big[\rho_\uparrow^L(-\boldsymbol{q})\rho_\downarrow^L(\boldsymbol{q})+\rho_\uparrow^R(-\boldsymbol{q})\rho_\downarrow^R(\boldsymbol{q})\big]\Bigg\}.\end{aligned} \tag{12}$$

The form of $\mathcal{H}_1$ emphasizes the excitonic attraction between densities from opposite layers (electron-hole attraction), which we expect to dominate physics at small distances. On the level of effective dipoles - composite particles (c's) this will translate to a strong instability to a Cooper pair formation between c's from different layers. On the other hand, the form of $\mathcal{H}_2$ is suggestive of excitonic pairing between c's from opposite layers. Indeed, in a mean-field treatment of $\mathcal{H}_1$ and $\mathcal{H}_2$, these instabilities can be identified as shown in Fig. 1. Details of the mean-field treatment are provided in the Appendix. For all distances considered, the s-wave ($l = 0$) Cooper pairing between layers has lower energy than the p-wave ($l = 1$) Cooper pairing and s-wave ($l = 0$) excitonic pairing. The s-wave excitonic phase of quasiparticles is similar to the one proposed in Ref. [45], which describes an interlayer correlated CF liquid (ICCFL). However, in our work, we operate within an LL, and the quasiparticles involved are (neutral) dipoles.

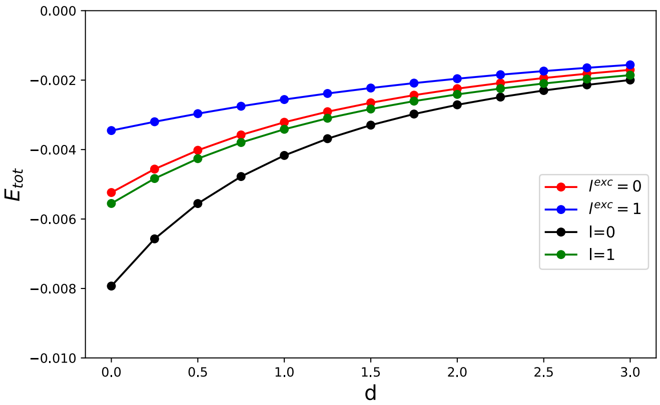

FIG. 1. The total energies of the ground states of effective Hamiltonians H_1 and H_2 as functions of the distance between layers; s-wave Cooper pairing of H_1 in black, p-wave Cooper pairing of H_1 in green, s-wave exciton pairing of H_2 in red, and p-wave exciton pairing of H_2 in blue.

In calculating total energies we applied a short-distance "cutoff" if necessary (if we encountered divergences). Though consistently defined on the whole $\boldsymbol{k}$ plane [61], the enlarged space description must be supplied with a natural "cutoff" (due to an intrinsic "lattice constant" l_B for this system): radius $k = \sqrt{2}/l_B$ of a circle in the $\boldsymbol{k}$ space, i.e., a volume of the available states in a single LL. In most cases the presence of Gaussians allows the extension of the integration over the whole space.

The exciton instability in the plotted range $d \in [0, 3l_B]$ can be described as an occupation of a single, lower band that is associated with the symmetric superposition: $[c_\uparrow(\boldsymbol{k}) + c_\downarrow(\boldsymbol{k})]/\sqrt{2}$. Thus a single, large Fermi sea exists in this range according to the mean-field calculation. Related to this is the excitonic binding of c's implied by $\mathcal{H}_0$ (with a dipole-dipole interaction that screens the bare Coulomb interaction) with the gap parameter, $\Delta_{\boldsymbol{k}} \sim |\boldsymbol{k}|^2$ (not a constant as in the case of $\mathcal{H}_2$). The total energy of this solution is negligible and may be relevant only for very large d when a transition to two decoupled Fermi seas takes place, i.e., for an equal population of symmetric and antisymmetric bands.

We applied the mean-field approach to the effective Hamiltonians and thus we may expect that our results are more reliable for larger d, i.e., weak coupling between layers. The weak-coupling assumption is completely justified for $d \sim 3l_B$ [see Fig. 1, weak attraction (pairing amplitudes), i.e., weak coupling can be recognized in small differences in total energies with respect to the asymptotic value, i.e., the free-fermion limit], and we may ask whether (at all, because of the strong coupling for $d \lesssim l_B$) a conclusion for the state of the system at any d can be drawn. But the nature of the predicted phase for $d \lesssim l_B$ (in the strong-coupling regime) in our formalism is the same as the one that is firmly confirmed in many calculations and approaches, a binding of the density of electrons with the density of holes in the opposite layers (opposite charge binding), and given that this phase (in our formalism) persists to large d (weak-coupling regime where the approach is fully reliable), we can conclude (assuming continuity, i.e., that a reentrant scenario is unlikely) that one and the same phase is present for all relevant distances including $d \gg l_B$.

In our approach, the binding of charges from opposite layers is described (effectively) as s-wave binding of dipoles of momenta $\boldsymbol{k}$ and $-\boldsymbol{k}$ and thus involves opposite dipole moments from opposite layers. This is similar to the binding described in Ref. [50], where a CF in one layer binds to a CH in the other one. The underlying physics of pairing is the same, and the descriptions should correspond to the same phase [64].

We did not include a requirement for the boost invariance (K invariance [63,65]) as in the single-layer case [59], because in this case, a real increase of the energy of the system is possible due to a relative motion between layers. In the mean field, the dispersion of the Goldstone mode is $\omega_{\boldsymbol{k}} \sim \sqrt{\Delta_s/M}$, where Δ_s is the BCS gap and M is the mass of quasiparticles due to the Coulomb interaction between the same layer particles. The boost invariance should be ensured in the limiting cases, $d = 0$ and $d = \infty$, but at intermediate distances, we may rely on the mean-field estimates.

IV. DISCUSSION AND CONCLUSIONS

Thus, we may conclude that within the scope of dipole representation and mean-field method, there is no transition in the QHB at finite distance between layers; the excitonic phase of electrons (or Cooper s-wave pairing of fermionic quasiparticles and dipoles in the long-distance approximation) dominates the physics at relevant distances. On the other hand, the suppressed yet competing, s-wave excitonic phase of quasiparticle inside LLL can be described as a large Fermi sea of quasiparticles (with no layer index, i.e., with symmetric superpositions). An intermediate state in the QHB has been identified and described by exact diagonalization on a torus in Ref. [46]. In our description the Fermi sea of (neutral) dipoles, in the absence of the boost invariance (or K invariance), leads to the incompressibility in the charge channel [63,65] of the competing phase, and that is consistent with findings of Ref. [46] (and distinct from the ICCFL phase of Ref. [45]). The exciton condensation induces a gapped, topological behavior in the neutral channel, just as in the case of the ICCFL phase (of Ref. [45]) and consistent with findings of Ref. [46].

Based on previous analyses [47,48], one may expect that the inclusion of LL mixing will lead to the formation of the p-wave pairing state of CFs (from opposite layers, i.e., interpairing). This state can be found in an unprojected (to a fixed LL) Chern-Simons field-theoretical description. A Dirac type of the gauge theory leads to the conclusion that the p-wave Cooper pairing of CFs from opposite layers describes the system at any distance between layers [49] (except at $d = \infty$). The no-transition scenario continues to exist under LL mixing [51]. The results of our work, within the LLL, and the results of Ref. [51], with no projection in a Chern-Simons treatment, are in correspondence. This continuous (one and only for all distances) phase can be simulated by selecting an appropriate shift (i.e., bias) in the spherical geometry, inside the LLL, as described in Ref. [50].

In short, we have demonstrated the usefulness of the dipole representation in the case of the long-standing problem of the QHB, with potential to be used for half-filled problems of general Chern bands. Inside an LLL, the QHB physics is dominated by a single phase: the Cooper s-wave pairing of effective dipoles. While for the system of electrons in a single layer that occupy half of the available states in a LL a compressible behavior is only possible [69], here we find that a nontrivial double, a nontrivial superposition of two such systems with incompressible, topological behavior based on the noncommutative nature of projection(s) inside LL(s) is in a competition with a compressible phase, but again the compressible (in the neutral channel) phase is realized.

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APPENDIX: MEAN-FIELD APPROACH TO EFFECTIVE HAMILTONIANS

In this Appendix, we give a brief account of the mean-field treatment of the Hamiltonians, $\mathcal{H}_1$, (11), and $\mathcal{H}_2$, (12). Due to the attractive nature of the effective interaction in $\mathcal{H}_1$, and the repulsive nature of the effective interaction in $\mathcal{H}_2$, we introduce a mean-field reduction of the Hamiltonians, assuming the pairing in the Cooper channel of $\mathcal{H}_1$, i.e., $\langle c^\dagger_{\boldsymbol{k},\uparrow} c^\dagger_{-\boldsymbol{k},\downarrow}\rangle = \Delta^{\rm bcs}_{\boldsymbol{k}} \neq 0$, and the excitonic pairing of $\mathcal{H}_2$, i.e., $\langle c^\dagger_{\boldsymbol{k},\uparrow} c_{\boldsymbol{k},\downarrow}\rangle = \Delta^{\rm exc}_{\boldsymbol{k}} \neq 0$.

In the BCS case, we need to solve self-consistently the following equation, for the order parameter $\Delta^{\rm bcs}_{\boldsymbol{q}}$:

$$\Delta^{\rm bcs}_{\boldsymbol{k}} = \int \frac{d\boldsymbol{q}}{(2\pi)^2} V_{\uparrow\downarrow}(|\boldsymbol{q}-\boldsymbol{k}|)\frac{\Delta^{\rm bcs}_{\boldsymbol{q}}}{2E_{\boldsymbol{q}}}, \tag{A1}$$

where $E_{\boldsymbol{q}} = \sqrt{\xi_{\boldsymbol{q}}^2 + |\Delta^{\rm bcs}_{\boldsymbol{q}}|^2}$ and $\xi_{\boldsymbol{q}} = \epsilon_{\boldsymbol{q}} - \epsilon_{q_F}$, with $\boldsymbol{q}_F = 1$ (a half-filled condition for each layer). Also $\epsilon_{\boldsymbol{q}}$ represents the single-particle energy of quasiparticles in each layer that is calculated using the Hartree-Fock method, applied to the single-layer part of the Hamiltonian that describes the intralayer interaction. See below an explicit formula in (A5). The (total) ground-state energy of the system is

$$E_0^{\rm bcs} = \int \frac{d\boldsymbol{q}}{(2\pi)^2}(\xi_{\boldsymbol{q}} - E_{\boldsymbol{q}}) + \int \frac{d\boldsymbol{q}}{(2\pi)^2}\frac{\left|\Delta^{\rm bcs}_{\boldsymbol{q}}\right|^2}{2E_{\boldsymbol{q}}}. \tag{A2}$$

In the excitonic case, we need to self-consistently solve the following equation, for the order parameter $\Delta^{\rm exc}_{\boldsymbol{q}}$:

$$\Delta^{\rm exc}_{\boldsymbol{k}} = \int \frac{d\boldsymbol{q}}{(2\pi)^2} V_{\uparrow\downarrow}(|\boldsymbol{q}-\boldsymbol{k}|)\frac{\Delta^{\rm exc}_{\boldsymbol{q}}}{2\left|\Delta^{\rm exc}_{\boldsymbol{q}}\right|}[n_\alpha(\boldsymbol{q}) - n_\beta(\boldsymbol{q})], \tag{A3}$$

where $n_\alpha(\boldsymbol{q})$ and $n_\beta(\boldsymbol{q})$ denote the occupations of the states with momentum $\boldsymbol{q}$, in the band with energies $\mathcal{E}_\alpha(\boldsymbol{q}) = \epsilon_{\boldsymbol{q}} - |\Delta^{\rm exc}_{\boldsymbol{q}}|$, and in the band with energy $\mathcal{E}_\beta(\boldsymbol{q}) = \epsilon_{\boldsymbol{q}} + |\Delta^{\rm exc}_{\boldsymbol{q}}|$, respectively. In solving (A3), we have to keep the density of the system constant, i.e., the occupation of the lower and upper band, described by appropriate Fermi momenta, q^F_+ and q^F_-, should satisfy the following equation: $(q^F_+)^2 + (q^F_-)^2 = 2$.

The (total) ground-state energy of the system is

$$\begin{aligned} E_0^{\rm exc} = \int \frac{d\boldsymbol{q}}{(2\pi)^2}\big[&\big(\xi_{\boldsymbol{q}} - \left|\Delta^{\rm exc}_{\boldsymbol{q}}\right|/2\big)n_\alpha(\boldsymbol{q}) \\ &+ \big(\xi_{\boldsymbol{q}} + \left|\Delta^{\rm exc}_{\boldsymbol{q}}\right|/2\big)n_\beta(\boldsymbol{q})\big], \end{aligned} \tag{A4}$$

where, as before, $\xi_{\boldsymbol{q}} = \epsilon_{\boldsymbol{q}} - \epsilon_{q_F}$, with $\boldsymbol{q}_F = 1$ (a half-filled condition for each layer).

The following equation describes the single-particle energy obtained after the application of the (Hartree-)Fock procedure to the intralayer part of the Hamiltonian:

$$\begin{aligned} \epsilon_{\boldsymbol{k}} = \frac{1}{2}\int &\frac{d\boldsymbol{q}}{(2\pi)^2}\tilde{V}(|\boldsymbol{q}|)\left[\sin\left(i\frac{\boldsymbol{k}\times\boldsymbol{q}}{2}\right)\right]^2 \\ &- \int \frac{d\boldsymbol{q}}{(2\pi)^2}\tilde{V}(|\boldsymbol{q}-\boldsymbol{k}|)\left[\sin\left(i\frac{\boldsymbol{k}\times\boldsymbol{q}}{2}\right)\right]^2 n(\boldsymbol{q}). \end{aligned} \tag{A5}$$

The occupation $n(\boldsymbol{q})$ describes the filled Fermi sphere with radius $q_F = 1$. The first contribution comes from the normal ordering of the density-density form of the intralayer term and may represent the self-energy of a dipole [62], and the second term represents a Fock contribution.

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