

Ferromagnetic spin-orbital liquid of dipolar fermions in zigzag lattices

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Two-component dipolar fermions in zigzag optical lattices allow for the engineering of spin-orbital models. We show that dipolar lattice fermions permit the exploration of a regime typically unavailable in solid-state compounds that is characterized by a spin-liquid phase with a finite magnetization and spontaneously broken SU(2) symmetry. This peculiar spin liquid may be understood as the Luttinger liquid of composite particles consisting of bound states of spin waves and orbital domain walls moving in an unsaturated ferromagnetic background. In addition, we show that the system exhibits a boundary phase transitions involving nonlocal entanglement of edge spins.

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I. INTRODUCTION

Frustrated spin systems provide a wealth of novel phenomena, both at the classical and quantum levels [1]. Frustration becomes particularly important in low-dimensional systems, where quantum and thermal fluctuations are strongly enhanced and long-range order is suppressed. One of the most interesting frustration-inducing mechanisms involves the interaction of spins with orbital degrees of freedom [1–4], which may result in spin-liquid states that lack long-range magnetic order [5–9]. However, in solid-state systems, controlling the strength of spin-orbital interactions is hardly possible, limiting the exploration of spin-liquid phases.

Several recent works [10–13] have shown that ultracold atomic gases in optical lattices can serve as quantum simulators of spin-orbital models, providing the required freedom for controlling the effective interactions by tweaking the optical lattice or by using Feshbach resonances. Moreover, rapidly developing experimental techniques make it possible to study the physics of higher energy bands, and to exploit orbital degeneracy [14].

In particular, it has been recently shown [13] that spin-orbital models of the Kugel-Khomskii type [15], relevant in transition metal oxides [2,3], can be realized in systems of dipolar spin- $\frac{1}{2}$ fermions loaded in doubly degenerate p bands of optical zigzag lattices. For comparable on-site intraorbital repulsion U and interorbital repulsion V , which is the typical situation in solid-state scenarios [16], it was shown that dipolar fermions have a rich ground-state phase diagram containing states with ferromagnetic (FM), antiferromagnetic (AF), dimerized, and quadrumerized spin order [13]. Spin-liquid phases are, however, absent in this regime.

Interestingly, contrary to the usual case in solid-state systems, a large ratio U/V may be attained for the case of dipolar fermions in zigzag lattices by properly controlling the ratio between dipolar and contact interactions. In this paper we show that for $U/V > 2$ the ground-state diagram contains a spin-orbital liquid phase with a finite magnetization. This phase has a spontaneously broken SU(2) spin symmetry and algebraically decaying longitudinal spin correlations, while the orbital correlations decay exponentially. This behavior is interesting, since in one dimension (1D) spontaneous breaking of continuous symmetry is usually forbidden, with the only

known exception being ferromagnets and ferrimagnets, where the magnetization of the ground state is locked at a certain value fixed by the Lieb-Schulz-Mattis theorem [17]. The mechanism driving the transition into this phase is given by the softening of composite excitations formed by bound states of spin waves and orbital domain walls. We support our analytical arguments by numerical results obtained by means of the density matrix renormalization group (DMRG) technique [18,19]. In addition, for open boundary conditions we observe peculiar boundary phase transitions that involve the formation of edge spins that decouple from the bulk and become nonlocally entangled.

II. SPIN-ORBITAL MODEL

We consider two-component (pseudo-spin-1/2) dipolar fermions loaded in doubly degenerate p bands of a quasi-1D zigzag lattice [see Fig. 1(a)]. The system is described by the Hubbard-type Hamiltonian with twofold orbital degeneracy. The energy scales that determine the system are the nearest-neighbor (NN) hoppings t and ε between equal orbitals, the on-site repulsion energies U (V) between the same (different) orbitals, the Hund coupling J_H , and an in-plane deformation of the optical lattice, distorting the XY rotational symmetry of a single-site potential that mixes the orbitals within the same site with an amplitude γ .

Dipolar spinor fermions may be realized using polar molecules (see Ref. [13] for a detailed discussion) or employing atoms with large magnetic dipole moments, such as chromium [20], dysprosium [21], or erbium [22]. For the particular case of ^{53}Cr , in a strong magnetic field, any two of the four lowest energy states $|F, m_F\rangle = |\frac{9}{2}, -\frac{9}{2}\rangle, |\frac{9}{2}, -\frac{7}{2}\rangle, |\frac{9}{2}, -\frac{5}{2}\rangle$, and $|\frac{9}{2}, -\frac{3}{2}\rangle$, can be chosen to simulate the \uparrow and \downarrow pseudospin- $\frac{1}{2}$ states. Those states have approximately the same large magnetic moments, given by the electronic spin projection $m_s = -3$, differing only by their nuclear moment. The total interparticle potential is of the form

$$V(\mathbf{r}_1 - \mathbf{r}_2) = \frac{\mu_0 \mu^2}{4\pi |\mathbf{r}_1 - \mathbf{r}_2|^3} + g \delta(\mathbf{r}_1 - \mathbf{r}_2),$$

where $g = 4\pi a_s \hbar^2 / m$ characterizes the contact interactions, a_s is the s -wave scattering length, m is the atomic mass,

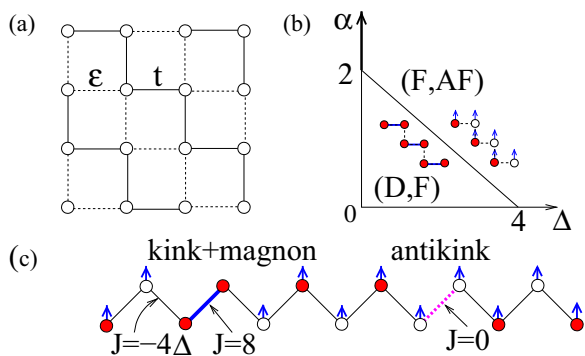


FIG. 1. (Color online) (a) Spin-orbital model on a quasi-1D zigzag lattice with weak interchain hoppings $\varepsilon \ll t$. The model (4) corresponds to $\varepsilon = 0$. (b) Phase diagram of the model for $\lambda = 0$. (c) A sketch of the kink-magnon bound state in the (F,AF) phase, where J denotes the effective spin exchange on the corresponding link. A magnon binds only to the orbital kink, but not to the antikink. Open and solid circles in (b) and (c) show the occupied orbital states $\sigma^z = \pm 1$.

μ_0 is the vacuum permittivity, and μ is the magnetic dipole moment. The average on-site repulsion energies between the same (different) orbitals U and V are given by [13]

$$U = \int d\mathbf{r}_1 d\mathbf{r}_2 p_x^2(\mathbf{r}_1) V(\mathbf{r}_1 - \mathbf{r}_2) p_x^2(\mathbf{r}_2), \quad (1)$$

$$V = \int d\mathbf{r}_1 d\mathbf{r}_2 p_x^2(\mathbf{r}_1) V(\mathbf{r}_1 - \mathbf{r}_2) p_y^2(\mathbf{r}_2), \quad (2)$$

where $p_{x,y}(\mathbf{r})$ are the orbital wave functions centered at the same site.

Two fermions occupying the same orbital may form a symmetric or an antisymmetric state with respect to the orbital index with corresponding energies $U + J_H$ and $U - J_H$, where

$$J_H = \int d\mathbf{r}_1 d\mathbf{r}_2 p_x(\mathbf{r}_1) p_y(\mathbf{r}_1) V(\mathbf{r}_1 - \mathbf{r}_2) p_x(\mathbf{r}_2) p_y(\mathbf{r}_2). \quad (3)$$

When two fermions occupy different orbitals, they may form a spin-singlet or a spin-triplet state with corresponding energies $V + J_H$ and $V - J_H$, which are split by Hund's exchange.

The interaction, resulting from the electronic degrees of freedom, is pseudospin independent, providing the desired SU(2) spin symmetry of the problem. Further details on the experimental implementation of this system can be found in Ref. [13].

We start by considering the purely 1D case, $\varepsilon = 0$. In the Mott insulator regime (one fermion per site and strong coupling $U \pm J_H, V \pm J_H \gg t, \gamma$), the system is described by an effective spin-orbital Hamiltonian (for details of the derivation we refer the reader to Ref. [13]):

$$\mathcal{H} = \sum_l \left(2\mathbf{S}_l \cdot \mathbf{S}_{l+1} + \alpha - \frac{1}{2} \right) [1 + (-1)^l \sigma_l^z] [1 + (-1)^l \sigma_{l+1}^z] - \Delta \sum_l 2\mathbf{S}_l \cdot \mathbf{S}_{l+1} (1 - \sigma_l^z \sigma_{l+1}^z) - \lambda \sum_l \sigma_l^x, \quad (4)$$

where \mathbf{S}_l are spin- $\frac{1}{2}$ operators acting on the lattice site l , and $\sigma_l^{z,x}$ are the Pauli matrices describing the orbitals. The parameters of the model, in the leading order in J_H/U , are given by $\alpha \approx U/V$, $\Delta \approx J_H U/V^2$, $\lambda \approx \gamma U/t^2$, and the Hamiltonian (4) has overall units of $t^2/2U$.

It should be remarked that the dipole-dipole coupling is crucial because for a purely contact interaction there is no repulsion between fermions in the spin-triplet state, and hence the Mott phase with one particle per site could not stabilize. For ^{53}Cr , the natural value of the ratio $U/V \approx \alpha$ is in the regime $U/V > 2$ considered in this work.

III. ANALYTICAL ESTIMATES

For the case $\lambda = 0$, i.e., when the orbitals are classical, the phase diagram of the 1D model (4) can be easily established and is shown in Fig. 1(b). The $\alpha > 2$ region is dominated by a phase with FM spin order and AF orbital order, which we label (F,AF) $|\uparrow\uparrow\uparrow\uparrow\cdots\rangle_S \otimes |\uparrow\downarrow\uparrow\downarrow\cdots\rangle_\sigma$, following the notation of Ref. [13]. A smaller α favors the spontaneously dimerized (D,F) state, with the spin sector described by a product of singlets on even (odd) NN bonds and ferromagnetic orbitals. On the line $\Delta = 0$, $\lambda = 0$, $\alpha > 2$ the spins are fully decoupled, whereas adding infinitesimally small Δ (λ) favors FM (AF) spin exchange. This competition between λ and Δ leads to a first-order transition from the (F,AF) phase to the (iH,AF) phase where the spin sector behaves as an isotropic Heisenberg antiferromagnet, and the orbitals retain AF order $|\uparrow\downarrow\uparrow\downarrow\cdots\rangle_S \otimes |\uparrow\downarrow\uparrow\downarrow\cdots\rangle_\sigma$. For $\lambda, \Delta \rightarrow 0$ this transition line can be easily estimated by computing the leading order correction in λ to the energy $E_m(k)$ of a magnon in the (F,AF) state. For small momenta k , one obtains $E_m(k) \rightarrow (2\Delta - \frac{\lambda^2}{8(\alpha-2)})k^2$, collapsing at $\lambda = \lambda_F = 4\sqrt{(\alpha-2)\Delta} + O(\Delta^{3/2})$. A further increase of λ at fixed small Δ eventually leads to an Ising transition in the orbital sector, bringing the system into the (iH,P) phase with paramagnetic orbitals $|\uparrow\downarrow\uparrow\downarrow\cdots\rangle_S \otimes |\rightarrow\rightarrow\rightarrow\rightarrow\cdots\rangle_\sigma$.

The (F,AF) ground state factorizes into a product of spin and orbital wave functions, so there is a purely orbital Ising-type transition from the (F,AF) phase to the (F,P) phase where orbitals are paramagnetic (disordered) and spins fully polarized, $|\uparrow\uparrow\uparrow\uparrow\cdots\rangle_S \otimes |\rightarrow\rightarrow\rightarrow\rightarrow\cdots\rangle_\sigma$; the transition line thus can be obtained exactly as $\lambda = \lambda_{\text{Ising}} = \alpha + \Delta/2$.

However, there is another instability of the (F,AF) phase which is of crucial interest here. This instability can be traced down to the fact that in the (F,AF) phase magnons tend to bind to kinks in the orbital order [see Fig. 1(c)]. If a kink-antikink pair is excited on top of the (F,AF) state, on the link at the kink position the effective exchange J changes from ferromagnetic ($J \approx -4\Delta$ in zeroth order in λ) to antiferromagnetic ($J \approx 8$), acting as an impurity which can bind a magnon. There is another impurity link with $J \approx 0$ at the antikink position, but it does not support bound states.

To the leading order in λ , the energy of the kink-antikink pair with a magnon bound to the kink is

$$E_{\text{bs}}(p, k) = 4\alpha + 2\Delta - 8 + 8\Delta/(\Delta + 4) + 2\lambda\{[(8 - \Delta^2)/(4 + \Delta)^2] \cos p - \cos k\}, \quad (5)$$

where p and k are the kink and antikink momenta, respectively. The lower edge of this continuum is achieved at $p = \pi$, $k = 0$, i.e., when the magnon is essentially a propagating singlet dimer. This excitation softens at $\lambda = \lambda_c = \frac{4}{3}(\alpha - 2) + \frac{2}{9}(\alpha + 4)\Delta + O(\Delta^2)$. Hence, for $\lambda > \lambda_c$ a different phase is expected with a finite density of composite kink-dimer particles “floating” in the ferromagnetic background [23]. An infinitesimal density of moving kinks and antikinks immediately suppresses the orbital order, so the orbital AF order parameter experiences a jump at the transition. Indeed, the (F,AF) product wave function remains an exact eigenstate all the way up to $\lambda = \lambda_c$, and λ_c remains smaller than the Ising transition value λ_{Ising} in a finite range of Δ . The ferromagnetic order in spins is retained, but the magnetization is no more fully saturated.

In the phase mentioned above, the SU(2) symmetry in the spin sector remains spontaneously broken, exactly as in the (F,AF) phase, but the ground state belongs to a degenerate multiplet with some spin $S_{\text{tot}} < N/2$, where N is the number of particles ($N = L$ at unit filling considered here). This phase is expected to have *two* branches of gapless excitations, one with a quadratic dispersion at small momenta (“spin” mode, ferromagnetic magnons), and the other with a linear dispersion (“charge” mode, sound waves in the Luttinger liquid of kink-dimer particles). This resembles the situation found in spin- $\frac{1}{2}$ Bose gas, where such a spin-charge separation has been found both in the 1D [24–27] and two-dimensional (2D) [28] cases. Since the longitudinal spin correlator is related to the kink-dimer density fluctuations, it must decay algebraically on top of the long-range order. This highly unusual phase can be called a ferromagnetic spin-orbital liquid (FSOL) [29].

When zigzag chains are coupled into a 2D structure by weak interchain hopping $\varepsilon \ll t$ as shown in Fig. 1(a), assuming $(\alpha - 2), \Delta \ll 1$, similar calculations as those presented for purely 1D case show that the FSOL-type phase, characterized by a finite density of orbital domain walls carrying bound magnons, survives next to the (F,AF) state in a finite interval of Δ at least for $(\varepsilon/t)^2 < \frac{2}{3}(\alpha - 2)$. In contrast to its 1D counterpart, this phase is both magnetically and orbitally ordered, but it retains the unique feature of the FSOL phase, namely, its “diluted” ferromagnetism with a reduced magnetization. At larger 2D coupling, $5(\alpha - 2) \lesssim (\varepsilon/t)^2 \ll 1$, the FSOL-type phase gives way to a striped dimer phase consisting of (D,F) chains as shown in Fig. 1(b), with alternating orientation of spins in neighboring chains.

IV. NUMERICAL RESULTS FOR 1D CASE

Our DMRG results confirm the analytical arguments given above. Figure 2 shows our numerical results for the (λ, Δ) phase diagram of the 1D version of the model (4) at $\alpha = 3$. We considered open systems consisting of up to $L = 96$ sites, monitoring different correlation functions, total spin of the ground state, and fidelity susceptibility [30] to detect phase boundaries. In addition, we have checked our data on systems of up to $L = 48$ sites with periodic boundary conditions. We have typically kept up to 800 states (within a subspace with fixed S^z) in our DMRG calculations.

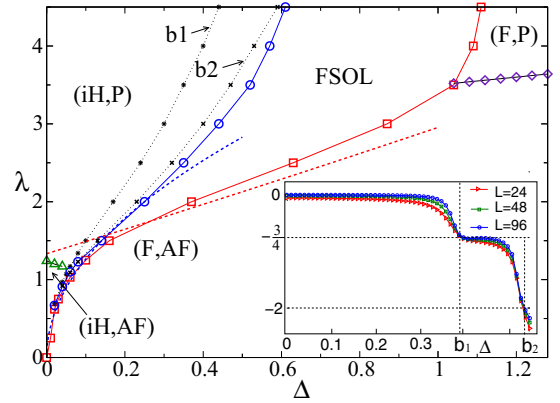


FIG. 2. (Color online) Phase diagram of the 1D spin-orbital model for $\alpha = 3$ and $L = 96$ sites (for open boundaries). Symbols denote numerical results (solid and dotted lines are a guide to the eye), whereas dashed lines correspond to the analytical estimates λ_F and λ_c . Curves $b1$ and $b2$ mark the boundary phase transitions that involve nonlocal entanglement between edge spins $\tau_1 = S_1 + S_2 + S_3$ and $\tau_N = S_N + S_{N-1} + S_{N-2}$. The inset shows the ground-state correlation between edge spins $\langle \tau_1 \tau_N \rangle$ as a function of Δ for $\lambda = 4$.

We indeed observe the FSOL phase in a wide region of Δ and λ . As shown in Fig. 3(a), spontaneous magnetization in the FSOL phase changes smoothly, confirming that there is no gap for single-particle excitations. In accordance with the composite-particle transition mechanism outlined above, there is a clear correlation between the peaks in the densities of orbital domain walls and magnons [see Fig. 3(b)]. We have checked that such a correlation persists at all magnetization

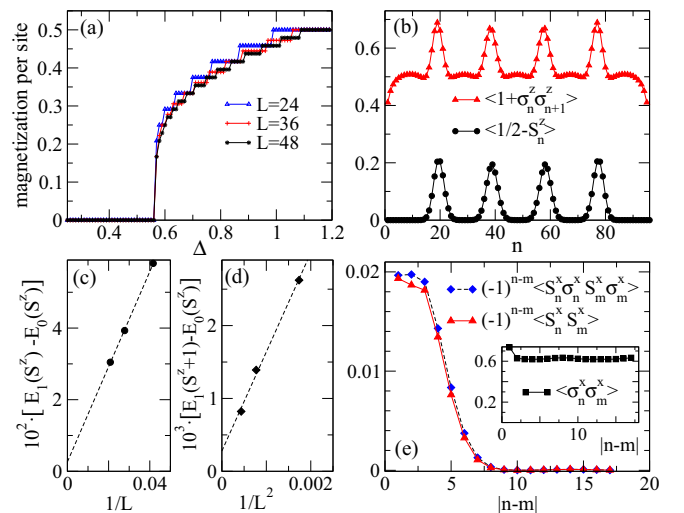


FIG. 3. (Color online) Properties of the FSOL phase for $\alpha = 3$ and $\lambda = 4$: (a) Magnetization curve for different system sizes L , $\sum_i \langle S_i^z \rangle / L$, calculated in the highest weight states of ground-state SU(2) multiplets; (b) magnon density (circles) and orbital domain wall density (triangles) in the ground state at $\Delta = 1.02$, $S^z = 44$, $L = 96$ (open boundary conditions break translation symmetry and pin kink magnons); finite-size scaling of the particle-hole (c) and magnon (d) excitation gaps at $S^z = N/3$; (e) ground-state correlators for $\Delta = 0.86$, $L = 48$. See text for details.

values, and that the number of peaks in the domain wall density is always equal to the number of magnons in the ground state.

Moreover, the energy of the lowest excitation in the same S^z sector as the ground state (the particle-hole gap) scales as L^{-1} with the system size L , while that in the sector corresponding to adding a magnon scales as L^{-2} , as shown in Figs. 3(c) and 3(d). Thus these are two gapless excitation branches with linear and quadratic dispersion, respectively.

The phase transition from (iH,P) into (F,P) is first order, as the total spin jumps abruptly from 0 to $L/6$. Similarly, the transition from (F,AF) into FSOL is first order since the AF orbital order in σ^z changes discontinuously. In contrast to that, the transition from (F,P) into FSOL seems second order of the commensurate-incommensurate type (even though the system sizes studied are not enough to observe a square root behavior of the kink-magnon density close to the fully polarized state), since all quantities observed change in a continuous manner. The minimal model capturing this transition is a system of two-component repulsive SU(2)-symmetric bosons undergoing a transition from vacuum into a finite density state driven by a chemical potential. Note that this finite density state is not a two-component Luttinger liquid, since the continuous SU(2) symmetry is spontaneously broken.

In the FSOL phase the correlators $\langle S_i^x S_j^x \rangle$ and $\langle S_i^x \sigma_i^x S_j^x \sigma_j^x \rangle$ are very close to each other, despite the fact that $\langle \sigma_i^x \sigma_j^x \rangle$ can be significantly lower than one [see Fig. 3(e)]. In fact, for the parameters presented in Fig. 3(e), $\langle S_i^x \sigma_i^x S_j^x \sigma_j^x \rangle$ is larger in absolute value than $\langle S_i^x S_j^x \rangle$ even though $|\langle \sigma_i^x \sigma_j^x \rangle| \sim \langle \sigma_i^x \rangle^2 \simeq 0.6$, where the finite value of $\langle \sigma_i^x \rangle$ is induced by the coupling λ in Eq. (4). One can straightforwardly check that this follows from the fact that the wave function of the bound state is very close to a singlet bond across the orbital domain wall, so that the operator $S_i^+(1 - \sigma_i^x)$ nearly annihilates the ground state.

V. BOUNDARY PHASE TRANSITIONS

In addition to the existence of the FSOL phase, the spin-orbital model with $\alpha > 2$ is characterized by the appearance of peculiar boundary phase transitions within the (iH,P) phase (curves $b1$ and $b2$ in Fig. 2) at which the behavior of the edge spins in open chains changes drastically. When increasing Δ at fixed λ , localized and strongly correlated $S = \frac{1}{2}$ edge spins emerge when crossing the $b1$ curve. Further increasing Δ leads to a second transition at the $b2$ line, where the value of the boundary spin changes from $S = \frac{1}{2}$ to $S = 1$. This effect is illustrated in the inset of Fig. 2, where the correlation between edge spins is depicted as a function of Δ for $\lambda = 4$ [31].

The boundary transitions inside the (iH,P) phase are peculiar in 1D, since edge spins are separated by a macroscopic distance, and the only way to communicate between them is through the bulk from which they effectively decouple. To prove that we are dealing with a boundary phenomenon we compare the excitation gaps for open and periodic boundary conditions. One can clearly see from Fig. 4 that low-lying states below the bulk modes develop for open boundary conditions. Another illustration of this boundary transition is provided by Fig. 5, which shows the behavior of the first excited states in the $S^z = 1$ and $S^z = 2$ sector.

To describe the physics of this transition at the qualitative level, it is instructive to consider the limit of large λ . In the

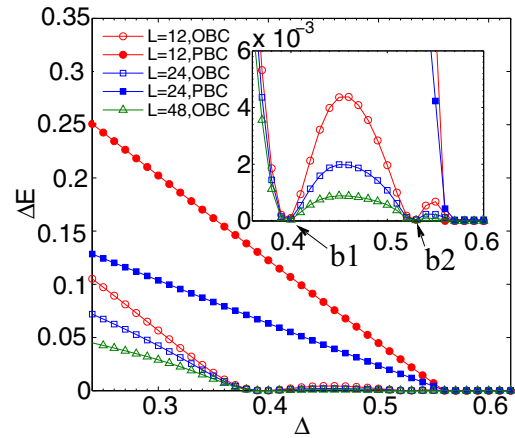


FIG. 4. (Color online) Excitation gap for open boundary conditions (OBCs) and periodic boundary conditions (PBCs) as a function of Δ and the system size L . The inset zooms in the region $0.36 < \Delta < 0.6$, revealing the existence of the two boundary transitions at $b1$ and $b2$.

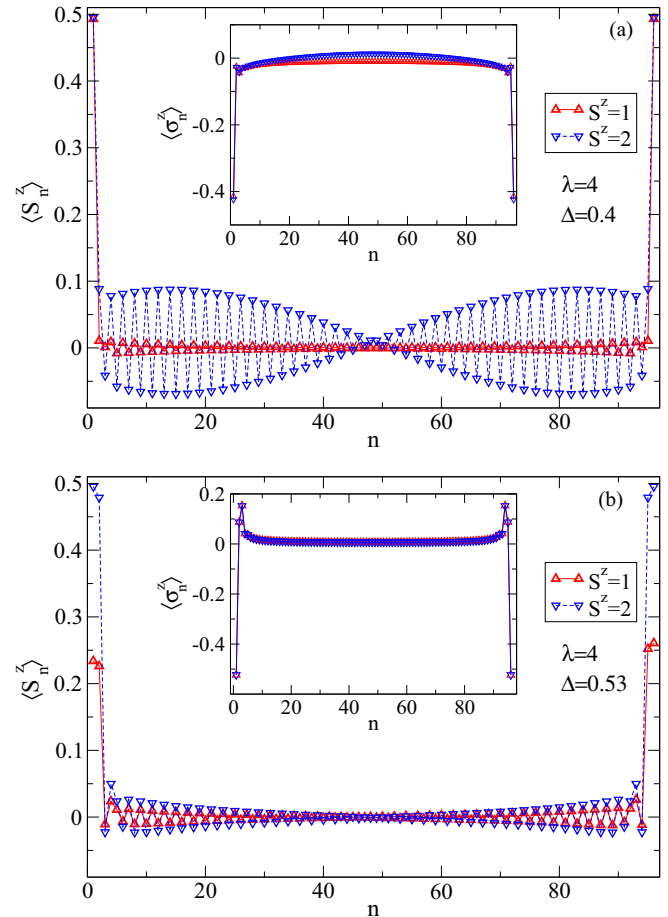


FIG. 5. (Color online) Spin and orbital distribution profiles in the ground states of the $S^z = 1$ and $S^z = 2$ sectors, at two points of the $\alpha = 3$ phase diagram, along the $\lambda = 4$ line: (a) At a point between the $b1$ and $b2$ boundary transition lines, the $S^z = 1$ excitation is localized at the system edges, while the $S^z = 2$ excitation belongs to the bulk; (b) at another point between the $b2$ line and the boundary of the FSOL phase, both $S^z = 1$ and $S^z = 2$ excitations are localized at the edges.

strong λ limit one can integrate out orbital degrees of freedom to obtain an effective spin- $\frac{1}{2}$ model. In the leading order in $1/\lambda$, its Hamiltonian has the form of a J_1 - J_2 model with modified first and last nearest-neighbor links:

$$H_S = j_1 \sum_{n=2}^{N-2} \mathbf{S}_n \cdot \mathbf{S}_{n+1} + j_2 \sum_{n=2}^{N-1} \mathbf{S}_{n-1} \cdot \mathbf{S}_{n+1} + j'_1 (\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_{N-1} \cdot \mathbf{S}_N), \quad (6)$$

where

$$j_1 = 2(1 - \Delta) + \frac{4 + (1 + \Delta)(\Delta + 2 - 2\alpha)}{2\lambda},$$

$$j_2 = 1/\lambda, \quad j'_1 = j_1 + \frac{1 - 2\alpha}{2\lambda}. \quad (7)$$

One can see that with increasing Δ , the boundary link strength j'_1 goes through zero at some point and changes its sign to a ferromagnetic coupling. This effectively creates “impurity” spins attached ferromagnetically at the ends of the spin- $\frac{1}{2}$ chain. Interaction between the end spins is mediated by the bulk. For an even number of sites the effective interaction is antiferromagnetic, whereas for an odd number of sites the effective interaction between the end spins is ferromagnetic.

The second boundary transition, b_2 , is similar in nature to the first one, but now the last two spins decouple from the bulk, creating an effective spin-1 localized at each boundary that is ferromagnetically attached to the antiferromagnetic spin- $\frac{1}{2}$ chain. The interaction between the spin-1 edge impurities is antiferromagnetic for an even number of sites and ferromagnetic for an odd number of sites. The lowest excitations are boundary

excitations: a boundary triplet with total spin $S^T = 1$, and a boundary quintet with $S^T = 2$ with a slightly higher energy.

VI. SUMMARY

We have shown that dipolar two-component fermions loaded in the p bands of a zigzag optical lattice may allow for the realization of a different, inaccessible in solid-state systems, spin-orbital liquid phase characterized by a finite but unsaturated magnetization. This phase, as a ferromagnet, has spontaneously broken SU(2) symmetry, but, unlike a ferromagnet, it has algebraically decaying longitudinal spin correlations. Remarkably, its magnetization changes continuously from saturation value with a change of the model parameters, *in the absence of any magnetic field*. This phase can be viewed as the Luttinger liquid of bound composites of singlet spin dimers and orbital domain walls on top of a fully polarized ferromagnetic phase.

Finally, we remark that observation of this magnetized spin-orbital liquid demands to cool down the system to the temperatures of the order of the spin-coherence scale $4t^2/U$, which constitutes a major experimental challenge presently [32].

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