Ferromagnetic spin-orbital liquid of dipolar fermions in zigzag lattices

G. Sun,1 A. K. Kolezhuk,2,3 L. Santos,1 and T. Vekua1

1Institut für Theoretische Physik, Leibniz Universität Hannover, 30167 Hannover, Germany
2Institute of High Technologies, Taras Shevchenko National University of Kiev, 03022 Kiev, Ukraine
3Institute of Magnetism, National Academy of Sciences and Ministry of Education, 03142 Kiev, Ukraine

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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 novel spin-liquid phase with a finite magnetization and spontaneously broken SU(2) symmetry. This peculiar spin liquid may be understood as a 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 non-local entanglement of edge spins.

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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 [2, 3], which may result in spin-liquid states that lack long-range magnetic order [2, 3]. 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 of controlling the effective interactions by tweaking the optical lattice or by using Feshbach resonances. Moreover, rapidly-developing experimental techniques make 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-1/2 fermions loaded in doubly-degenerate p-bands of optical zigzag lattices. For comparable on-site intra-orbital repulsion U and inter-orbital 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 zig-zag lattices by properly controlling the ratio between dipolar and contact interactions. In this Letter we show that for U/V > 2 the ground state diagram contains a novel 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. 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 [17, 18]. 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 get non-locally entangled.

Spin-orbital model.– We consider two-component (pseudo-spin-1/2) fermions loaded in doubly degenerate p-bands of a zig-zag lattice (see Fig. 1(a), details on the experimental implementation of this system can be found in Ref. [13]). The energy scales that determine the system are the nearest-neighbor (NN) hopping t between equal

![FIG. 1. (Color online).](image-url)
orbitals, the average on-site repulsion energies $U$ ($V$) between 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 $\gamma$. In the Mott insulator regime (one fermion per site and strong coupling $U, V \gg J_H \gg t, \gamma$), the system is described by an effective spin-orbital Hamiltonian (for details of the derivation we refer to Ref. [13]):

$$H = \sum_l (2S_l \cdot S_{l+1} + \alpha - \frac{1}{2})(1 + (-1)^{i} \sigma^z_l) (1 + (-1)^{i} \sigma^z_{l+1})$$

$$- \Delta \sum_l 2S_l \cdot S_{l+1} (1 - \sigma^z_l \sigma^z_{l+1}) - \lambda \sum_l \sigma^x_l$$

(1)

where $S_l$ are spin-1/2 operators acting on the lattice site $l$, and $\sigma^x, \sigma^z$ 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 (1) has overall units of $t^2/2U$. The dipole-dipole coupling is crucial because for 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.

**Analytical estimates.** Figure (1b) shows the phase diagram for the case $\lambda = 0$, for which the orbitals are classical. The $\alpha > 2$ region is dominated by a phase with FM spin order and AF orbital order, which we label (F,AF) following the notation of Ref. [13]. A smaller $\alpha$ 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 $\Delta (\lambda)$ favors FM (AF) spin exchange. This competition between $\lambda$ and $\Delta$ 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. For $\lambda, \Delta \to 0$ this transition line can be easily estimated by computing the leading order correction in $\lambda$ to the energy $E_m(k)$ of a magnon in the (F,AF) state. For small momenta $k$, one obtains $E_m(k) \to (2\Delta - \frac{\lambda^2}{2(\alpha - 2)})k^2$, collapsing at $\lambda = \lambda_f = 4\sqrt{(\alpha - 2)\Delta + O(\Delta^3/2)}$. A further increase of $\lambda$ at fixed small $\Delta$ eventually leads to an Ising transition in the orbital sector, bringing the system into the (iH,P) phase with paramagnetic orbitals.

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 remain fully polarized; the transition line thus can be obtained exactly as $\lambda = \lambda_{\text{Ising}} = \alpha + \Delta/2$.

However, there is another, previously unknown, 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. (1c)). 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 $\lambda$) 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 $\lambda$, the energy of the kink-antikink pair with a magnon bound to the kink is

$$E_{bs}(p, k) = 4\alpha + 2\Delta - 8 + 8\Delta/(\Delta + 4)$$

$$+ 2\lambda \{ [(8 - 2\Delta)/4 + \Delta^2] \cos p - \cos k \},$$

(2)

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 $\lambda = \lambda_c = \frac{4}{3}(\alpha - 2) + \frac{4}{3}(\alpha + 4)\Delta + O(\Delta^2)$. Hence, for $\lambda > \lambda_c$ a novel phase is expected with a finite density of composite kink-dimer particles “floating” in the ferromagnetic background [10]. 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 $\lambda_c$ remains smaller than the Ising transition value $\lambda_{\text{Ising}}$ in a finite range of $\Delta$. The ferromagnetic order in spins is retained, but the magnetization is no more fully saturated.

In the novel phase mentioned above, the SU(2) sym-
configuration in the FSOL phase changes smoothly, confirming with fixed different correlation functions, total spin of the ground state of systems consisting of up to \( L = 48 \) sites with periodic boundary conditions. We have checked that such a correlation persists at all magnetization 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 (d). Thus these are two gapless excitation branches with linear and quadratic dispersion, respectively.

Finally, in the FSOL phase the correlators \( \langle S^+_l S^z_l \rangle \) and \( \langle S^+_l \sigma^+_l S^-_m \sigma^-_m \rangle \) are very close to each other, despite the fact that \( \langle \sigma^+_l \sigma^-_m \rangle \) can be significantly lower than one, see Fig. 3(e) (in fact, for the parameters presented in Fig. 3(c) \( \langle S^+_l \sigma^+_l S^-_m \sigma^-_m \rangle \) is larger in absolute value than \( \langle S^+_l S^-_l \rangle \) even though \( \langle \sigma^+_l \sigma^-_m \rangle \) \( \sim 6 \) ). 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 \( S^+_l S^-_l (1 - \sigma^+_l) \) nearly annihilates the ground state.

**Boundary 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 \( \Delta \) at fixed \( \lambda \), localized and strongly correlated \( S = \frac{1}{2} \) edge spins emerge when crossing the b1 curve. Further increasing \( \Delta \) leads to a second transition at the b2 line, where the value of the boundary spin changes from \( \sigma \) to \( \frac{1}{2} \). This effect is illustrated in the inset of Fig. 2, where the correlation between edge spins is depicted as a function of \( \Delta \) for \( \lambda = 4 \). We refer to the Supplemental Material [28] for further details.

**Realization.**—Dipolar spinor fermions may be realized using polar molecules (see Ref. [12] for a detailed discussion) or employing atoms with large magnetic dipole moments, such as chromium [29], dysprosium [30], or erbium [31]. For the particular case of \( ^{58}\text{Cr} \), in a strong magnetic field, any two of the four lowest energy states \( |F, m_F \rangle = |\frac{9}{2}, -\frac{9}{2} \rangle, |\frac{9}{2}, -\frac{7}{2} \rangle, |\frac{9}{2}, -\frac{3}{2} \rangle \), and \( |\frac{9}{2}, -\frac{1}{2} \rangle \), can be chosen to simulate the \( | \uparrow \rangle \) and \( | \downarrow \rangle \) pseudospin 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 \( V(r_1 - r_2) = \frac{\mu_0}{4\pi |r_1 - r_2|^3} + g \delta(r_1 - r_2) \), where \( g = 4\pi a_s \hbar^2 / m \) characterizes the contact interactions, where \( a_s \) is the \( s \)-wave scattering length, \( m \) is the atomic mass, \( \mu_0 \) is the vacuum permeability and \( \mu \) is the magnetic dipole moment. The
interaction, resulting from the electronic degrees of freedom, is pseudospin-independent, providing the desired SU(2) spin symmetry of the problem. For $^{53}\text{Cr}$ the natural value of ratio $U/V$, where

$$U(V) = \int dr_1 dr_2 p^2_{\alpha} (r_1) V(r_1 - r_2) p^2_{\alpha}(r_2),$$

(here $\alpha, \beta = x, y$ and $p_{x,y}(r)$ are the orbital wave functions centered at the same site) is in the regime $U/V > 2$ considered in this letter.

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 novel, inaccessible in solid-state systems, spin-orbital liquid phase characterized by a finite but unsaturated magnetization. This phase, like ferromagnet, has spontaneously broken SU(2) symmetry, but, unlike a ferromagnet, it has algebraically decaying longitudinal spin correlations. This phase can be viewed as a Luttinger liquid of bound composites of singlet spin dimers and orbital domain walls on top of a fully polarized ferromagnetic phase.

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SUPPLEMENTARY MATERIALS ON: DETAILS OF BOUNDARY TRANSITIONS IN THE (iH,P) PHASE

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. 1 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 $\lambda$. In the strong $\lambda$ 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:

$$H_S = j_1 \sum_{n=2}^{N-2} S_n \cdot S_{n+1} + j_2 \sum_{n=2}^{N-1} S_{n-1} \cdot S_{n+1} + j'_1 (S_1 \cdot S_2 + S_{N-1} \cdot S_N),$$

where

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

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

One can see that with increasing $\Delta$, 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 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-$\frac{1}{2}$ localized at each boundary and ferromagnetically attached to the antiferromagnetic spin-$\frac{1}{2}$ chain. The interaction between the spin-$1$ edge impurities is antiferromagnetic for even number of sites and ferromagnetic for odd number of sites. The lowest excitations are boundary excitations: a boundary triplet with total spin $S_T = 1$ and a little higher boundary quintet with spin $S_T = 2$.

FIG. 4. (Color online). Excitation gap for open boundary conditions (OBC) and periodic boundary conditions (PBC) as a function of $\Delta$. The inset zooms in the region $0.36 < \Delta < 0.6$, revealing the existence of the two boundary transitions at $b_1$ and $b_2$.

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 $b_1$ and $b_2$ 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 $b_2$ line and the boundary of the FSOL phase, both $S^z = 1$ and $S^z = 2$ excitations are localized at the edges.