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Current carrying ground state in a bilayer model of strongly correlated systems

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Strongly interacting systems have been conjectured to spontaneously develop current carrying ground states under certain conditions. We demonstrate the existence of a commensurate staggered interlayer current phase in a bilayer model by using the recently discovered quantum Monte Carlo algorithm without the sign problem *for fermionic systems*. A pseudospin $SU(2)$ algebra and the corresponding anisotropic spin-1 Heisenberg model are constructed to show the competition among the staggered interlayer current, rung singlet, and charge density wave phases.

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Strongly correlated systems can spontaneously break symmetries of the microscopic Hamiltonian. A particularly interesting class of ground states spontaneously break the time reversal symmetry and carry a persistent current in the ground state. Such states are known by different synonyms, e.g. the orbital antiferromagnetic phase, the staggered flux (SF), or the *D*-density wave (DDW) phase. In the context of high T_c superconductivity, these current carrying ground states have been proposed as competing states for the pseudogap phase.[1–6] The SF or the DDW phase has the attractive feature that the nodal quasiparticles have an energy spectrum similar to that of the *d*-wave superconducting state. The incommensurate SF phase was also proposed to explain the hidden order phenomenon in the URu_2Si_2 system.[7]

Whenever new ground states are proposed, it is important to establish for which microscopic Hamiltonian such states are realized. Because of the availability of reliable analytical and numerical methods, the ladder system has been used as a theoretical laboratory to investigate the DDW phase. Weak coupling bosonization methods combined with the renormalization group analysis on extended two-leg Hubbard ladders show the existence of a commensurate DDW phase at half-filling[8–10] and incommensurate power law fluctuating DDW order away from half-filling.[9,11,12] While the DDW state does not appear to be the ground state of the *t-J* ladder,[13,14] numerical works using the density matrix renormalization group found commensurate DDW order at half-filling[15] and incommensurate DDW order at low doping[16] in a ladder model first proposed by Scalapino, Zhang, and Hanke,[17] which is commonly referred as to the SZH model. The work of Schollwöck *et al.* has generated significant interest in connection with the DDW proposal for the cuprates.[5]

To the best of our knowledge, the existence of a current carrying ground state has not been conclusively demonstrated in any higher dimensional models. We investigate the current carrying ground state in a bilayer version of the SZH model, which was constructed and extensively investigated because of the exact $SO(5)$ symmetry when coupling constants satisfy a simple relation.[18–21] Here we show that the recently discovered fermionic quantum Monte Carlo (QMC) algorithm without the sign problem[22] can also be applied here at and away from half-filling. Thus we can conclusively demonstrate the existence of a current carrying ground state as illustrated in Fig. 1 with staggered interlayer currents (SIC) between the bilayers and alternating source to drain currents within the bilayers. Viewed from the top, this current pattern has an *s*-wave symmetry. While the DDW currents are divergence-free within the layer, the SIC current is curl-free within the layer. These two patterns can be considered as dual to each other in two dimensions. In this paper, we shall first discuss the physics of the SIC phase by mapping onto an effective spin one antiferromagnetic (AF) Heisenberg model, and then proceed with the QMC results.

The Hamiltonian for the SZH model[17] generalized straightforwardly to the bilayer system reads

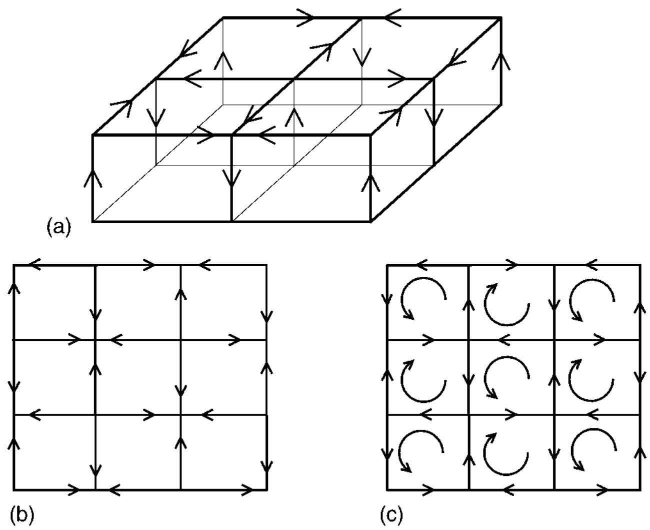

FIG. 1. (a) Sketch of a SIC phase. For clarity, we do not show the bottom layer current. By conservation, each site acts as a source or drain for the current within the bilayers. (b) The top view of the the bilayer. (c) A sketch of the SF or the DDW current pattern for comparison.

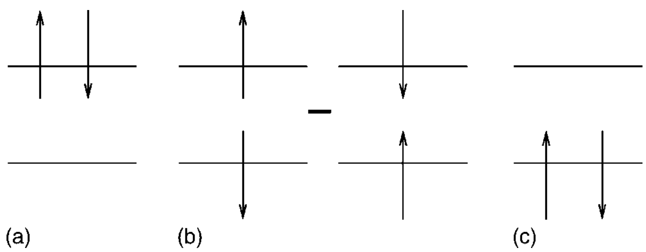

FIG. 2. The double occupancy states a and c and the rung singlet b (a), (b) and (c) are spin $SU(2)$ singlets and form the triplet representation of the pseudospin $SU(2)$ group.

$$H = -t_{\parallel}\sum_{\langle ij\rangle}\{c^{\dagger}_{i\sigma}c_{j\sigma} + d^{\dagger}_{i\sigma}d_{j,\sigma} + \mathrm{H.c.}\} - t_{\perp}\sum_{i}\{c^{\dagger}_{i,\sigma}d_{i,\sigma} + \mathrm{H.c.}\} - \mu\sum_{i}\{c^{\dagger}_{i,\sigma}c_{i,\sigma} + d^{\dagger}_{i,\sigma}d_{i,\sigma}\} + J\sum_{i}\vec{S}_{i,c}\cdot\vec{S}_{i,d} + U\sum_{i}(n_{i,\uparrow,c}-1/2)(n_{i,\downarrow,c}-1/2) + (n_{i,\uparrow,d}-1/2)(n_{i,\downarrow,d}-1/2) + V\sum_{i}(n_{i,c}-1)(n_{i,d}-1), \quad (1)$$

where c and d denote fermionic operators in the upper and the lower layers, respectively, and σ corresponds to up and down spins. At half-filling, $\mu=0$, and the model is particle-hole symmetric. $t_{\parallel}=1$ sets the unit of energy. The SZH model was known to have a $SO(5)$ symmetry when $J=4(U+V)$ and $\mu=0$, which unifies antiferromagnetism with superconductivity.[17] Remarkably, it also has another $SO(5)$ symmetry in the particle-hole (p-h) channel when

$$J = 4(U - V), \quad t_{\perp} = 0 \quad (2)$$

is valid for all filling factors. We denote the former particle-particle $SO(5)$ symmetry as $SO(5)_{pp}$ and the later p-h $SO(5)$ symmetry as $SO(5)_{ph}$. The mathematical structure associated with the $SO(5)_{p\text{-}h}$ algebra, not necessarily the symmetry itself, plays a crucial role in constructing the fermionic QMC algorithm without minus sign problem.

We construct a four component fermion field $\Psi=\{c_{\sigma},d_{\sigma}\}$. Using the five Dirac Γ_a matrices given in Ref. 22, we construct the fermion bilinears

$$n_a = \Psi^{\dagger}\frac{\Gamma_a}{2}\Psi \quad L_{ab} = \Psi^{\dagger}\frac{\Gamma_{ab}}{2}\Psi.$$

It is straightforward to check that $[H,L_{ab}]=0$ when Eq. (2) is satisfied, thus demonstrating the exact $SO(5)_{ph}$ symmetry. The SZH model can be mapped exactly to the spin $3/2$ Hubbard model,[22] by the identification $c_{\uparrow}=c_{3/2}$, $c_{\downarrow}=c_{1/2}$, $d_{\uparrow}=c_{-1/2}$, $d_{\downarrow}=c_{-3/2}$, and the $SO(5)_{ph}$ symmetry maps exactly onto the $SO(5)$ symmetry of the spin $3/2$ Hubbard model. Thanks to this mapping, we are able to use the QMC algorithm discovered in Ref. 22, which has no minus sign problem in a large parameter regime

Scalapino *et al.* identified the phases where either the rung singlet state [Fig 2(b)], or the charge-density wave (CDW) states [Figs. 2(a) and 2(c)] are the lowest energy states.[17] References 15 and 16 reveal that the competition between these two phases could result in the DDW phase. In view of this insight, let us consider the following operators:

$$n_1(i) = i/2\sum_{\sigma}\{c^{\dagger}_{\sigma}(i)d_{\sigma}(i) - d^{\dagger}_{\sigma}(i)c_{\sigma}(i)\},$$

$$n_5(i) = 1/2\sum_{\sigma}\{c^{\dagger}_{\sigma}(i)d_{\sigma}(i) + d^{\dagger}_{\sigma}(i)c_{\sigma}(i)\},$$

$$Q(i) = L_{15} = 1/2\sum_{\sigma}\{c^{\dagger}_{\sigma}(i)c_{\sigma}(i) - d^{\dagger}_{\sigma}(i)d_{\sigma}(i)\}.$$

These operators describe rung current (n_1), rung kinetic energy (n_5), and the CDW order parameter (Q), which form a pseudospin $SU(2)$ algebra and commutes with the spin $SU(2)$ algebra. The three-spin singlet rung states shown in Fig. 2 form a spin-1 representation of this algebra with eigenvalues $Q=1,\ 0,\ -1$.

At half-filling and under the condition that $\max(U,V-3/4J)<\min(V+J/4,U+2V,U/2+V)$, these states are the three lowest energy states, which become degenerate at $U=V-3/4J$. In the strong coupling limit, we can construct an effective pseudospin-1 antiferromagnetic (AF) Heisenberg model as

$$H_{ex} = J_p\sum_{\langle i,j\rangle}\{n_5(i)n_5(j) + n_1(i)n_1(j) + Q(i)Q(j)\}, \quad (3)$$

with $J_p=2t_{\parallel}^2/(V+\frac{3}{4}J)$. Several terms break the pseudospin $SU(2)$ symmetry. The intrarung hopping $t_{\perp}$ term acts as an uniform external magnetic field which couples to n_5. Also, the deviation of U from $V-3/4J$ removes the degeneracy between the a, c, and b states. These can be described by the on site part as

$$H_{on} = \sum_{i}\{-2t_{\perp}n_5(i) + \Delta U[Q^2(i) - 1/2]\} \quad (4)$$

where $\Delta U=U-(V-3/4J)$. The nonzero value of ΔU also gives different corrections to the three exchange terms at the order of $J_p\Delta U/U$, which are small compared to the ΔU term and thus neglected. $H=H_{ex}+H_{on}$ describes a two-dimensional (2D) AF spin one Heisenberg model in an uniform magnetic field $t_{\perp}$, with either easy axis ($\Delta U<0$) or easy plane ($\Delta U>0$) anisotropy.

For the easy axis case, the effective Hamiltonian reduces to an Ising model with $Q=\pm 1$ states, in a transverse magnetic field as in Refs.10 and 17. For $t_{\perp}=0$ and $\Delta U>0$, the rung singlet state (b) has the lowest energy. However, there is a competition between the ΔU term and the exchange J_p term. For $\Delta U>zJ_p$, where $z=4$ is the coordination number, the ground state can be described as a product of each rung singlet state. On the other hand, for $\Delta U<zJ_p$, it is more favorable to develop a staggered ground state expectation value of $\langle n_1\rangle$ and $\langle n_5\rangle$ spontaneously. In this case with $t_{\perp}=0$, the pseudospin vector can lie along in any direction in the (n_1,n_5) plane. On the other hand, at $\Delta U=0$, a finite value of $t_{\perp}>0$ corresponds to a pseudospin magnetic field along the n_5 direction, which creates an easy (n_1,Q) space. The staggered component of the pseudospin lies in the (n_1,Q) plane, while the uniform one points along the n_5 direction.

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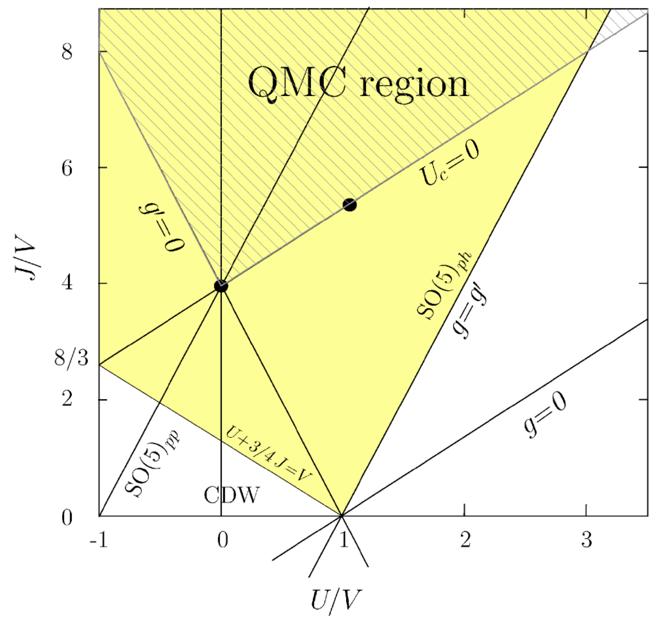

FIG. 3. (Color online) Phase diagram in the strong coupling limit. Two $SO(5)$ lines are shown as well as QMC region with no minus sign problem for any filling (hatched area): $g>0$, $g'>0$, and $U_c>0$. There is also another region with $V<0$ (not shown). In the yellow region, the low-energy bosonic states are a, b, and c as shown in Fig. 2. This is where we expect the competition between the SIC and the rung-singlet phase. Black dots correspond to where the QMC simulations are performed.

The pseudospin moment becomes fully polarized when $t_\perp > (z/2)J_p$, and the AF component vanishes beyond this point. We see that $t_\perp>0$ favors the (n_1,Q) easy plane, while $\Delta U<zJ_p$ favors the (n_1,n_5) easy plane. Therefore, when both conditions are present, the intersection between the two easy planes, namely the n_1 easy axis, is selected. This is exactly the staggered interlayer current order. Combining all these considerations, we can summarize the subtle criteria for the SIC phase as

$$V-\frac{3}{4}J<U<\min\left(V+\frac{J}{4},2V\right), \quad V>0$$

$$t_\perp<\frac{1}{2}zJ_p\sqrt{1-(\Delta U/zJ_p)^2}, \quad \Delta U<zJ_p, \tag{5}$$

The first two robust conditions ensure that the a, b, and c states are the three lowest energy states, while the last two conditions are the rough mean field estimates discussed above.

In Fig. 3, we show some specific regions on the phase diagram in the strong coupling limit. There are two additional axes for $t_\parallel$ and $t_\perp$. If $t_\parallel$ and/or $t_\perp$ gets larger, we can expect some phases to have larger or smaller extensions. In the case of ladders, a similar phase diagram has been proposed.[10,16] In order to obtain significant current correlations, one should be close enough from the line $V=U+3/4J$ where states a, b, and c become degenerate.

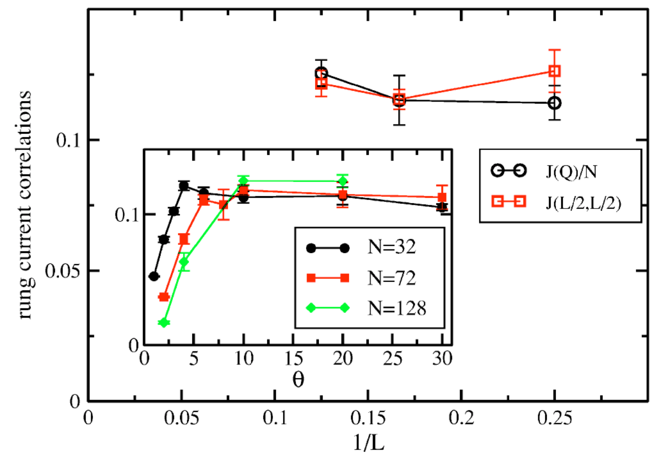

FIG. 4. (Color online) Parameters are $t_\perp=0.1$, $U=0$, $V=0.5$, and $J=2.0$ and correspond to $g=0.25$, $g'=0$, and $U_c=0$. The scaling of $\mathcal{J}(\vec{Q})/N$ and $J(L/2,L/2)$ vs $1/L$ shows almost no finite-size effects and proves long-range order in the thermodynamic limit. (The inset shows the convergence of $\mathcal{J}(\vec{Q})/N$ with the projection parameter θ. Typically the GS value is obtained for $\theta=20$.)

Now we proceed to discuss the QMC calculation of the SIC phase. We first express the interaction terms of the SZH model as

$$H_{int}=-\frac{g}{2}(n_1^2+n_5^2)-\frac{g'}{2}(n_2^2+n_3^2+n_4^2)-\frac{U_c}{2}(n-2)^2, \tag{6}$$

with $4U_c=-U-3V+3J/4$, $4g=V-U+3J/4$ and $4g'=U-V+J/4$. The $SO(5)_{ph}$ symmetry is recovered when $g=g'$, i.e., $U=V+J/4$. We now introduce auxiliary Hubbard-Stratonovich fields to decouple each of the three terms above. Wu, Hu, and Zhang[22] have shown that the QMC algorithm is free of the minus sign problem provided all three coefficients: g, g', and U_c are positive. It corresponds to a wedge in the phase diagram shown in Fig. 3, and most remarkably, it includes a region with purely repulsive interactions, where U, V, and J are all positive. A simpler case containing only n_4^2 interaction, which explicitly breaks the $SU(2)$ spin rotation invariance, has been studied in another context.[23] The ground-state (GS) properties of our model are conveniently studied with the projector auxiliary field QMC algorithm. The basic idea is to apply the operator $\exp(-\theta H)$ to a trial state. When θ becomes large enough and with a proper normalization, this state converges exponentially to the GS. Details of the algorithm may be found in Ref. 24.

We compute correlations between rung currents $n_1(\vec{r})$ and perform its Fourier transform

$$\mathcal{J}(\vec{q})=\frac{1}{N}\sum_{\vec{r}} e^{i\vec{q}\cdot\vec{r}}\sum_i \langle n_1(i)n_1(i+\vec{r})\rangle. \tag{7}$$

The strongest signal in the Fourier transform is found for $\vec{Q}=(\pi,\pi)$, suggesting a staggered current pattern as shown in Fig. 1. This quantity converges to its GS value as the projector parameter θ increases as shown in the inset of Fig.

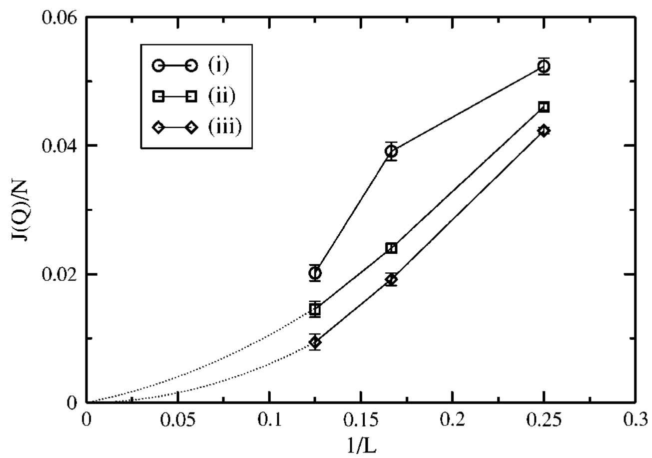

FIG. 5. Finite-size scaling of the current correlations $\mathcal{J}(\vec{Q})/N$ showing no long-range order in the thermodynamic limit. The parameters are (i) the same as Fig. 4 except for $t_\perp=0.5$; (ii) $U=V=0.3$, $J=1.6$, and $t_\perp=0.5$ at half-filling; (iii) $U=0.75$, $V=0$, $J=1$, and $t_\perp=0$ at 1/8 doping. Typically the GS value is obtained for $\theta=20$.

4. In order to obtain information in the thermodynamic limit, one has to make an extrapolation of these GS values with a $1/L$ finite-size scaling, where L is the linear size ($L=4$, 6, and 8 in our simulations). Note that the total number of sites is $N=2L^2$.

Following our previous mean-field arguments, in order to prefer a phase with staggered current, we choose $g>g'$ and $U_c=0$, with a small $t_\perp$. As shown on Fig. 4 for $U=0$, $V=0.5$, and $J=2$, and $t_\perp=0.1$, our values are rather constant with size, as expected in an Ising-like phase. Both the largest distance real-space correlations $J(L/2,L/2)$ and the Fourier transform $\mathcal{J}(\vec{Q})/N$ converge to the same finite value (within error bars), meaning long-range order in the thermodynamic limit.

As expected from our analytical estimates in (5), if ΔU or $t_\perp$ gets too large, long-range order disappear as shown in Fig. 5. Since we can also perform the QMC simulation at finite doping without the sign problem, we have chosen to work at 1/8 doping for some parameters shown on Fig. 5. Again, rung-current correlations vanish in the thermodynamic limit since the Fermi surface is not nested anymore.

From the analytical estimates based on the mapping to the spin one antiferromagnetic Heisenberg model and the detailed fermion QMC calculations without the sign problem, we can demonstrate the existence of the SIC phase at half-filling in a bilayer model. We have also shown that this rather subtle phase can be easily destabilized by large U and doping; therefore, the findings of this work severely constrain the possibility of current carrying ground states in the high T_c cuprates. The parameter range of stability discovered in this work could guide the search of the current carrying ground states in other strongly correlated systems, for example, the heavy fermion systems.

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