Current Carrying Ground State in a Bi-layer Model

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Strongly interacting systems have been conjectured to spontaneously develop current carrying ground states under certain conditions. We conclusively demonstrate the existence of a commensurate staggered interlayer current phase in a bi-layer model by using the recently discovered quantum Monte-Carlo algorithm without the sign problem. 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 (OAF), the staggered flux (SF) or the D-density wave (DDW) phase. In the context of high Tc superconductivity, these current carrying ground states have been proposed as competing states for the pseudogap phase. The SF or the DDW phase has the attractive feature that the nodal quasi-particles have an energy spectrum similar to that of the $d$-wave superconducting state.

Whenever new ground states are proposed, it is important to establish for which microscopic Hamiltonian such states are realized. Because of their relative simplicity and 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 (RG) analysis on extended two-leg Hubbard ladders show the existence of commensurate DDW phase at half-filling and incommensurate power law fluctuating DDW order away from half-filling. While the DDW state does not appear to be the ground state of the t-J ladder, numerical works using the density matrix renormalization group (DMRG) found commensurate DDW order at half-filling and incommensurate DDW order at low doping in a ladder model first proposed by Scalapino, Zhang and Hanke. The work of Schollwöck et al has generated significant interest in connection with the DDW proposal for the cuprates.

To the best of our knowledge, the existence of a current carrying ground state has not been conclusively demonstrated in any higher dimensional models. Following the insights we learned from the 1D systems, we investigate the current carrying ground state in a bi-layer version of the model constructed in Ref. [16]. This model was originally constructed and extensively investigated because of the exact $SO(5)$ symmetry when coupling constants satisfy a simple relation, and is commonly referred to as the SZH model. Here we show that the recently discovered fermionic quantum Monte Carlo (QMC) algorithm without the sign problem can also be applied to this model at and away from half-filling, for a large set of parameters, including purely repulsive interactions. Using this highly accurate numerical method, we can conclusively demonstrate the existence of a current carrying ground state in this model. The current carrying ground state is illustrated in Fig. with staggered interlayer currents (SIC) between the bi-layers and alternating source to drain currents within the bi-layers. Viewed from the top of the bi-layers, this current pattern is different from the SF or the DDW current pat-
tern, since it has a s-wave symmetry. While the SF or the DDW currents are divergence free within the layer, the SIC current is curl free within the layer. These two flow 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 Heisenberg model, and then proceed with the QMC results.

The Hamiltonian for the SZH model generalized straightforwardly to the bi-layer system reads

\[
H = -t_\parallel \sum_{\langle ij \rangle} \{ c_i^\dagger c_{i+\sigma} + d_i^\dagger d_{j+\sigma} + h.c. \} - t_\perp \sum_i \{ c_i^\dagger d_{i+\sigma} + h.c. \} - \mu \sum_i \{ c_i^\dagger c_{i+\sigma} + d_i^\dagger d_{i+\sigma} \} + J \sum_i \vec{S}_{i,c} \cdot \vec{S}_{i,d} + U \sum_i (n_{i,c}-1)(n_{i,d}-1),
\]

where \(c\) and \(d\) denotes fermionic operators in the upper and the lower layers, respectively, \(\sigma\) 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. Before discussing the SIC phase, we first discuss some general properties of the SZH model which were not known before. The SZH model was known to have a \(SO(5)\) symmetry when \(J = 4(U + V)\) and \(\mu = 0\), which unifies antiferromagnetism with superconductivity. Especially, it also has another \(SO(5)\) symmetry when \(\mu = 0\) and \(J\) is set to a constant. The SZH model can be mapped exactly to the \(\text{SU}(2)\) algebra, not necessarily the \(\text{SU}(2)\) algebra defined above, with eigenvalues \(\pm \frac{\pi}{4}\), and act as pseudospin raising and lowering operators \(\bar{\sigma}_i\). Using the five Dirac \(\Gamma_a\) matrices given in Ref. [21], we construct the fermion bi-linears

\[
\begin{align*}
\Psi &= (c_\sigma, d_\sigma), \\
n_a &= \Psi^\dagger \frac{\Gamma_a}{2} \Psi, \\
L_{ab} &= \Psi^\dagger \frac{\Gamma_{ab}}{2} \Psi
\end{align*}
\]

It is straightforward to check that \([H, L_{ab}] = 0\) when Eq. (2) is satisfied, thus demonstrating the exact \(SO(5)\) symmetry. The SZH model can be mapped exactly to the spin 3/2 Hubbard model [21], by the identification \(c_\uparrow = c_{3/2}, c_\downarrow = c_{-1/2}, d_\uparrow = d_{-1/2}, d_\downarrow = d_{3/2}\), and the \(SO(5)\) symmetry maps exactly onto the \(SO(5)\) symmetry of the spin 3/2 Hubbard model. Because of the exact mapping from the SZH model to the spin 3/2 Hubbard model, we are able to use the QMC algorithm discovered in Ref. [21], which works without the minus sign problem in a large parameter regime.

In studying the strong coupling phase diagram, SZH identified the \(E_0\) phase where the rung singlet state, depicted in Fig. 2b, is the lowest energy state, and the \(E_3\) phase, where the CDW states, depicted in Fig. 2a, and 2c are the lowest energy states. The new insight gained from Ref. [14, 15] reveals that the competition between these two phases could result in the DDW phase. In view of this insight, let us consider the following operators

\[
\begin{align*}
n_1(i) &= i/2 \sum_{\sigma} \{ c_\uparrow(i) d_\uparrow(i) - d_\uparrow(i) c_\uparrow(i) \}, \\
n_5(i) &= 1/2 \sum_{\sigma} \{ c_\downarrow(i) d_\downarrow(i) + d_\downarrow(i) c_\downarrow(i) \}, \\
Q(i) &= L_{15} = 1/2 \sum_{\sigma} \{ c_{\bar{\sigma}}(i) c_\sigma(i) - d_{\bar{\sigma}}(i) d_\sigma(i) \},
\end{align*}
\]

where \(\bar{\sigma}\) are the Pauli matrices. These operators describe rung current \((n_1)\), rung kinetic energy \((n_5)\) and the CDW order parameter \((Q)\). These three operators form a pseudo-spin \(\text{SU}(2)\) algebra which are important for our discussion of the SIC phase.

There are 16 states on each rung, including 8 bosonic states with particle number 0, 2 or 4 and eight fermionic states with particle number 1 or 3. We are interested in the three rung states shown in Fig. 2a, b, c, which form a spin-1 representation of the pseudospin \(\text{SU}(2)\) algebra defined above, with eigenvalues \(Q = 1, 0, -1\). \(n_1 \pm in_5\) act as pseudospin raising and lowering operators which connect these three states to each other. At half-filling and under the condition that \(\text{max}(U, V - 3/4J) < \min(V + J/4, U + 2V, U/2 + V)\), these are the three lowest energy states. Furthermore, at \(U = V - 3/4J\), these

\[
\begin{align*}
\psi_0 &= \frac{1}{\sqrt{2^n}} \sum_{\sigma_1, \sigma_2, \ldots, \sigma_n} \prod_{i=1}^n \{ c_{\sigma_i}(i) d_{\sigma_i}(i) \}, \\
\psi_1 &= \frac{1}{\sqrt{2^n}} \sum_{\sigma_1, \sigma_2, \ldots, \sigma_n} \prod_{i=1}^n \{ c_{\sigma_i}(i) d_{\bar{\sigma}_i}(i) \}, \\
\psi_2 &= \frac{1}{\sqrt{2^n}} \sum_{\sigma_1, \sigma_2, \ldots, \sigma_n} \prod_{i=1}^n \{ c_{\sigma_i}(i) d_{\sigma_i}(i) \}, \\
\psi_3 &= \frac{1}{\sqrt{2^n}} \sum_{\sigma_1, \sigma_2, \ldots, \sigma_n} \prod_{i=1}^n \{ d_{\sigma_i}(i) c_{\bar{\sigma}_i}(i) \}
\end{align*}
\]

FIG. 2: The double occupany state a) and c) and the rung singlet (b). a), b), c) are spin \(\text{SU}(2)\) singlets and form the triplet representation of the pseudospin \(\text{SU}(2)\) group.
three states are degenerate. In the strong coupling limit, we can construct an effective theory to describe the low energy physics by using a pseudospin-1 antiferromagnetic Heisenberg model

\[ H_{ex} = J_p \sum_{(i,j)} \left\{ n_5(i)n_5(j) + n_1(i)n_1(j) + Q(i)Q(j) \right\}, \]

with \( J_p = 2t_\parallel^2/(V + \frac{4}{3}J) \). Several terms break the pseudospin SU(2) symmetry. The intra-rung 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 \( a, \) \( c \) and \( b \) states. These symmetry breaking terms are described by the on-site part as

\[ H_{on} = \sum_i \left\{ -2t_\perp n_5(i) + \Delta U(Q^2(i) - 1/2) \right\} \]

where \( \Delta U = U - (V - 3/4J) \). The nonzero value of \( \Delta U \) also gives different corrections to the three exchange terms at the order of \( J_p\Delta U/U \). We will neglect these corrections below because the more important symmetry breaking effect from \( \Delta U \) has already been taking into account in the on-site part. \( H = H_{ex} + H_{on} \) describes a 2D antiferromagnetic 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 with \( \Delta U < 0 \), the effective Hamiltonian reduces to an Ising model with \( Q = \pm 1 \) states, in a transverse magnetic field \([5, 14]\). For \( t_\perp = 0 \), and \( \Delta U > 0 \), the rung singlet state \( (b) \) has the lowest energy. However, in this case, there is a competition between the \( \Delta U > 0 \) term and the Heisenberg exchange term \( J_p \). For \( \Delta U > zJ_p \), where \( z = 4 \) is the coordination number, the ground state is a featureless Mott insulating state which can be described as a product of the rung singlet state on each site. On the other hand, for \( \Delta U < zJ_p \), it is more favorable to form linear combinations between the \( (a), (b) \) and \( (c) \) states, such that a staggered ground state expectation value of \( \langle n_1 \rangle \) and \( \langle n_5 \rangle \) is spontaneously developed, thus lowering the Heisenberg exchange energy \( H_{ex} \). In this case, and for \( t_\perp = 0 \), the pseudo-spin vector can lie along in any direction in the \( (n_1, Q) \) plane. The antiferromagnetic component of the pseudo-spin moment lies in the \( (n_1, Q) \) plane, but the uniform component of the pseudo-spin moment points along the \( n_5 \) direction. The pseudo-spin moment becomes fully polarized when \( t_\perp > \frac{5}{2}J_p \), and the antiferromagnetic component vanishes beyond this point. We see that \( t_\perp > 0 \) favors the \( (a, Q) \) easy plane while \( \Delta U < zJ_p \) favors the \( (n_1, n_5) \) easy plane, therefore, when both conditions are satisfied, the intersection between the two easy planes, namely the \( n_1 \) easy axis, is selected. This is exactly the staggered inter-layer current (SIC) order. Combining all these considerations, we can summarize the subtle criteria for the SIC phase as

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

\[ t_\perp < \frac{1}{2}zJ_p\sqrt{1 - \frac{\Delta U}{zJ_p}^2}, \quad \Delta U < zJ_p \]

The first two robust conditions ensure that the \( (a), (b) \) and \( (c) \) states are the lowest and next lowest energy states among the 16 states on the rung, while the last two conditions are the rough mean field estimates discussed above.

On Fig. 3 we show some specific regions on the phase diagram, obtained in the strong coupling limit. There are two additional axis 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 extension. In the case of ladders, a similar phase diagram has been proposed \([9, 15]\). In order to obtain significant current correlations, one should be close enough from the line \( V = U + 3/4J \) shown on Fig. 3 where states \( a, b \) and \( c \) become degenerate.

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

\[ H_{int} = -g(n_1^2 + n_5^2) - g'(n_2^2 + n_3^2 + n_4^2) - U_2(n - 2)^2, \]

up to a constant term. Here \( 4U_2 = -U - 3V + 3J/4, 4q = V - U + 3J/4 \) and \( 4q' = U - V + J/4 \). The \( SO(5)_{ph} \) symmetry is clearly recovered when \( g = g' \), i.e., when \( U = V + J/4 \). We now introduce auxiliary Hubbard-Stratonovich fields to decouple each of the three terms

\[ 3 \]
checked that it does not change the results. and are rather constant with size, as expected in an Ising-like

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above. Wu, Hu and Zhang have shown that the QMC algorithm is free of the minus sign problem provided all three coefficients, , , and are positive. It corresponds to a wedge in the phase diagram shown on Fig. except for . Typically the GS value is obtained for .

We compute correlations between rung currents  and perform its Fourier transform

\[ \mathcal{F}(\vec{q}) = \frac{1}{N} \sum_{\vec{r}} e^{i \vec{q} \cdot \vec{r}} \sum_i \langle n_1(i) n_1(i + \vec{r}) \rangle. \] (8)

The strongest signal in the Fourier transform is found for \( \vec{Q} = (\pi, \pi) \), suggesting a staggered current pattern as shown in Fig. 4. This quantity converges to its GS value as the projector parameter increases as shown in the inset of Fig. 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).

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 \( t_L \). As shown on Fig. 4 for \( U = 0, V = 0.5 \) and \( J = 2 \) when \( t_L \) is small at 0.1, our values are rather constant with size, as expected in an Ising-like phase. Both the largest distance real-space correlations \( \mathcal{F}(\vec{Q})/N \) and the Fourier transform \( \mathcal{F}(\vec{Q})/N \) converge to the same finite value (within our error bars), meaning long-range order in the thermodynamic limit.

As expected from our analytical estimates in (6), if \( \Delta U \) or \( t_L \) gets too large, long-range order disappear as shown on Fig. 4. 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 QMC calculations shown above, we can conclusively demonstrate the existence of the SIC phase at half-filling, and also note that this is a rather subtle phase which can be easily destabilized by large \( U \) and doping.

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