Staggered flux state in the two-leg Hubbard ladder at half filling

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Abstract

We investigate the staggered flux state in the half-filled extended Hubbard ladder using the strong-coupling perturbation theory. The staggered flux state has long-range order of currents on rungs flowing in the alternating direction. We derive a low-energy effective Hamiltonian and study an Ising-type quantum phase transition between the staggered flux state and the d-wave-pairing Mott insulating state.

Key words: staggered flux state; half-filled Hubbard ladder; quantum phase transitions

The staggered flux (SF) state or the D-density wave state [1] has been proposed to characterize the underdoped pseudo-gap region in the two-dimensional high-T_c cuprates [2]. In the SF state, there is a spontaneous current flowing around each plaquette of a lattice. Two-leg t-J ladder systems have been studied as a simple prototype model which can exhibit the SF fluctuations [3]. Recently, the half-filled Hubbard ladder has been suggested to show the SF states with long-range order from the weak-coupling approach [4].

In this paper we investigate the SF state in the half-filled Hubbard ladder using the strong-coupling perturbation theory. The Hamiltonian is given by $H = H_{t_\parallel} + H_{t_\perp} + H_{\rm int}$. The first two terms describe hopping: $H_{t_\parallel} = -t_\parallel \sum_{j,\sigma,l}(c^\dagger_{j,l,\sigma}\, c_{j+1,l,\sigma} + \text{h.c.})$ and $H_{t_\perp} = -t_\perp \sum_{j,\sigma}(c^\dagger_{j,1,\sigma}\, c_{2,j,\sigma} + \text{h.c.})$, where $c_{j,l,\sigma}$ annihilates an electron of spin $\sigma(=\uparrow,\downarrow)$ on site j of chain $l(=1,2)$. We take into account interactions between electrons on the same rung by $H_{\rm int} = H_U + H_{V_\perp} + H_{J_\perp} + H_{\rm pair}$, where the respective terms denote the onsite repulsion $H_U = U \sum_{j,l} n_{j,l,\uparrow}\, n_{j,l,\downarrow}$, the nearest-neighbor repulsion $H_{V_\perp} = V_\perp \sum_j n_{j,1}\, n_{j,2}$, the rung exchange $H_{J_\perp} = J_\perp \sum_j \boldsymbol{S}_{j,1}\cdot \boldsymbol{S}_{j,2}$ and the pair hopping between chains $H_{\rm pair} = t_{\rm pair} \sum_j \left(c^\dagger_{j,1,\uparrow}\, c^\dagger_{j,1,\downarrow}\, c_{j,2,\downarrow}\, c_{j,2,\uparrow} + \text{h.c.}\right)$. The density operators are $n_{j,l,\sigma} = c^\dagger_{j,l,\sigma}\, c_{j,l,\sigma}$ and $n_{j,l} = n_{j,l,\uparrow} + n_{j,l,\downarrow}$, and $\boldsymbol{S}_{j,l}$ is the spin-$\frac{1}{2}$ operator. The coupling constants, U, $V_\perp$, $J_\perp$, and $t_{\rm pair}$, are assumed to be either zero or positive.

A single rung (e.g., jth rung) has four states at half filling:

$$
\begin{aligned}
|1\rangle_j &\equiv c^\dagger_{j,1,\uparrow}\, c^\dagger_{j,2,\downarrow}\, |0\rangle, \quad |2\rangle_j \equiv c^\dagger_{j,1,\downarrow}\, c^\dagger_{j,2,\uparrow}\, |0\rangle, \\
|3\rangle_j &\equiv c^\dagger_{j,1,\uparrow}\, c^\dagger_{j,1,\downarrow}\, |0\rangle, \quad |4\rangle_j \equiv c^\dagger_{j,2,\uparrow}\, c^\dagger_{j,2,\downarrow}\, |0\rangle.
\end{aligned} \tag{1}
$$

The eigenvalues of $H_{\rm int}$ are given by $V_\perp - \frac{3}{4}J_\perp$, $V_\perp + \frac{1}{4}J_\perp$, $U - t_{\rm pair}$ and $U + t_{\rm pair}$, and the corresponding eigenstates are $\frac{1}{\sqrt{2}}(|1\rangle_j - |2\rangle_j)$, $\frac{1}{\sqrt{2}}(|1\rangle_j + |2\rangle_j)$, $\frac{1}{\sqrt{2}}(|3\rangle_j - |4\rangle_j)$ and $\frac{1}{\sqrt{2}}(|3\rangle_j + |4\rangle_j)$, respectively. The lowest-energy state for $U > V_\perp - \frac{3}{4}J_\perp + t_{\rm pair}$ is $|\text{D-Mott}\rangle = \prod_j \frac{1}{\sqrt{2}}(|1\rangle_j - |2\rangle_j)$, which is a direct product of rung singlets and thus called D-Mott state [4].

Most interesting situation is the case where the energy gain of the rung-singlet state $\frac{1}{\sqrt{2}}(|1\rangle_j - |2\rangle_j)$ and that of the onsite-singlet state $\frac{1}{\sqrt{2}}(|3\rangle_j - |4\rangle_j)$ become comparable. The rung-singlet (onsite-singlet) state is stabilized by the exchange interaction $J_\perp$ (the pair-hopping term $t_{\rm pair}$) with the energy gain $-\frac{3}{4}J_\perp$ ($-t_{\rm pair}$). Thus, we first take into account the effects of these interaction terms and consider the case where $t_{\rm pair} \simeq \frac{3}{4}J_\perp$. In order to describe this situation, we take the unperturbed Hamiltonian as $H_0 = H_{J_\perp} + H^{(0)}_{\rm pair}$

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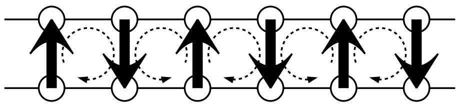

Fig. 1. Staggered flux state described as a Néel ordered state of the pseudo-spin states, $|\uparrow\rangle$ and $|\downarrow\rangle$.

where $H^{(0)}_{\text{pair}} = H_{\text{pair}}|_{t_{\text{pair}}=3J_\perp/4}$. The rung-singlet state $\frac{1}{\sqrt{2}}(|1\rangle_j - |2\rangle_j)$ and the onsite-singlet state $\frac{1}{\sqrt{2}}(|3\rangle_j - |4\rangle_j)$ are the *degenerate* lowest-energy states of H_0. In order to describe the SF state, we change the basis into the following one that breaks time reversal symmetry:

$$|\uparrow\rangle_j \equiv \frac{1}{2}\big[\big(|1\rangle_j - |2\rangle_j\big) + \mathrm{i}\big(|3\rangle_j - |4\rangle_j\big)\big], \tag{2}$$

$$|\downarrow\rangle_j \equiv \frac{1}{2}\big[\big(|1\rangle_j - |2\rangle_j\big) - \mathrm{i}\big(|3\rangle_j - |4\rangle_j\big)\big]. \tag{3}$$

These states represent states with finite currents running along a rung, as they are eigenstates of the rung-current operator defined by $\hat{J}_j \equiv \mathrm{i}\sum_\sigma(c^\dagger_{j,1,\sigma}c_{j,2,\sigma} - c^\dagger_{j,2,\sigma}c_{j,1,\sigma})$ with eigenvalues ± 2: $\hat{J}_j\,|\uparrow\rangle_j = +2\,|\uparrow\rangle_j$ $\hat{J}_j\,|\downarrow\rangle_j = -2\,|\downarrow\rangle_j$. We can regard $|\uparrow\rangle_j$ and $|\downarrow\rangle_j$ as up and down states of a pseudo-spin $\widetilde{\boldsymbol{S}}_j$. The SF state has long-range order of currents counter-circulating around each plaquette, which corresponds to the long-range Néel order of pseudo-spins in our description (Fig. 1). To verify the existence of the SF phase, we apply the perturbation theory and derive a low-energy effective theory (pseudo-spin Hamiltonian) for the lowest-energy states $|\uparrow\rangle_j$ and $|\downarrow\rangle_j$. The perturbation expansion is performed by splitting the Hamiltonian as $H = H_0 + H'$ where $H' = H_U + H_{V_\perp} + H_{t_\parallel} + H_{t_\perp} + H_{\text{pair}}|_{t_{\text{pair}}=\delta t_{\text{pair}}}$ with $\delta t_{\text{pair}} \equiv t_{\text{pair}} - \frac{3}{4}J_\perp$. Up to the lowest-order perturbation for each term in H', we find that the effective Hamiltonian is the antiferromagnetic Ising chain in a transverse field,

$$H^{\text{eff}} = \sum_j \left(K\,\tilde{\sigma}^z_j\,\tilde{\sigma}^z_{j+1} - h\,\tilde{\sigma}^x_j\right), \tag{4}$$

$$K = \frac{4t^2_\parallel}{3J_\perp}, \qquad h = \frac{1}{2}(U - V_\perp - \delta t_{\text{pair}}) + \frac{4t^2_\perp}{3J_\perp}, \tag{5}$$

where $\tilde{\sigma}^a_j$ are the Pauli matrices ($a = x, z$) acting on the pseudo-spin states: $\tilde{\sigma}^z_j\,|\uparrow\rangle_j = +\,|\uparrow\rangle_j$, $\tilde{\sigma}^z_j\,|\downarrow\rangle_j = -\,|\downarrow\rangle_j$, $\tilde{\sigma}^x_j\,|\uparrow\rangle_j = |\downarrow\rangle_j$ and $\tilde{\sigma}^x_j\,|\downarrow\rangle_j = |\uparrow\rangle_j$. This model exhibits an Ising phase transition at $K = |h|$ between the Néel ordered phase ($K > |h|$) and the disordered phase ($K < |h|$). The ground state in the disordered phase $h > K > 0$ is adiabatically connected with that in the limit $h \to \infty$, i.e., the eigenstate of $|\tilde{\sigma}^x = +1\rangle_j$. This state corresponds to the D-Mott state since

$$|\tilde{\sigma}^x{=}1\rangle_j = \frac{|\uparrow\rangle_j + |\downarrow\rangle_j}{\sqrt{2}} = \frac{|1\rangle_j - |2\rangle_j}{\sqrt{2}} \to |\text{D-Mott}\rangle. \tag{6}$$

Therefore we conclude that the Ising disordered phase is the D-Mott phase.

Finally we discuss the order parameter which characterizes the D-Mott insulating phase. Here we consider the following string order parameter:

$$V_j \equiv \exp\left[\mathrm{i}\frac{\pi}{2}\sum_{i=1}^{j}\sum_\sigma \sigma\left(c^\dagger_{i,1,\sigma}c_{i,2,\sigma} + \text{h.c.}\right)\right]. \tag{7}$$

Under the constraints $\sum_{l,\sigma} n_{i,l,\sigma} = 2$ and $\sum_l S^z_{i,l} = 0$ for any i, the string order parameter is rewritten as $V_j = \prod_{i=1}^j v_i$, where $v_i = (c^\dagger_{i,1,\uparrow}c^\dagger_{i,1,\downarrow}c_{i,2,\downarrow}c_{i,2,\uparrow} + \text{h.c.}) - (S^+_{j,1}\,S^-_{j,2} + S^-_{j,1}\,S^+_{j,2})$. Since v_j acts as the x-component of the pseudo-spin operator, $v_j\,|\uparrow\rangle_j = |\downarrow\rangle_j$ and $v_j\,|\downarrow\rangle_j = |\uparrow\rangle_j$, we find that V_j reduces to

$$V_j = \prod_{i=1}^{j}\tilde{\sigma}^x_i = \tilde{\mu}^z_j, \tag{8}$$

where $\tilde{\mu}^z_j$ is the Ising disorder parameter which takes a finite expectation value in the Ising disordered phase. Thus we can identify V_j as the order parameter for the D-Mott phase. We note that in the weak-coupling bosonization approach this string order parameter corresponds to the vertex operator $\exp(\mathrm{i}\phi_{\sigma-})$ where $\phi_{\sigma-}$ is a bosonic field describing spin degrees of freedom [5].

In summary, we have shown by using the strong-coupling perturbation theory that the SF state in the half-filled Hubbard ladder is described as a Néel ordered state of the rung currents. The SF–D-Mott transition is in the Ising universality class where the Ising disordered phase corresponds to the D-Mott state.

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