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LETTER TO THE EDITOR

Effective hole–hole interaction in the spiral phase of a doped antiferromagnet

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Abstract. The effective hole–hole interaction mediated by the spin wave in the spiral phase of a doped antiferromagnet is derived in the framework of the t–t'–J model by using the Schiwinger boson–slave fermion theory. For small doping, the effective interaction for the hole Cooper pairs is attractive, which leads to the competition and coexistence of superconductivity and spiral order.

Very soon after the discovery of copper oxide superconductors [1] Anderson [2] suggested that the physics of these materials is contained in a two-dimensional, large U, single-band Hubbard model. In the large U limit, the Hubbard model may be transformed into the t–J model

$$H = -t \sum_{ij} C^{\dagger}_{i,\sigma} C_{j,\sigma} + \text{HC} + J \sum_{ij} (S_i S_j - n_i/n_j) \tag{1}$$

acting on the space with no doubly occupied sites, with S_i the electron spin and n_i the electron number. Since then most work [3] has been based on the t–J model because there are reasons to believe that the low energy behaviour of the full three-band model, which is used in the case of band structure calculation, may be transferred onto the one-band model [2, 4]. For the half-filled case, the t–J model reduces to the antiferromagnetic Heisenberg Hamiltonian. Away from half-filling, the model is characterized by a competition between kinetic (t) and magnetic energy (J). Magnetic energy J favours antiferromagnetic order for the spins, whereas kinetic energy t favours delocalization of the holes and tends to destroy the spin order. The interplay between doping and antiferromagnetism is a central issue in the theories of the oxide superconductors [5]. Recently, Kane *et al* [6] argued that quantum fluctuations may repair a pair of overturned spins, which allows the holes to hop coherently on the same sublattice. Further energy may be gained if holes can hop coherently onto the opposite sublattice when neighbouring spins are not completely antiparallel. One way which this may be accomplished is for the spins to form a spiral as suggested by Shraiman and Siggia [7]. They have argued that small doping may lead to a ground state with spiral spin structure and a spiral spin structure would have a chiral character [8], as well as a broken translational invariance. These indirect hopping processes may be treated in an effective way by considering a same sublattice hopping term, $\Sigma_{ij} t'_{ij} C^{\dagger}_{i,\sigma} C_{j,\sigma}$. This leads one to study the more general t–t'–J model [6]. Thus an intriguing question is how the hole–hole is to interact in the spiral phase of spins. In this letter we study this problem by using the Schiwinger boson–slave fermion theory.

In the doped RVB state [9, 10], the elementary excitations are the neutral spin-$\frac{1}{2}$ solitons (spinons), and the charged particles (holons) which are bosons. Thus one can express the electron operators as a product of two operators [10], the spin may be represented by a fermion operator and the hole by a boson operator. In the spiral phase of a lightly doped antiferromagnet, however, a more natural starting point may be the slave fermion method (Schiwinger boson method) [11, 6], where the spin can be represented by a boson operator and the hole by a fermion operator. Following Kane *et al* [6], the t–t'–J model Hamiltonian in the Schiwinger boson–slave fermion representation may be written as

$$H = -t\sum_{\langle ij\rangle} f_i f_j^\dagger b_{i,\sigma}^\dagger b_{j,\sigma} + \mathrm{HC} + \sum_{ij} t'_{ij} f_i f_j^\dagger b_{i,\sigma}^\dagger b_{j,\sigma} + \mathrm{HC} + \frac{J}{4}\sum_{\langle ij\rangle}(S_iS_j - n_in_j) \tag{2}$$

where the Schiwinger boson operators, $b_{i,\sigma}^\dagger$ keep track of the spins, while the slave fermion operators, $f_i^\dagger$ keep track of the holes, λ_i is the Lagrangian multiplier on the site i. In the following, we shall derive the effective hole–hole interaction mediated by the spin-wave in the spiral phase. The Hamiltonian (2) thus can be written as

$$H = H_{\mathrm{M}} + H_{\mathrm{I}} \tag{3}$$

where

$$H_{\mathrm{I}} = t\sum_{\langle ij\rangle}(f_i^\dagger f_j - F_\eta)\Big(\sum_\sigma b_{i,\sigma}^\dagger b_{j,\sigma} - Q_\eta) + \mathrm{HC} \tag{4}$$

$$H_{\mathrm{M}} = H_b + H_f \tag{5}$$

$$H_f = -\sum_k (t'_{fk} + \mu')f_k^{\mathrm{A}\dagger} f_k^{\mathrm{A}} - \sum_k (t'_{fk} + \mu')f_k^{\mathrm{B}\dagger} f_k^{\mathrm{B}} + \sum_k tQ_k f_k^{\mathrm{B}\dagger} f_k^{\mathrm{A}} + \mathrm{HC}$$
$$+ V_\infty \sum_i f_i^{\mathrm{A}\dagger} f_i^{\mathrm{A}} f_i^{\mathrm{A}\dagger} f_i^{\mathrm{A}} + V_\infty \sum_i f_i^{\mathrm{B}\dagger} f_i^{\mathrm{B}} f_i^{\mathrm{B}\dagger} f_i^{\mathrm{B}} \tag{6}$$

$$H_b = -\sum_{k\sigma}(t'_{bk} + \lambda) b_{k\sigma}^{\mathrm{A}\dagger} b_{k\sigma}^{\mathrm{A}} - \sum_{k\sigma}(t'_{bk} + \lambda) b_{k\sigma}^{\mathrm{B}\dagger} b_{k\sigma}^{\mathrm{B}} + \sum_{k\sigma}\left(tF_k + \frac{JQ_k}{4}\right) b_{k\sigma}^{\mathrm{A}\dagger} b_{k\sigma}^{\mathrm{B}} + \mathrm{HC}$$
$$- J\sum_k (D_k^\dagger b_{k\uparrow}^{\mathrm{A}} b_{-k\downarrow}^{\mathrm{B}} + \mathrm{HC}) \tag{7}$$

is the mean-field approximation to the Hamiltonian (2) treated by Kane *et al* [6], where λ_i has been treated as a constant independent of position and decoupling the spin interaction in a Hartree-like approximation by introducing the order parameter

$$D_k = \sum_\eta \mathrm{e}^{\mathrm{i}k\cdot\eta} D_\eta \qquad (D_\eta \equiv \langle b_{i\uparrow}^{\mathrm{A}} b_{i+\eta\downarrow}^{\mathrm{B}} - b_{i\downarrow}^{\mathrm{A}} b_{i+\eta\uparrow}^{\mathrm{B}}\rangle)$$

on each bond

$$F_k = \sum_\eta \mathrm{e}^{\mathrm{i}k\cdot\eta} F_\eta \qquad (F_\eta \equiv \langle f_i^{\mathrm{A}\dagger} f_{i+\eta}^{\mathrm{B}}\rangle)$$

$$t'_{bk} = \sum_{k'} t'_{k-k'} \langle f_{k'}^{A\dagger} f_{k'}^{A} \rangle \qquad t'_{fk} = \sum_{k'} t'_{k-k'} \langle b_{k'\sigma}^{A\dagger} b_{k'\sigma}^{A} \rangle$$

where t'_k is the bandstructure corresponding to t'_{ij}, and

$$Q_k = \sum_\eta e^{ik\cdot\eta} Q_\eta \qquad (Q_\eta \equiv \langle b_{i\uparrow}^{A\dagger} b_{i+\eta\uparrow}^{B} + b_{i\downarrow}^{A} b_{i+\eta\downarrow}^{B} \rangle)$$

is the order parameter which describes the spiral, since it is non-zero when neighbouring spins have finite overlap. In (6) the on-site repulsion V_∞ are added to prevent double occupation of the holes at the same site. Kane *et al* [6] have discussed the Hamiltonian H_M in detail; they argued that one may specify D_η has s symmetry, then state that a spiral along the (1, 1) direction corresponds to $Q_x = Q_y = -Q_{-x} = -Q_{-y}$, and along the (1, 0) direction corresponds to $Q_x = -Q_{-x}$, $Q_{\pm y} = 0$. Within reasonable parameters, they have shown that spiral states have lower energy due to the quantum fluctuations.

In the spiral phase of spins, the Hamiltonian H_M may be diagonalized by using the Bogolubov-like transformation to give

$$H_b = -\sum_k \omega_k^- (d_k^\dagger d_k + e_k^\dagger e_k) - \sum_k \omega_k^+ (x_k^\dagger x_k + y_k^\dagger y_k) \tag{8}$$

$$\omega_k^\pm = \sqrt{(\varepsilon_k^\pm)^2 - |JD_k/2|^2} \qquad \varepsilon_k^\pm = t'_{bk} + \lambda \pm |tF_k + JQ_k/4| \tag{9}$$

and the new operators d_k, e_k, x_k, y_k are related to the spin operators by

$$\begin{pmatrix} b_{k\uparrow}^{A} \\ b_{-k\downarrow}^{A\dagger} \\ b_{k\uparrow}^{B} \\ b_{-k\downarrow}^{B\dagger} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} u_k^- & -v_k^- & u_k^+ & -v_k^+ \\ v_k^- & -u_k^- & v_k^+ & -u_k^+ \\ u_k^- & -v_k^- & -u_k^+ & v_k^+ \\ v_k^- & -u_k^- & -v_k^+ & u_k^+ \end{pmatrix} \begin{pmatrix} d_k \\ e_{-k}^\dagger \\ x_k \\ y_{-k}^\dagger \end{pmatrix} \tag{10}$$

where

$$(u_k^\pm)^2 = \tfrac{1}{2}(\varepsilon_k^\pm/\omega_k^\pm + 1) \qquad (v_k^\pm)^2 = \tfrac{1}{2}(\varepsilon_k^\pm/\omega_k^\pm - 1) \tag{11}$$

the Hamiltonian H_f can be diagonalized as

$$H_f = -\sum_k (E_k^- \alpha_k^\dagger \alpha_k + E_k^+ \beta_k^\dagger \beta_k) \tag{12}$$

$$E_k^\pm = t'_{fk} \pm t|Q_k| \tag{13}$$

and operators α_k, β_k are related to the hole operators by

$$\alpha_k = (1/\sqrt{2})(f_k^A + f_k^B) \qquad \beta_k = (1/\sqrt{2})(f_k^A - f_k^B). \tag{14}$$

The hole energy band has been split into two bands due to coupling with Q_η. For small doping, the holes will occupy only the lower energy band (E_k^-), then our interesting problem is how to get the effective hole–hole interaction in the lower band.

We seek a canonical transformation [12, 13] to obtain the effective hole–hole interaction

$$H_{\text{eff}} = \tfrac{1}{2}\langle 0|[H_1, S]|0\rangle \tag{15}$$

where $|0\rangle$ is the spin ground state, and the transformation factor S is found by choosing S such that it obeys

$$H_{\mathrm{I}} + [H_b^{\mathrm{A}}, S] = 0 \qquad H_b^{\mathrm{A}} = -\sum_k E_k^- \alpha_k^\dagger \alpha_k. \tag{16}$$

After somewhat lengthy but straightforward algebra we get the effective hole–hole interaction

$$H_{\mathrm{eff}} = \frac{1}{2N} \sum_{k,k',q} V(k, k', q) \alpha_{k+q}^\dagger \alpha_k \alpha_{k'-q}^\dagger \alpha_{k'}. \tag{17}$$

Thus we find that the effective interaction of the hole Cooper pairs

$$V(k, -k) = -\frac{t^2}{4N} \sum_p (\gamma(p-k) + \gamma(p+k))^2 \left(\frac{(u_p^+ v_p^+)^2}{\omega_p^+} + \frac{(u_p^- v_p^-)^2}{\omega_p^-} \right) \tag{18}$$

$$\gamma(k) = \sum_\eta \mathrm{e}^{\mathrm{i}k\cdot\eta} \tag{19}$$

is attractive. The range of the attractive interaction may be of the order of the spin energy in the spiral phase, then the condensation of the hole Cooper pairs may lead to the superconductivity. However, as shown by Kane *et al* [6], and Shraiman and Siggia [7], spiral phase is such a state with at least short-range antiferromagnetic order. Thus for small doping an important question raised concerns the competition and coexistence of superconductivity and spiral order. This result is very similar to those of the competition and coexistence of superconductivity and magnetized RVB states studied by Lee and Feng [5]. At present, there is no experimental evidence for the coexistence, this means inaccuracy of our results based on the mean-field approximation or other effects beyond our consideration. The fact is that dynamic renormalization will play an important role, as pointed out by Su *et al* [14], thus a better method to further this study may be in the framework of self-consistent renormalization [14].

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