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Spin polarons in the t–t'–J model

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Abstract

We investigate the effect of the next-nearest neighbour hopping terms t' and the three-site hopping terms in the t–t'–J model. We derive a more realistic hole–magnon vertex which leads to vanishing of the quasiparticles in some parts of the Brillouin zone even for relatively small $t' \simeq 0.2t$, while quasiparticles survive for $t' < 0$.

There is accumulating evidence that the low-energy electronic structure of the Cu-based high-temperature superconductors (HTS) can be successfully described by an effective one-band model. The multi-band charge-transfer model for CuO_2 planes can be mapped on the single-band model with large on-site interactions [1,2]. The latter model leads in turn to the the isotropic two-dimensional (2D) $S = \frac{1}{2}$ Heisenberg model (J term) for the undoped systems, while an *effective* single-band model, with the nearest- ($\sim t$), next-nearest neighbour ($\sim t'$), and three-site hopping ($\sim t^2/U$), here called the extended t–t'–J model, results at finite doping.

It is well known that in the t–J model the kinetic energy of doped carriers competes with the magnetic order and an added hole propagates coherently in the antiferromagnetic (AF) background only by its coupling to local quantum fluctuations [3]. This results in a low-energy quasiparticle with low dispersion $\sim J$. The two extensions of the t–J model discussed below have a different physical origin. First, it has been argued [4] that the t' term might be responsible for different physical properties as a hole can propagate on the same sublattice without spin flips (in contrast to t). Recently, further justification for the t' hopping was given, as it is necessary for reproducing the observed Fermi surfaces in the cuprates [5]. Second, the usually neglected three-site terms are essential for reproducing the correct behaviour of the optical conductivity in the strongly correlated Hubbard model [6]. Here we address the question of to what extent the low-energy quasiparticles survive in the extended t–t'–J model.

We study the dynamics of a single hole in a Heisenberg antiferromagnet using the linear spin-wave (LSW) self-consistent Born approximation (SCBA) of Schmitt-Rink et al. [7] which turned out to be surprisingly accurate for $S = \frac{1}{2}$ [8] and has been extended to $S = 1, \frac{3}{2}$ models [9]. The success of this approximation has roots in the vanishing of low-order magnon vertex corrections for systems with a hole coupled to an AF spin background, as pointed out by several authors. We find in $\boldsymbol{k}$ space the following Hamiltonian in LSW order, written in terms of Schwinger bosons,

$$H_{\mathrm{LSW}} = \sum_{k} \epsilon(k) f_k^\dagger f_k + \sum_{q} \omega_q \beta_q^\dagger \beta_q + \frac{1}{\sqrt{N}} \sum_{kq} \left[M(k, q) f_k^\dagger f_{k-q} \beta_q + \mathrm{h.c.} \right], \quad (1)$$

where ω_q is the magnon dispersion in the unfolded zone, $\omega_q = 4J(1-\gamma_q^2)^{1/2}$. Unlike in the t–J model, we do have the bare band for spinless f_k-fermions, with the dispersion at low doping δ given by

$$\epsilon(k) = 2zt'\gamma'_k + \frac{2zt^2}{U}(1-\delta)(z\gamma_k^2 - 1). \quad (2)$$

This reflects the possibility of hole propagation without disturbing the underlying spin background, as, for example, by $A(B) \to A(B)$ processes realized by t'-hopping (A, B are two sublattices). The three-site $A(B) \to B(A) \to A(B)$ hoppings $\sim t^2/U$ involve even magnon processes around the saddle point, and thus do not couple to magnons in leading order. The hole–magnon bare vertex $M(\boldsymbol{k}, \boldsymbol{q})$ depends on the geometrical factors which follow from the Bogoliubov transformation:

$$M(k, q) = zt(u_q\gamma_k - q + v_q\gamma_k) + \frac{ztt'}{U}(1-\delta)(\gamma'_{k-q} - \gamma'_k)(u_q\gamma_{k-q} - v_q\gamma_k). \quad (3)$$

Here $z = 4$ (in 2D), $\gamma_q = \frac{1}{2}(\cos q_x + \cos q_y)$, and $\gamma'_q = \cos q_x \cos q_y$, with the lattice constant $a = 1$. The hole

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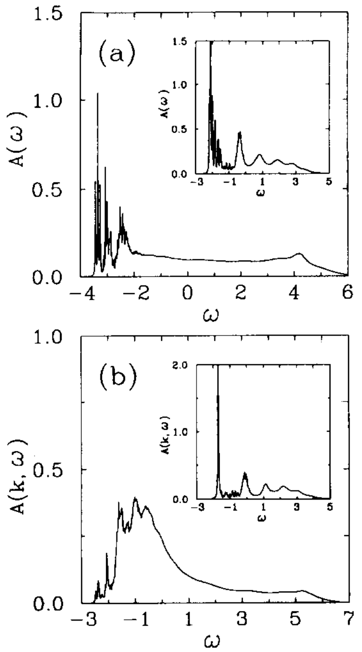

Fig. 1. Density of states $A(\omega)=(1/N)\Sigma_k A(k, \omega)$ (a) and the spectral function $A(k,\omega)$ for $k=(\pi/2, 0)$ (b) as obtained for the generic $t-t'-J$ model with $t=1$, $t'=0.2$ and $J=0.4$ (all in eV). The insets show the results for the $t-J$ model.

dynamics is determined by emission or absorption of spin waves. Within the SCBA we find the hole Green function of the form

$$G(k, \omega)=[\omega-\epsilon(k)-\Sigma(k, \omega)]^{-1} \tag{4}$$

with the selfenergies

$$\Sigma(k, \omega)=\frac{1}{N}\sum_q M^2(k, q)G(k-q, \omega-\omega_q). \tag{5}$$

The above system of equations was solved self-consistently in 2D on a 16×16 lattice.

In the t–J model extended by the t^2/U terms one finds that the free hole band has a width of $W\simeq 3.2$ eV for $J=0.4$ eV ($t=1$ eV), and this causes the QP state to disappear at $k=(0,0)$, and is rather damped at $k=(\pi/2, 0)$. If we turn on instead the $t'=0.2$ eV hopping, we find $W\simeq 3.0$ eV and similar spectral functions to those obtained with t^2/U-terms, with strong damping and splitting for $k=(\pi/2, 0)$. This can be understood qualitatively by considering the Green function where $\epsilon(k)$ is strongly k-dependent and therefore in the SCBA gives such great alterations in some parts of the Brillouin zone (BZ).

Next we consider the full t–t'–J model including both parts of $\epsilon(k)$ in Eq. (2), and the tt'/U corrections to the hole–magnon vertex (3). As one can see in Fig. 1a, the density of states $A(\omega)$ changes considerably. The lowest QP peak now lies ~ 0.5 eV lower than in the t–J model (Fig. 1a inset), while in addition the incoherent processes now give a flat spectrum which spreads up to ~ 6 eV (~ 1.5 eV higher than in the t–J model). In Fig. 1b we present the spectral function $A(k, \omega)$ for $k=(\pi/2, 0)$, where the effect of t' is the most significant. In contrast to the t–J model, our full Hamiltonian gives a *completely incoherent spectrum* with a broad irregular maximum for $\omega\sim -1$ eV. Furthermore, we found that the existence of QP peaks at particular k values depends on the actual value and sign of the next-nearest hopping t'. The reason is that the free dispersion $\epsilon(k)$ (2) which results from the three-site hopping is increased (decreased) by $t'>0$ ($t'<0$). As a consequence, changing the sign of t' (to $t'=-0.2$ eV) gives a drastically different spectrum, with a strong QP peak at $\omega\sim -1.5$ eV. This transformation corresponds to the change from an s-like to a d-like lattice realized in the t–t'–J model for HTS [2]. Therefore, for $t'<0$ the QP peaks occur in the whole BZ, and may be stronger than in the t–J model.

In conclusion, we have demonstrated that the t–t'–J model leads to qualitatively different behaviour from that of the standard t–J model. Depending on the sign of the next-nearest neighbour t' hopping, the quasiparticles are damped or enhanced, and their dispersion changes. The higher-order (three-site) and next-neighbour hopping terms are thus important for more realistic description of doped charge-transfer insulators, including HTS. Moreover, t' terms which do not involve spin flips may have implications for the superconducting state in HTS. It would be interesting to extend the present study to finite hole concentrations and for nonzero temperatures.

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