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Generalizing the t - J model: triplet holes

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As a consequence of the local conservation of total spin in doped Mott-Hubbard insulators, the carriers may have an internal spin degree of freedom. We study the motion of an $s = 1$ carrier in an $s = 1/2$ background, finding that its propagation is quite different from that of the singlet holes of the t - J model: for a single hole, the tendency to form ferromagnetic polarons is *suppressed* and the single-hole spectral function in the two dimensional Heisenberg antiferromagnet is completely incoherent.

The electronic properties of doped Mott-Hubbard insulators (doped MHI's) are subject to considerable current interest. A key difference between doped MHI's and conventional semiconductors lies in the strong constraints on the phase space for charge fluctuations in the former, imposed by the on-site Coulomb interactions. The simplest model incorporating these "charge projections" is the popular (singlet) t - J model (StJ), describing the hopping of vacancies (singlets) in an $s = 1/2$ Heisenberg spin system. This model is only of relevance under the special condition that the underlying electronic system is effectively spin degenerate. Much less is known about the general case where orbital degeneracy does matter. In such cases a second local constraint enters (conservation of total spin) leading to models which are qualitatively distinct from the StJ model. An important ingredient in these generalized t - J models is that *the carriers possess an internal spin degree of freedom*. The simplest example is that of a triplet carrier, moving in an $s = 1/2$ background, the "triplet t - J model" (TtJ).¹ By studying limits where the physics of the StJ model is well understood, we will show that the internal degree of freedom of the triplet hole changes the problem drastically. We will first consider a triplet hole in a ferromagnetic background in the presence of a spin flip.² Contrary to the intuitive notion that larger spin should help ferromagnetism,³ we find that the spin flip is attracted by the hole if J is positive, indicating that the tendency to form ferromagnetic polarons is *suppressed*. We then study the spectral function of a single hole in the two-dimensional (2D) antiferromagnet using the linear spin wave (LSW) approach of Schmitt-Rink *et al.*⁴ Although the coherent bandwidth of the triplet hole seems to be at first sight of order t (instead of J in the case of singlets⁵), it is actually overdamped due to nonlinear processes in the coupling to spin waves.

As van Vleck explained a long time ago, total spin (and orbital angular momentum) is locally conserved in MHI's. Hund's rule and crystal field interactions cause gaps (in addition to the MH gap) which are larger than the relevant kinetic scale ($\sim J$), enforcing those local conservation laws. In doped MHI's, the latter scale is the carrier bandwidth ($\sim t$) and it is less obvious that the Hund's rule gaps survive. Nevertheless, these total spin projections seem to be remarkably robust as exemplified by, e.g., the mapping procedure of Zhang and Rice.⁶ For instance, it is believed that the carriers in p-type NiO are low spin doublets, moving in an $s = 1$ spin system, while holes in CoO are singlets in an $s=3/2$ background.⁷ So the canonical doped MHI is not only specified by the allowed charge states, but also by the total spin (and orbital) states of the individual spins (s) and carriers (s').⁸

According to fractional parentage rules, the carrier can only delocalize by single electron hopping if s and s' differ by not more than $\pm 1/2$, a criterion which is fulfilled in many doped MHI's. Consider configurations characterized by $|s + 1/2, m\rangle$ and $|s, m'\rangle$ at neighboring sites i and j , respectively. After the hopping of a physical up (down) spin hole, site i will be occupied by the state $|s, m - 1/2\rangle$ ($|s, m + 1/2\rangle$) and site j by $|s + 1/2, m' + 1/2\rangle$ ($|s + 1/2, m' - 1/2\rangle$). Because of the total s projections, the hopping is modified by the product of the overlaps of the states at sites i and j , before and after the hopping, which are given by Clebsch-Gordon coefficients. Representing the $(2s + 1)$ -fold degenerate states $|s, m\rangle$ by $SU(2s + 1)$ Schwinger bosons $b_{i,m}^\dagger$ and the $|s + 1/2, m'\rangle$ by products of $SU(2s + 2)$ bosons (a) and auxiliary fermions (h) $h_i^\dagger a_{i,m'}$ we obtain the hopping Hamiltonian for arbitrary s

$$H_t = \frac{t}{2s + 1} \sum_{\langle ij \rangle} \sum_{m,n=-s}^s \left[b_{j,n}^\dagger \left(\sum_{\pm} \sqrt{(s \pm m + 1)(s \pm n + 1)} a_{i,m \pm 1/2}^\dagger a_{j,n \pm 1/2} \right) b_{i,m} h_i h_j^\dagger + \text{H.c.} \right]. \quad (1)$$

By adding the Heisenberg term, H_J , for the spin background in this Schwinger boson representation, one obtains the generalized t - J model. Instead of using these $SU(2s+1)$ Schwinger bosons (representing individual local m_s eigenstates), one may as well use the conventional $SU(2)$ Schwinger boson representation. Kane *et al.*⁵ following these lines arrived at a large s expansion for the t - J model. In their derivation the linear spin-wave approximation (LSW) is introduced in an early stage appropriate for the singlet hole problem. In this case, Eq. (1) reduces to the usual t - J model, with the replacement $(J/t) \rightarrow (2s+1)s/\sqrt{2s}(J/t)$. We find that if the hole carries an internal spin degree of freedom, essential nonlinearities are introduced by the motion of the hole. In these cases, the above expansion is invalid.⁹ The simplest relevant model is that of an $s = 1$ hole moving into an $s = 1/2$ background, described by Eq. (1), setting $s = 1/2$ (TtJ model). In this special case, our $su(2s+1)$ representation is convenient, because it explicitly keeps track of the internal spin degree of freedom of the hole, while the spin background is of the usual $s = 1/2$ variety.

The triplet hole can hop in *three* distinct ways [Eq. (1)]: $(1_i, \uparrow_j \rightarrow \uparrow_i 1_j)$, $(1_i, \downarrow_j \rightarrow \uparrow_i, 0_j)$, $(0_i, \uparrow_j \rightarrow \uparrow_i, 0_j)$, with hopping amplitudes t , $t/\sqrt{2}$, and $t/2$, respectively (i and j denote nearest-neighbor lattice sites, \uparrow, \downarrow and $1, 0, -1$ are spin-1/2 and spin-1 states, respectively. The other five hops can be obtained by time and/or spin reversal). Elsewhere¹⁰ we studied the ramifications of this complex hopping behavior in the simple (Brinkman-Rice¹¹) case of a single triplet hole propagating in a noninteracting ($J = 0$) antiferromagnetic chain. We showed that, although the physical motion is confined to 1D, the distinct hopping possibilities lead to a connectivity of the Hilbert space similar to that of a 2D noninteracting tight-binding system. Accordingly, we found an electronic density of state similar to that of a 2D noninteracting problem.

We first consider the problem of a triplet hole in a ferromagnetic (FM) background in the presence of one additional spin flip, the Nagaoka problem.² For singlet holes, the spin flip is repelled by the hole if $J > 0$, reflecting the tendency to form a ferromagnetic polaron. Surprisingly, we find that the triplet hole in fact *attracts* the spin flip. The fully polarized (Nagaoka) state consists of an $M_s = 1$ hole in a spin-up background, $|\text{FM}\rangle = \prod_i a_{i\uparrow}^\dagger |0\rangle$. The bound-state wave functions in the presence of an additional spin flip are of the form $|\Phi\rangle = \sum_{ij} \phi(ji) S_j^- h_i^\dagger |\text{FM}\rangle$. From the condition $H^{\text{TtJ}}|\Phi\rangle = E|\Phi\rangle$ a Schrödinger equation for the coefficients $\phi(ji)$ is found, in momentum space

$$(E - E_{\mathbf{k},\mathbf{q}})\phi_{\mathbf{q}}(\mathbf{k}) = \frac{1}{N} \sum_{\mathbf{k}'} \{zt[(1/\sqrt{2} - 1)(\gamma_{\mathbf{k}} + \gamma_{\mathbf{k}'}) + \frac{1}{2}\gamma_{\mathbf{q}}] + zJ(\gamma_{\mathbf{k}-\mathbf{k}'} - \gamma_{\mathbf{q}-\mathbf{k}'})\}\phi_{\mathbf{q}}(\mathbf{k}'), \quad (2)$$

where \mathbf{q} and \mathbf{k} are center of mass and relative momenta, respectively, $E_{\mathbf{k},\mathbf{q}} = zt\gamma_{\mathbf{k}} - zJ(1 - \gamma_{\mathbf{q}-\mathbf{k}})$ and $\gamma_{\mathbf{k}} = (1/z) \sum_{\delta} \exp(i\mathbf{k}\delta)$. This expression looks similar to the one obtained for the StJ model.² The first difference originates in the constraints on the hopping [first

term on the right-hand side of Eq. (2)]. In contrast to StJ, the hole and the spin flip can localize on the same site (forming an $M_s = 0$ hole), although the hopping in or out of this state is modified by a factor of $1/\sqrt{2} - 1$. Further, an additional term ($\gamma_{\mathbf{q}}/2$) is found, coming from the hopping of the $M_s = 0$ hole. The solutions of Eq. (2) are either of even or odd parity. In contrast to StJ, we find that the bound states of the triplet problem are characterized by *even* parity, with a finite probability to find the hole and the spin flip on the same site. The bound-state condition is

$$0 = [1 - zt(1/\sqrt{2} - 1)\Gamma_{\mathbf{q}}^{(1)}]^2 - zt\Gamma_{\mathbf{q}}^{(0)}[\gamma_{\mathbf{q}}/2 + zt(1/\sqrt{2} - 1)^2\Gamma_{\mathbf{q}}^{(2)}] + zJ(\gamma_{\mathbf{q}}\Gamma_{\mathbf{q}}^{(1)} - \Gamma_{\mathbf{q}}^{(2)}) + z^2tJ\gamma_{\mathbf{q}}(1/\sqrt{2} - \frac{1}{2})(\Gamma_{\mathbf{q}}^{(0)}\Gamma_{\mathbf{q}}^{(2)} - \Gamma_{\mathbf{q}}^{(1)}\Gamma_{\mathbf{q}}^{(1)}), \quad (3)$$

where $\Gamma_{\mathbf{q}}^{(n)} = (1/N) \sum_{\mathbf{k}} \gamma_{\mathbf{k}}^n / (E - E_{\mathbf{k},\mathbf{q}})$ and assuming s-wave symmetry in $D > 1$. Equation (3) only has bound-state solutions [$E < \min_{\mathbf{k},\mathbf{q}}(E_{\mathbf{k},\mathbf{q}})$] for positive J , indicative of a net attractive interaction between spin flip and hole. In 1D one finds for the binding energy of the bound state for small positive J [occurring at $\mathbf{q} = (\pi, \pi)$ for $t > 0$]

$$E_b = \frac{2(3 - 2\sqrt{2})J^2}{t - 2(1 + \sqrt{2})J} + O(J^3/t^2). \quad (4)$$

As for the StJ model, we find that $E_b \sim J^2/t$, showing that for $J = 0$ the lowest-energy maximum S state is degenerate with the $S_{\text{max}} - 1$ state, indicative of charge-spin separation.¹² This is rather remarkable, involving an exact cancellation of the kinetic-energy cost because of the reduced hopping amplitude for $M_s = 1 \leftrightarrow M_s = 0$ and the gain coming from the hopping of the $M_s = 0$ hole.¹⁰ The latter process effectively propagates the spin flip. For $J > 0$ this process interferes constructively with the propagation of the spin flip, leading to a net attraction. This mechanism survives in higher dimensions, although the formation of a bound state requires now a finite J (in 2D $\sim 0.3t$).

Let us now turn to the physically more relevant case of an isolated triplet hole in a 2D square lattice Heisenberg antiferromagnet. The properties of the singlet hole in this limit are well understood. Numerical simulations have provided evidence in favor of the hole forming a quasiparticle (QP) of the small polaron variety, with a coherent bandwidth $\sim J$ and a pole-strength $z \sim J/t$ for small J/t .¹³ This problem can also be treated by self-consistent perturbation theory, where the spin degrees of freedom are bosonized and treated within LSW. Such a polaronlike approach has been worked out by Schmitt-Rink *et al.*⁴ and detailed comparisons with finite-size results show that this approach is quite accurate, even in quantitative respects.¹⁴ The novel features of the triplet hole problem are all related to the structure of the hopping Hamiltonian. The advantage of the $SU(3)$ representation for the triplet hole is that these features do not get lost if the ($s = 1/2$) spin background is approximated by linear spin waves. After linearizing^{4,5} we obtain for the TtJ model

$$\begin{aligned}
 H_{\text{LSW}} = & \sum_{\mathbf{k}, \sigma = \pm 1/2} \varepsilon_{\mathbf{k}} \xi_{\mathbf{k}\sigma}^\dagger \xi_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} \beta_{\mathbf{q}}^\dagger \beta_{\mathbf{q}} - \frac{zt}{4\sqrt{N}} \sum_{\mathbf{k}, \mathbf{q}} \left(\xi_{\mathbf{k}, \frac{1}{2}} \xi_{\mathbf{k}-\mathbf{q}, -\frac{1}{2}}^\dagger [(\gamma_{\mathbf{k}-\mathbf{q}} u_{\mathbf{q}} + \gamma_{\mathbf{k}} v_{\mathbf{q}}) \beta_{\mathbf{q}}^\dagger + (\gamma_{\mathbf{k}-\mathbf{q}} v_{\mathbf{q}} + \gamma_{\mathbf{k}} u_{\mathbf{q}}) \beta_{-\mathbf{q}}] \right. \\
 & \left. + 2 \sum_{\pm} \xi_{\mathbf{k}, \pm \frac{1}{2}} \xi_{\mathbf{k}-\mathbf{q}, \pm \frac{3}{2}}^\dagger \gamma_{\mathbf{k}} (v_{\mathbf{q}} \beta_{\mathbf{q}}^\dagger + u_{\mathbf{q}} \beta_{-\mathbf{q}}) + \text{H.c.} \right). \quad (5)
 \end{aligned}$$

Here, $\varepsilon_{\mathbf{k}} = -zt\gamma_{\mathbf{k}}/\sqrt{2}$, $\omega_{\mathbf{q}}$ is the magnon dispersion, $\beta_{\mathbf{q}}^\dagger$ a magnon creation operator, and $u_{\mathbf{k}}, v_{\mathbf{k}}$ are the LSW coherence factors.⁴ This equation is considerably more complicated than the equivalent expression for the singlet model. First, with respect to the classical vacuum there are *twice as many hole degrees of freedom*. Calling the up- (down-) spin sublattice A (B), an $M_s = 1$ on A and an $M_s = 0$ on B triplet states (or 0 and -1 on A and B , respectively) have total $M_s = 1/2$ ($-1/2$), and these correspond with the physical hole. In addition, an $M_s = 1$ state can be created on sublattice B (or -1 on A), corresponding with a total $M_s = 3/2$ ($-3/2$). This explains the labels of the ξ 's in Eq. (5). Secondly, the $\pm 1/2$ holes have a *large free dispersion* characterized by a bandwidth which is only smaller by a factor $\sqrt{2}$ compared to the free particle bandwidth $8t$. This bandwidth results from the $(1/2)$ hole propagating by $1_A \rightarrow 0_B \rightarrow 1_A \rightarrow \dots$ with no damage to the spin lattice. At the same time, the $\pm 1/2$ holes are coupled to the magnons due to the StJ-like propagation of the $M_s = 0$ hole ($0_A \rightarrow 0_B \rightarrow \dots$). On the other hand, the $\pm 3/2$ holes have infinite mass and delocalize exclusively by emitting and/or absorbing a magnon and turning into a $\pm 1/2$ hole.

Using the self-consistent Born approximation^{4,14} and neglecting the partial constraint on spin flips and holes occupying the same site,¹⁵ we find for the $1/2$ and $3/2$ hole Green's functions $G_{1/2}(\mathbf{k}, \omega) = [\omega - \varepsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, \omega) - \Pi_{1/2}(\mathbf{k}, \omega)]^{-1}$ and $G_{3/2}(\mathbf{k}, \omega) = [\omega - \Pi_{3/2}(\mathbf{k}, \omega)]^{-1}$, respectively. The self-energies are given by

$$\Sigma(\mathbf{k}, \omega) = \left(\frac{zt}{4}\right)^2 \frac{1}{N} \sum_{\mathbf{q}} f(\mathbf{k}, \mathbf{q}) G_{1/2}(\mathbf{k} - \mathbf{q}, \omega - \omega_{\mathbf{q}}),$$

$$\Pi_{1/2}(\mathbf{k}, \omega) = \left(\frac{zt}{2}\right)^2 \frac{1}{N} \sum_{\mathbf{q}} \gamma_{\mathbf{k}}^2 v_{\mathbf{q}}^2 G_{3/2}(\mathbf{k} - \mathbf{q}, \omega - \omega_{\mathbf{q}}), \quad (6)$$

$$\Pi_{3/2}(\mathbf{k}, \omega) = \left(\frac{zt}{2}\right)^2 \frac{1}{N} \sum_{\mathbf{q}} \gamma_{\mathbf{k}-\mathbf{q}}^2 u_{\mathbf{q}}^2 G_{1/2}(\mathbf{k} - \mathbf{q}, \omega - \omega_{\mathbf{q}}),$$

where $f(\mathbf{k}, \mathbf{q}) = (\gamma_{\mathbf{k}-\mathbf{q}} u_{\mathbf{q}} + \gamma_{\mathbf{k}} v_{\mathbf{q}})^2$. We solved this system of integral equations numerically in 2D and in Fig. 1 we show some typical results for the physical hole spectral function $A(\mathbf{k}, \omega) = (1/\pi) \text{Im} G_{1/2}(\mathbf{k}, \omega)$ and for $B(\mathbf{k}, \omega) = (1/\pi) \text{Im} G_{3/2}(\mathbf{k}, \omega)$. To understand these results it is instructive to neglect first the $1/2 \leftrightarrow 3/2$ vertex in Eq. (5) altogether. In this case the Π 's are zero, and the same form is obtained as for the StJ model,⁴ except that the coherent hopping $\sim \varepsilon_{\mathbf{k}}$ is added. It turns out that the large free bandwidth overrules the spin-flip scattering and, accordingly, the triplet hole seems to be in the large polaron limit, in marked contrast with the small polaron behavior of a singlet hole.¹⁴ As can be seen

from Fig. 1(a), the spin-flip scattering seems to add only broadenings to the free-particle-like dispersion, which are especially near the band edges quite small. If we turn on the Π 's, this picture is altered in a subtle, but drastic way. First, we notice that the $3/2$ spectral function is *completely incoherent* [Fig. 1(b)]. This can be understood qualitatively by considering the Ising limit. Studying all possible hopping histories, one finds that the $3/2$ hole splits apart in a spin flip, localized at the origin and a delocalized $1/2$ hole. A confining ("string") potential is absent and, accordingly, the $3/2$ hole is a composite particle. Fig. 1(b) can be understood in this way. $B(\mathbf{k}, \omega)$ can be thought of as arising from a localized state (at $\omega = 0$) interacting with a continuum given by $\text{Im} \Pi_{3/2}$, which is essentially the kinematical convolution of $A(\mathbf{k}, \omega)$ and the magnon density of states (e.g., its lower bound disperses like the magnon). Bound states (below the spin-flip- $1/2$ hole continuum) are not formed because a confining interaction is absent, and B is fully incoherent. The non-QP character of the (unphysical) $3/2$ hole would have

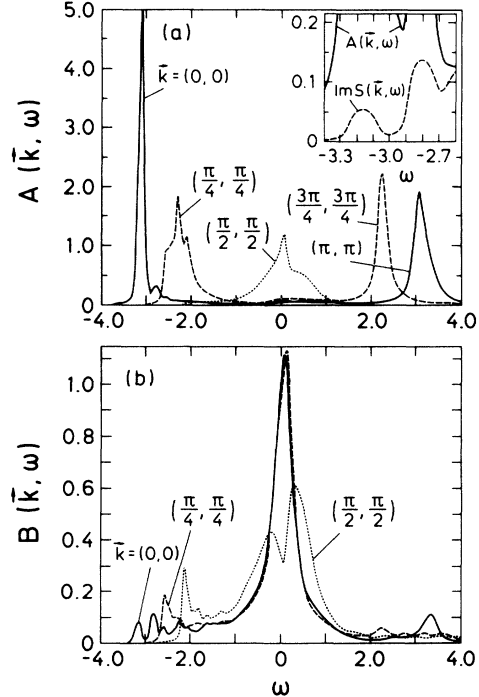


FIG. 1. Spectral function of the $1/2$ (a) and $3/2$ (b) hole, for different momenta and $t/J = 0.5$. The inset in (a) shows the low-energy part of the $1/2$ spectral function and the corresponding self-energy $S(\mathbf{k}, \omega) = \Sigma(\mathbf{k}, \omega) + \Pi_{1/2}(\mathbf{k}, \omega)$. The coupling between the $1/2$ and $3/2$ holes results in broadening of the peak in $A(\mathbf{k} = 0, \omega)$ and the quasiparticle behavior is lost even at the bottom of the band.

been rather meaningless, were it not that the (physical) $1/2$ hole turns out to be affected. We find that *the incoherency of the $3/2$ "particle" destroys the quasiparticle character of the physical $(1/2)$ hole*. In the quantum antiferromagnet, the physical hole can decay in the $3/2$ channel, emitting and/or absorbing a magnon [Eq. (5)], and this process becomes increasingly important at lower energies and longer wavelength. If $k, \omega \rightarrow 0$, we find in second order that $\text{Im}\Sigma \rightarrow \omega^4$, but $\text{Im}\Pi_{1/2} \rightarrow \text{const.}$ Under iteration this leads to the loss of QP behavior [Fig. 1(a)]. The reason is that the $1/2 \rightarrow 3/2$ vertex diverges as $1/q$, which is reminiscent of the coupling to spin waves in the spin-fermion model.¹⁶ However, unlike the vertex in the latter case,¹⁷ the divergence in the TtJ model does not vanish in the Born approximation. As a consequence, by using the dominant pole approximation one finds that the QP weight vanishes as $z \sim (v_s/t)^2 L^{-1/2}$, where v_s is the spin-wave velocity and L is the linear dimension of the 2D lattice. No bound states are formed in A and instead the spectral function behaves as $1/\omega$ at low energy and long wavelength, signaling the breakdown of the quasiparticle picture.

The above theory is not expected to describe correctly the low-energy response. It is significant, however, that perturbation theory breaks down, signaling an orthogonality between the ground state with one hole and the quantum antiferromagnet. Apparently, the relaxation of the hole involves an infinity of magnon excitations, although the one-hole ground state is definitely not ferromagnetic. To our knowledge, this is the first time that non-QP behavior has been established in a 2D strongly correlated system (except for the fractional quantum Hall effect), and one might wonder if this survives finite carrier concentration.

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¹This situation might be experimentally realized by doping a low-spin Ni(III) compound (e.g., YSrNiO₄). Moreover, different groups have pointed to the possibility that triplet holes might play a role in cuprate high- T_c superconductivity: A. Bianconi *et al.*, *Physica C* **162-164**, 209 (1989); T. Egami *et al.*, in *Electronic Structure and Mechanisms of High T_c Superconductivity*, edited by J. Ashkenazi and G. Vezzoli (Plenum, New York, 1991); H. Kamimura and M. Eto, *J. Phys. Soc. Jpn.* **59**, 3053 (1990); V. I. Anisimov *et al.*, *Phys. Rev. Lett.* **68**, 345 (1992).

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