Polaron in the $t$-$J$ Models with Three-Site Terms: 
the $SU(2)$ and the Ising Cases

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Abstract. We compare the role of the three-site terms added to the $t$-$J$ models in the $SU(2)$ and the Ising cases in the extremely low doping regime, i.e. when a single hole added to the strongly interacting half-filled system becomes a polaron. We show that in the realistic Ising case the three-site terms play a vital role in the polaron movement and should never be neglected unlike in the $SU(2)$ case.

Keywords: polaron, $t$-$J$ model, three-site terms, $SU(2)$, Ising

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INTRODUCTION

The Hubbard model is regarded as the model which can describe many of the spectacular phenomena observed in transition metal oxides (TMO) – such as e.g. Mott insulating ground states, antiferromagnetism, and perhaps even high temperature superconductivity [1]. Usually, however, it is the $t$-$J$ model which is used to explain these phenomena [1]. This model: (i) is easier to solve than the Hubbard model [2], (ii) can be easily reduced to the Heisenberg model for the half-filled doping and hence naturally predicts the antiferromagnetic ground state of undoped TMO, (iii) is believed to give qualitatively similar predictions as the Hubbard model for it merely follows from a perturbative expansion of the Hubbard model in the physical regime of strong interactions [3].

A priori, one can have some doubts concerning the stated above 1 : 1 correspondence between these two models. Actually, in a rigorous perturbative expansion of the Hubbard model one obtains the so-called three-site terms, in addition to the kinetic and magnetic terms in the $t$-$J$ model [3]. These terms are often neglected in the small doping regime (close to the Mott insulating ground state) when they are much smaller than the two $t$-$J$ model terms and only yield a small longer range hopping. Indeed, it was shown in Ref. [4] that the inclusion of the three-site terms in this standard $SU(2)$ symmetric case of the $t$-$J$ models does not change qualitatively the low-energy physics of the system.

However, a different situation can arise when the Ising limit of the $t$-$J$ model is taken and the $SU(2)$ symmetry is broken, which is quite often done for computational purposes in e.g. more elaborate $t$-$J$ models [5]. Could the three-site terms play an important role and entirely change the solutions in the Ising limit? In this paper we answer this question by comparing the role of the three-site terms added to the $t$-$J$ models in the $SU(2)$ and the Ising cases, cf. [6]. We perform calculations in the extremely low doping regime namely for the case of a single hole added to a half-filled ordered ground state of the models, i.e. when a single hole couples to the excitations of the ordered state in a polaronic way.
**t-J MODELS WITH THREE-SITE TERMS**

In order to see how the three-site terms arise in the perturbation theory and why they are often neglected we introduce (a generalized version of) the Hubbard model:

\[
H = -t \sum_{i,j(l), \sigma, \sigma'} z_{ij}^{\sigma \sigma'} c_{i \sigma}^\dagger c_{j \sigma'} + U \sum_i n_i n_{i2},
\]

where we defined \( n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \), \( \sigma = 1, 2 \) – a quantum number with two values (not necessarily a spin quantum number), and \( z_{ij}^{\sigma \sigma'} \) is a hopping element between state \( \sigma \) on site \( i \) and state \( \sigma' \) on site \( j \). Hence, this model allows for e.g. \( \sigma \)-dependent values of the hopping elements. As already mentioned, usually in realistic systems the hopping \( t \) is much smaller than the on-site interaction \( U \) so that we can safely perform a perturbative expansion in the kinetic terms [3]. We obtain the effective Hamiltonian:

\[
H_{\text{eff}} = -t \sum_{i,j(l), \sigma, \sigma'} z_{ij}^{\sigma \sigma'} c_{i \sigma}^\dagger c_{j \sigma'} - \frac{J}{4} \sum_{i,j(l), j(i), j'(i)} \left( \sum_{\sigma} \sigma_1 \sigma_2 \sigma_3 \sigma_4 \tilde{c}_{i \sigma_1} c_{i \sigma_2} n_{i \sigma_1} n_{i \sigma_2} c_{i \sigma_2}^\dagger \tilde{c}_{j \sigma_4} \right)
\]

\[
= -t \sum_{i,j(l), \sigma, \sigma'} \left( \cdots - \frac{J}{4} \sum_{i,j(l), j(i), j'(i)} \left( \cdots - \frac{J}{4} \sum_{i,j(l), j(i), j'(i)} \left( \cdots \right) \right) \right),
\]

where \( \tilde{c}_{i \sigma} = c_{i \sigma} (1 - n_{i \sigma}) \) and \( J = 4t^2 / U \).

The first two terms in Eq. (3) form a generalized version of the \( t-J \) model (\( H_{t-J} \)) whereas the last one is the three-site term (\( H_{3s} \)). The physical interpretation of these terms is the following: (i) the first term describes the hopping of electrons with no double occupancies allowed and this term contributes to the total energy of the system as \( \propto t \delta \), where \( \delta \) is the number of doped holes (by definition we have no holes in the half-filled case), (ii) the second term \( \propto J(1-\delta)^2 \) describes the electron which makes a virtual hopping \( t \) from site \( j \) to an occupied site \( i \) which costs energy \( U \) and then comes back to site \( j \), (iii) the third term \( \propto J\delta \) describes the situation when the electron does not return to the same site \( j \) but goes to the site \( j' \) provided this site is unoccupied (hence in the half-filled case this term vanishes). Since in the low doping regime \( \delta \ll 1 \) and \( J < t \), then naturally the last term has the smallest contribution to the total energy of the system and this is the reason why (as explained in the introduction) it is often neglected.

Let us also note the reasons for introducing the generalized version of the Hubbard and \( t-J \) models. Firstly, it enables us to treat the Ising and the \( SU(2) \) cases on equal footing (see below). Secondly, it is possible to obtain the Ising limit from this model in such a way that it coincides with the model describing the correlated electrons in the systems with partial \( t_{2g} \) orbital degeneracy (with active \( \gamma_\ast, \gamma_x \) orbitals in the ferromagnetic plane) as e.g. in the \( d^1 \) system of \( Sr_2VO_4 \) [7]. This means that this specific Ising limit would not only correspond to a standard Ising spin approximation but would also constitute a realistic physical model [6].
POLARON IN THE $SU(2)$ CASE

In the $SU(2)$ symmetric case the quantum numbers $\sigma = \uparrow, \downarrow$ describe physical spins. Then

$$
\epsilon^{\sigma\sigma'}_{(ij)} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (4)
$$

where the hopping is restricted to the nearest neighbour sites $(ij)$. Substituting Eq. (4) to Eq. (3) we obtain for the $t$-$J$ part

$$
H_{t-J} = -t \sum_{(ij)} (\tilde{c}^{\dagger}_{i\uparrow} \tilde{c}_{j\uparrow} + \tilde{c}^{\dagger}_{i\downarrow} \tilde{c}_{j\uparrow} + h.c.) + J \sum_{(ij)} (S_i S_j - \frac{1}{4} \tilde{n}_i \tilde{n}_j), \quad (5)
$$

where $S_i^+ = \tilde{c}^{\dagger}_{i\uparrow} \tilde{c}_{i\downarrow}, S_i^- = \tilde{c}^{\dagger}_{i\downarrow} \tilde{c}_{i\uparrow}, S_i^z = \frac{1}{2}(\tilde{n}_{i\uparrow} - \tilde{n}_{i\downarrow})$. The three-site terms part reads

$$
H_{3s} = -\frac{1}{4} J \sum_{\{j'ij\}} (\tilde{c}^{\dagger}_{j'\uparrow} \tilde{n}_{ij} \tilde{c}_{j\uparrow} + \tilde{c}^{\dagger}_{j'\downarrow} \tilde{n}_{ij} \tilde{c}_{j\uparrow} - \tilde{c}^{\dagger}_{j'\uparrow} \tilde{c}_{i\downarrow} \tilde{c}_{j\downarrow} - \tilde{c}^{\dagger}_{j'\downarrow} \tilde{c}_{i\uparrow} \tilde{c}_{j\downarrow} - \tilde{c}^{\dagger}_{j'\uparrow} \tilde{c}_{i\downarrow} \tilde{c}_{j\uparrow} - \tilde{c}^{\dagger}_{j'\downarrow} \tilde{c}_{i\uparrow} \tilde{c}_{j\uparrow}), \quad (6)
$$

where we sum over all possible configurations of three adjacent sites $\{j'ij\}$ (with $i$ denoting the middle site).

In the half-filled case it is easily seen that the ground state of the model is a quantum antiferromagnet (AF). The calculation of the ground state of the model with one additional hole in the AF is more complicated and one needs to use the self-consistent Born approximation (SCBA) [8]. The hole spectral density $A(k, \omega)$ obtained in this way for the two-dimensional (2D) lattice is shown in Fig. 1(a) [Fig. 1(b)] without [with] three-site terms included, respectively. In both figures we see a finite though strongly renormalized dispersion of the lowest peak. This suggests a formation of a mobile polaron as a hole moves by dressing up with spin excitations and acquires a large but finite effective mass. The inclusion of the three-site terms Eq. (6) merely strongly increases the spectral weight of the incoherent part for particular $k$ values in the Brillouin zone, cf. Fig. 1(b).
POLARON IN THE ISING CASE

To obtain the Ising limit from the model Eq. (3) which at the same time serves as the realistic model for correlated electrons with $t_{2g}$ degeneracy (see last paragraph of the second section) we assume $\sigma = yz, zx$ and

$$z_{\langle ij|\hat{x}\rangle}^{\sigma\sigma'} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad z_{\langle ij|\hat{y}\rangle}^{\sigma\sigma'} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

where the hopping is between the nearest neighbour sites along the $\hat{x}$ and $\hat{y}$ directions depending on the value of $\sigma$ [6]. Substituting Eq. (7) to Eq. (3) we obtain for the $t-J$ part

$$H_{t-J} = -t \sum_{\langle ij|\hat{x}\rangle} (\tilde{c}_{ib}^{\dagger} \tilde{c}_{jb} + h.c.) - t \sum_{\langle ij|\hat{y}\rangle} (\tilde{c}_{ia}^{\dagger} \tilde{c}_{ja} + h.c.) + J \sum_{\langle i,j\rangle} (T_{i}^{x} T_{j}^{y} - \frac{1}{4} \tilde{n}_{i} \tilde{n}_{j}),$$

where $T_{i}^{x} = \frac{1}{2} (\tilde{n}_{ia} - \tilde{n}_{ib})$. The three-site terms part reads

$$H_{3s} = -\frac{1}{4} J \sum_{\langle fi|j\rangle} \tilde{c}_{ja}^{\dagger} \tilde{n}_{ia} \tilde{c}_{jb} - \frac{1}{4} J \sum_{\langle fi|j\rangle} \tilde{c}_{ja}^{\dagger} \tilde{n}_{ib} \tilde{c}_{ja}$$

$$+ \frac{1}{4} J \sum_{\langle fi|j\rangle} \tilde{c}_{ja}^{\dagger} \tilde{c}_{ib} \tilde{c}_{ia} \tilde{c}_{jb} + \frac{1}{4} J \sum_{\langle fi|j\rangle} \tilde{c}_{ia}^{\dagger} \tilde{c}_{ib} \tilde{c}_{ja} \tilde{c}_{jb},$$

where the three-site hop can be either straight (along $\hat{x}$ or $\hat{y}$ direction) or along the corner [e.g. first hop along the $\hat{x}$ direction and then along the $\hat{y}$ one, cf. the last term of Eq. (9)].

In the half-filled case the ground state of the model is a classical state with alternating orbitals occupied on each site (Ising AF in the spin language). The ground state of the model with one additional hole in the Ising AF can again be calculated using the SCBA. The hole spectral densities $A(k, \omega)$ for the 2D case are shown in Fig. 2 with and without three-site terms included. We see that in the case without the three-site terms the polaron is immobile [8] whereas adding the three-site terms yields a small dispersion.
CONCLUSIONS AND FINAL DISCUSSION

In conclusion, we studied a problem of a single hole doped into the half-filled ground state of two different cases of the $t$-$J$ model. On one hand, in the $SU(2)$ case we noticed a quite big quantitative difference in the polaron behaviour between the models with and without the three-site terms. However, the polaron was always mobile and the inclusion of the three-site terms did not change qualitatively the low-energy physics of the system, cf. [4]. On the other hand, in the Ising case the polaron became mobile only after including the three-site terms in the model.

This means that for a $t$-$J$ model in the Ising limit to become more realistic one should include the three-site terms even in the extremely low doping regime. In particular, one should also include these terms for the models describing the $t_{2g}$ systems such as e.g. Sr$_2$VO$_4$ where the Ising limit arises not as an approximation to the $SU(2)$ case but as a genuine $t$-$J$ model.

As a postscriptum one can discuss the reason why the three-site terms play any role in the Ising limit of the $t$-$J$ model despite the fact that they are very small in the low doping regime (as stated in the introduction and explicitly shown in the second section). We suggest the following answer: if there is a strong competition between two processes in the system (e.g. the magnetic interaction and the hole hopping in the $t$-$J$ model) then the neglected third term (e.g. the three-site hopping) can decide about the ground state of the system. This is because it is the difference between these two larger terms in the Hamiltonian which matters and with which the magnitude of the neglected term should be compared.

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