Spin, Orbital, and Spin-Orbital Polarons in Transition Metal Oxides

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Abstract. I give a brief overview of a polaron formation in three distinct transition metal oxides: (i) spin polaron when a hole is added to the antiferromagnetic (AF) ordered plane in La$_2$CuO$_4$, (ii) orbital polaron when a hole is added to the alternating orbital (AO) ordered plane in LaMnO$_3$, and (iii) spin-orbital polaron when a hole is added to the AF and AO ordered plane in LaVO$_3$. Comparison of the distinct features of the above polarons can shed some light on the basic differences between the experimental phase diagrams of the lightly doped transition metal oxides La$_{2-x}$Sr$_x$CuO$_4$, La$_{1-x}$Sr$_x$MnO$_3$, and La$_{1-x}$Sr$_x$VO$_3$.

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INTRODUCTION

The doped transition metal oxides have very rich phase diagrams which are fingerprints of the spectacular physics present in these strongly correlated electron systems [1]. In particular: (i) La$_{2-x}$Sr$_x$CuO$_4$ has an antiferromagnetic (AF) and Mott insulating ground state only for very low doping $x \in (0,0.02]$ although it is a high-temperature superconductor with optimal doping $x \sim 0.15$ [1], (ii) La$_{1-x}$Sr$_x$MnO$_3$ has a plane with a ferromagnetic (FM) $e_g$ alternating orbital (AO) and Mott insulating ground state in the lightly doped regime $x \in (0,0.18]$ [2], and (iii) La$_{1-x}$Sr$_x$VO$_3$ has a plane with an AF and a $t_{2g}$ AO Mott insulating ground state in the lightly doped regime $x \in (0,0.178]$ [3]. In the present paper we try to shed some light on the distinct features of the phase diagrams of these three lightly doped transition metal oxides.

From the theoretical point of view the description of the lightly doped transition metal oxides is relatively easy in the extreme case of only one hole doped into the half-filled state [4] and in what follows we reduce our studies to this limit only. Then the motion of such a single hole added to the half-filled Mott insulating ordered ground state is strongly renormalized as it couples to the excitations of the ordered state, magnons in the AF state and orbitons in the AO state [4, 5]. This means that a polaron is formed: (i) in La$_2$CuO$_4$ with one hole in the AF ground state – a spin polaron [4], (ii) in LaMnO$_3$ with one hole in the AO ground state – an orbital polaron [5], and (iii) in LaVO$_3$ with one hole in the AO and AF ground state – a spin-orbital polaron [6]. In the next three chapters, using the self-consistent Born approximation (SCBA) [4] applied to the polaron formulation of the respective t-J model, we compare features of these three different polarons [7].
FIGURE 1. Spectral density $A(k, \omega)$ of the model Eq. (1) with $J = 0.4t$ along the particular directions of the 2D Brillouin zone.

**SPIN POLARON**

It is believed that the basic effective model which describes the important physics present both in the undoped La$_2$CuO$_4$ and in the lightly doped La$_{2-x}$Sr$_x$CuO$_4$ is the two-dimensional (2D) $t$-$J$ model [8],

$$H_S = -t \sum_{\langle i, j \rangle, \sigma} \left( \tilde{c}^\dagger_{i \sigma} \tilde{c}_{j \sigma} + H.c. \right) + J \sum_{\langle i, j \rangle} S_i \cdot S_j,$$

where $S_i$ are spin $S = 1/2$ operators and the constrained operators $\tilde{c}^\dagger_{i \sigma} = c^\dagger_{i \sigma} (1 - n_{i \sigma})$ allow for the hopping only in the restricted Hilbert space with no double occupancies. The superexchange energy scale is $J = 4t^2/U$ where $U$ is the effective repulsion between two electrons with opposite spins on the same Cu site and $t$ is the effective hopping between the Cu ions.

In the undoped case the ground state of the model is the 2D AF ordered state – this can be easily seen by noting that the kinetic term in Eq. (1) does not contribute in the half-filled case and the $t$-$J$ model reduces then to the Heisenberg model. On the other hand, in the case of one hole doped into the AF ground state the model Eq. (1) can be reduced to the polaron-type model with the quadratic terms representing magnon spectrum and the polaron-type interaction between the holes and the magnons [4]. Such a model can be easily solved using the SCBA method [4] and the hole spectral functions can be calculated from the Green’s functions.

We solved the SCBA equations numerically on a mesh of $16 \times 16$ points – the results for the realistic case of $J = 0.4t$ are shown in Fig. 1. We see a well-developed dispersive quasiparticle peak on the right hand side of the spectrum which suggests that the polaron is formed. Since microscopically the polaron is formed due to the coupling between the hole and magnons we call it a spin polaron. Besides, we note that the excited states are almost entirely different than those found in the classical Ising case (the so-called ladder spectrum [4]). This is particularly pronounced for some values of momentum $\mathbf{k}$ such as e.g. $\mathbf{k} = (0, 0)$ or $\mathbf{k} = (\pi, \pi)$. 
FIGURE 2. Spectral density $A(k, \omega)$ of the model Eq. (2) with $J = 0.4t$ along the particular directions of the 2D Brillouin zone.

### ORBITAL POLARON

A different situation occurs in the undoped LaMnO$_3$ and its doped counterpart La$_{1-x}$Sr$_x$MnO$_3$: here the partially filled $e_g$ orbitals are degenerate and the orbital degrees should be taken into account. However, in the lightly doped case the 2D ferromagnetic state is stable and consequently the spin degrees of freedom can be integrated out. Thus, one arrives at the following orbital $t$-$J$ model for the $(a, b)$ plane [9, 5],

\[ H_0 = -\frac{1}{4} t \sum_{\langle i, j \rangle} \left[ 3x_i^\dagger x_j + z_i^\dagger z_j + \sqrt{3} \left( x_i^\dagger z_j + z_i^\dagger x_j \right) + \text{H.c.} \right] + \frac{1}{8} J \sum_{\langle i, j \rangle} \left[ 3T_i^x T_j^x + T_i^z T_j^z \mp \sqrt{3} \left( T_i^x T_j^z + T_i^z T_j^x \right) \right], \tag{2} \]

where $x_i^\dagger |0\rangle = \frac{1}{\sqrt{2}} (|x\rangle \pm |z\rangle)$, $z_i^\dagger |0\rangle = \frac{1}{\sqrt{6}} (3|z\rangle^2 - r^2)|0\rangle$, the $-$$(+)$ signs denote the bonds along the $a$ ($b$) direction, and tilde denotes the hopping in the Hilbert space with no double occupancies. Besides, $T_i$ are pseudospin $T = 1/2$ operators with $T_i^z = (\tilde{n}_{ix} - \tilde{n}_{iz})/2$, the superexchange energy scale is $J = 4t^2/U$ where $U$ is the effective repulsion between electrons in the $^6A_1$ state, and $t$ is the effective hopping between the Mn ions.

This time, in the undoped case the ground state of the model is the 2D AO ordered state formed by the $(|x\rangle + |z\rangle)/\sqrt{2}$ and $(|x\rangle - |z\rangle)/\sqrt{2}$ orbitals. When one hole is doped into such an AO ground state the model Eq. (2) can be again reduced to the polaron-type model with the quadratic terms representing orbiton spectrum and the polaron-type interaction between the holes and the orbitons [5].

We solved the respective SCBA equations numerically on a mesh of $16 \times 16$ points – the spectral function for the realistic case of $J = 0.4t$ [5] is shown in Fig. 2. As in the spin case there is a well-developed quasiparticle peak on the right hand side of the spectrum which suggests that the polaron is formed. However, it is an orbital polaron since it describes a hole dressed by orbiton excitations. Moreover, the quasiparticle peak has almost no dispersion and the excited states resemble the ladder spectrum [4] which suggests that the orbital polarons are much more "classical" than the spin ones.
In the undoped LaVO$_3$ and in the lightly doped La$_{1-x}$Sr$_x$VO$_3$ the situation is much more complex than in the cuprates or manganites: here both the spin and orbital degrees of freedom should be taken into account as the spin degrees of freedom form the AF order in the undoped plane and cannot be integrated out as in the manganites [10]. Thus, one needs to consider the full spin-orbital $t$-$J$ model with $t_{2g}$ orbital degrees of freedom [10, 11]. Furthermore, in the case of the $t$-$J$ models with $t_{2g}$ orbital degrees of freedom we have to supplement such models with the frequently neglected three-site terms [12]. Thus we arrive at the following strong-coupling model for the $(a, b)$ planes of the cubic vanadates [6],

$$H_{SO} = H_t + H_{J}^{(1)} + H_{J}^{(2)} + H_{J}^{(3)} + H_{3s}. \tag{3}$$

The first term in the above equation is the kinetic term [6],

$$H_t = -t \sum_{i, \sigma} P \left( \hat{b}_{i \sigma}^{\dagger} \hat{b}_{i+\hat{a} \sigma} + \hat{a}_{i \sigma}^{\dagger} \hat{a}_{i+\hat{b} \sigma} + \text{H.c.} \right) P, \tag{4}$$

where: (i) electrons in $d_{yz}$ $(d_{zx})$ orbitals can hop only along the $b$ ($a$) direction in the $(a, b)$ plane,(ii) the tilde above the operators denotes the fact that the hopping is allowed only in the constrained Hilbert space, and (iii) due to the large Hund’s coupling $J_H \gg t$ in the cubic vanadates [10] we project the final states resulting from the electron hopping onto the high spin states using the $P$ operators in Eq. (4). The middle terms in Eq. (3) are the superexchange terms and are somewhat lengthy [13],

$$H_{J}^{(1)} = -\frac{1}{6} J r_1 \sum_{(i,j)} \left( \mathbf{S}_i \cdot \mathbf{S}_j + 2 \right) \left( \frac{1}{4} - T_i^z T_j^z \right), \tag{5}$$

$$H_{J}^{(2)} = \frac{1}{8} J r_2 \sum_{(i,j)} \left( \mathbf{S}_i \cdot \mathbf{S}_j - 1 \right) \left( \frac{19}{12} + \frac{1}{2} T_i^z T_j^z + \frac{1}{2} T_j^z T_i^z - \frac{1}{3} T_i^z T_j^z \right), \tag{6}$$

$$H_{J}^{(3)} = \frac{1}{8} J r_3 \sum_{(i,j)} \left( \mathbf{S}_i \cdot \mathbf{S}_j - 1 \right) \left( \frac{5}{4} + \frac{1}{2} T_i^z T_j^z + \frac{1}{2} T_j^z T_i^z + \frac{1}{3} T_i^z T_j^z \right), \tag{7}$$

where: $\mathbf{S}_i$ is a spin $S = 1$ operator, $T_i^z = (\bar{n}_{ib} - \bar{n}_{ia})/2$ is a pseudospin $T = 1/2$ operator, and the superexchange constant $J = 4t^2/U$ with $U$ being the repulsion between electrons on the same site and in the same orbital and with $t \ll U$ being the effective hopping between the V ions. The factors $r_1 = 1/(1-3\eta)$ and $r_3 = 1/(1+2\eta)$ (where $\eta = J_H/U$) account for the Hund’s coupling $J_H$ and originate from the energy splitting of various $d^3$ excited states due to the various possible spin and orbital configurations [10]. The last term is the three-site term which would contribute to the free hole motion [6],

$$H_{3s} = -\frac{1}{12} J (r_1 + 2) \sum_{i, \sigma} P \left( \hat{b}_{i-\hat{a} \sigma}^{\dagger} \bar{n}_{ia} \hat{b}_{i+\hat{a} \sigma} + \text{H.c.} \right) P$$

$$- \frac{1}{12} J (r_1 + 2) \sum_{i, \sigma} P \left( \hat{a}_{i-\hat{b} \sigma}^{\dagger} \bar{n}_{ib} \hat{a}_{i+\hat{b} \sigma} + \text{H.c.} \right) P. \tag{8}$$
In the undoped case the ground state of the model is the 2D AF and AO ordered state [10]. When one hole is doped to the system the model Eq. (3) can again be expressed in the polaron language; however, this time the hole couples both to orbiton and magnon excitation simultaneously [6]. Thus, the SCBA equations are more complicated and require an additional sum over the 2D Brillouin zone, similarly as in the case of the coupling between a hole and two magnons [14]. Nevertheless, it is possible to solve them numerically also on a mesh of $16 \times 16$ points – the results for the realistic case of $J = 0.2t$ and $\eta = 0.15t$ are shown in Fig. 3.

As in the purely spin or orbital case, described in the preceding chapters, a well-developed quasiparticle peak on the right hand side of the spectrum suggests formation of the polaron also in the present case. This time it is a spin-orbital polaron since the hole couples both to the orbitons and magnons. Surprisingly, the quasiparticle peak has only a very small dispersion and the excited states reproduce almost exactly the ladder spectrum of the purely classical spin case [4]. Since in the model Eq. (3) only the orbital (pseudo)spins are Ising-type this means that these are the orbital degrees of freedom which are responsible for the observed classical behaviour.

CONCLUSIONS AND FINAL DISCUSSION

In conclusion, we studied a problem of a single hole doped into the half-filled ground state of the three different cases of the $t$-$J$ model: (i) the spin model relevant for the cuprates, (ii) the $e_g$ orbital model relevant for the manganites, and (iii) the spin-orbital model relevant for the vanadates. In all these three cases the hole moves by dressing up with the collective excitations of the ground state and forms a polaron.

However, there are striking differences between the discussed here polarons. On one hand, in the spin case the quasiparticle peak has a large dispersion and the excited spectrum does not resemble the classical ladder spectrum [4] at all. On the other hand, both in the orbital and in the spin-orbital case the quasiparticle has a very tiny dispersion and the rest of the spectrum resembles almost exactly the ladder spectrum of the classical...
Ising model [15]. Possibly this is one of the reasons why the ordered state disappears very quickly with hole doping in the cuprates whereas it is relatively stable in the manganites or vanadates: in the two latter cases the polarons are more classical and quantum fluctuations would not destroy the ordered state so easily.

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15. This is because the orbital pseudospins are more classical than the spins as the interaction between the earlier is of the Ising-type.