Effective one-band electron-phonon Hamiltonian for nickel perovskites

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Inspired by recent experiments on the Sr-doped nickelates, $La_{2-x}Sr_xNiO_4$, we propose a minimal microscopic model capable of describing the variety of the observed quasistatic charge/lattice modulations and the resulting magnetic and electronic-transport anomalies. Analyzing the motion of low-spin ($s=1/2$) holes in a high-spin ($S=1$) background as well as their coupling to the in-plane oxygen phonon modes, we construct a sort of generalized Holstein t-J Hamiltonian for the NiO_2 planes, which contains, besides the rather complex ''composite-hole'' hopping part, nonlocal spin-spin and hole-phonon interaction terms.
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Charge carrier doping of transition metal oxides with a perovskite related structure induces remarkable phenomena, such as high-temperature superconductivity in cuprates, intrinsic incommensurate charge and spin ordering in nonmetallic nickelates $La_{2-x}Sr_xNiO_4$ [LSNO(x)], metal-insulator transition, and colossal magnetoresistance in Mn oxides. All these phenomena are strongly concentration dependent and the experiments suggest the decisive role of interconnection between the spin and charge correlations and the lattice and transport properties for their emergence.[1,2]

In this paper we derive an effective Hamiltonian describing the interplay of charge, spin, and lattice degrees of freedom in doped Ni oxides. As revealed by recent neutron scattering of LSNO(x),[3] the stripe order of both charge and spin densities, in general, is found to be incommensurate in the low-density region ($x\lesssim 0.3$); commensurability is restricted to very special values of x, such as 1/3 and 1/2.[4] The rich variety of charge and spin ordering accompanied by the transport anomalies in nickelates[4–6] deserves the attention not only by itself, but also with respect to understanding the superconducting state in the isostructural cuprates.

The parent compound of the LSNO(x) system is the antiferromagnetic (AF) insulator La_2NiO_4 with a Néel temperature $T_N\approx 330$ K and an in-plane exchange constant $J\approx 30$ meV. The magnetic $3d^8$ Ni^{2+} ions, having holes in $3d_{x^2-y^2}$, $3d_{3z^2-1}$ orbitals, are in the high-spin state (HSS) with $S=1$ according to Hund's rule. Doping this parent compound induces additional holes in the NiO_2 plane, but, in contrast to the superconducting cuprates, the layered nickel oxides LSNO(x) become metallic only near $x\approx 1$.

An additional hole in the NiO_2 plane quasilocalized at some Ni ion aligns its spin antiparallel to the $S=1$ spin of the ion due to the strong effective on-site interaction originated by the crystal field effect (overcoming the Hund's rule coupling).[7] The resulting low-spin state (LSS) with total spin 1/2 is tightly bound to the moving charge carrier forming a so-called ''Zhang-Rice doublet'',[6] which is the counterpart to the usual Zhang-Rice singlet in the cuprates. Aiming at the construction of a one-band model, i.e., a sort of generalization of the t-J model for the NiO_2 plane, we have to take into account the constraints put on the motion of the composite-hole LSS by the background of correlated HSS of Ni^{2+} ions.

The two configurations, corresponding to an extra hole trapped at one of the two nearest neighbor (NN) nickel ions of the bond $\langle ij\rangle$ (i,j label the sites of the square lattice built up by the Ni ions in the a-b plane), are connected by an effective transition constant determined by the second order effect of the intermediate configuration with the hole in the p orbital of the central oxygen ion.[8] Assuming the orbital d^h_{jx} of the hole localized at the site j to be nearly the same as the orbital d_{jx} of the Ni-ion coupled to this extra hole, we shall take orbitals d^h_{jx}, d_{jx} to play equivalent roles in the hopping process (in the following the indices x,z stand for the orbitals $d_{x^2-y^2}, d_{3z^2-1}$, respectively), This assumption leads to two possible ways in which the two configurations are connected by direct-type (d) and exchange-type (e) transfers.

Moreover, the hopping rate of the hole from j to i also depends on the spin states of both configurations leading to different prefactors in front of the effective transfer constant t (which is determined by the overlap of the d- and p-orbital functions t_{pd}). According to Serber's method,[9] the transition matrix elements implying the effect of spin states associated with the initial and final configurations, are given by the matrix elements of the sum of the operators:

$$\mathcal{H}_t^{(d)} = t\,\mathcal{Q}_j^{\mathrm{HSS}}\mathcal{Q}_i^{\mathrm{LSS}}\mathcal{P}_{\mathrm{I}}^{s}\mathcal{Q}_j^{\mathrm{LSS}}\mathcal{Q}_i^{\mathrm{HSS}}, \tag{1}$$

$$\mathcal{H}_t^{(e)} = -t\,\mathcal{Q}_j^{\mathrm{HSS}}\mathcal{Q}_i^{\mathrm{LSS}}\mathcal{P}_{12}^{s}\mathcal{Q}_j^{\mathrm{LSS}}\mathcal{Q}_i^{\mathrm{HSS}}, \tag{2}$$

acting in the spin function space of two NN Ni ions and one extra hole. The identical permutation operator $\mathcal{P}_{\mathrm{I}}^{s}$ and the transposition operator $\mathcal{P}_{12}^{s}$, both acting on the spin variables with indices 1, 2, correspond to the direct-type and exchange-type hole transfers, respectively. The operators $\mathcal{Q}_k^{\mathrm{LSS}}$ ($\mathcal{Q}_k^{\mathrm{HSS}}$) project the spin functions pertaining to site k on the subspace of LSS (HSS). Consequently, the projection operators restrict the motion of the composite hole to the subspace of LSS and HSS.

The matrix elements of the transitions between configurations having the total spin projections $M_T=\pm 1/2$ and

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$M_T=\pm 3/2$ are given by the sum of matrices $[\mathcal{H}_t]=[\mathcal{H}_t^{(d)}]+[\mathcal{H}_t^{(e)}]$ as follows:

$$[\mathcal{H}_t^{(d)}]= \begin{array}{c} \\ \langle i+,j0| \\ \langle i-,j1| \\ \langle i+,j1| \end{array} \begin{array}{c} \begin{array}{ccc} |i0,j+\rangle & |i1,j-\rangle & |i1,j+\rangle \end{array} \\ \begin{bmatrix} \frac{1}{3}\,t & \frac{\sqrt{2}}{3}\,t & 0 \\ \frac{\sqrt{2}}{3}\,t & 0 & 0 \\ 0 & 0 & \frac{2}{3}\,t \end{bmatrix} \end{array}, \tag{3}$$

$$[\mathcal{H}_t^{(e)}]=\frac{1}{2}\,[\mathcal{H}_t^{(d)}]. \tag{4}$$

Here the whole numbers in the bra- and ket-vectors label the spin projection belonging to HSS, whereas spin-up and spin-down LSS are denoted by + and −, respectively. Adding Eqs. (3) and (4), three types of hopping processes with effective transition constants $t/2$ and $t/\sqrt{2}$, and t are obtained.[10]

Having determined the transition matrix elements of the hopping processes, the effective transport Hamiltonian in the space of LSS and HSS of Ni ions may be written down. To this end we introduce the tensor product space $\mathcal{H}^S\otimes\mathcal{H}^h$,

$$\mathcal{H}^S=\prod_i{}^{\otimes}\{|im\rangle\},\quad m=\pm 1,0, \tag{5}$$

$$\mathcal{H}^h=\prod_i{}^{\otimes}\{|i\sigma\rangle,|i0\rangle\},\quad \sigma=\uparrow,\downarrow, \tag{6}$$

where $|i,m\rangle$ are the eigenfunctions of spin $S=1$ operators $\vec{S}_i^{\,2}$, S_i^z at site i with spin projection m. On the other hand, $|i\sigma\rangle$ means an eigenfunction of the spin $s=1/2$ operators $\vec{s}_i^{\,2}$, s_i^z of an additional hole at site i with a spin projection σ. The hole state $|i0\rangle$ corresponds to no extra hole at i.

The HSS creation and annihilation in the hopping process will be described by means of the operators[7]

$$B_{i,1}^\dagger=b_{ix,\uparrow}^\dagger b_{iz,\uparrow}^\dagger,\quad B_{i,-1}^\dagger=b_{ix,\downarrow}^\dagger b_{iz,\downarrow}^\dagger, \tag{7}$$

$$B_{i,0}^\dagger=(b_{ix,\uparrow}^\dagger b_{iz,\downarrow}^\dagger+b_{ix,\downarrow}^\dagger b_{iz,\uparrow}^\dagger)/\sqrt{2}, \tag{8}$$

defined by the Schwinger boson creation operators $b_{ix,\sigma}^\dagger, b_{iz,\sigma}^\dagger$. Denoting by $|0\rangle_B$ the boson vacuum (with respect to the closed d-shells Ni configuration), the vectors

$$|i,m\rangle=B_{i,m}^\dagger|0\rangle_B, \tag{9}$$

and operators

$$S_i^+=\sqrt{2}(B_{i,1}^\dagger B_{i,0}+B_{i,0}^\dagger B_{i,-1}), \tag{10}$$

$$S_i^z=B_{i,1}^\dagger B_{i,1}-B_{i,-1}^\dagger B_{i,-1}, \tag{11}$$

constitute a spin-1 representation, and we have

$$B_{i,m}|0\rangle_B=0,\quad B_{i,m}|jm'\rangle=\delta_{ij}\delta_{mm'}|0\rangle_B. \tag{12}$$

Accordingly, the HSS can be represented by the vectors

$$|im\rangle|i0\rangle=B_{i,m}^\dagger|0\rangle_B|i0\rangle. \tag{13}$$

Now let us consider the LSS of composite holes. Defining the Hubbard operators

$$X_i^{\sigma 0}=|i\sigma\rangle\langle i0| \tag{14}$$

in the single-occupation space $\mathcal{H}^h$, the LSS will be expressed by means of the Clebsch-Gordon coefficients as follows:

$$|i+\rangle=\frac{1}{\sqrt{3}}\,(-B_{i,0}^\dagger X_i^{\uparrow 0}+\sqrt{2}B_{i,1}^\dagger X_i^{\downarrow 0})|0\rangle_B|i0\rangle, \tag{15}$$

$$|i-\rangle=\frac{1}{\sqrt{3}}(-\sqrt{2}B_{i,-1}^\dagger X_i^{\uparrow 0}+B_{i,0}^\dagger X_i^{\downarrow 0})|0\rangle_B|i0\rangle. \tag{16}$$

Then, using the transition matrix elements given by Eqs. (1)–(4) and the representation of HSS and LSS by Eqs. (13), (15), (16), the effective transport Hamiltonian $\mathcal{H}_t$ may be rewritten as

$$\mathcal{H}_t=t\sum_{\langle i,j\rangle}(C_{i,1/2}^\dagger C_{j,\,1/2}+C_{i,-\,1/2}^\dagger C_{j,-\,1/2}), \tag{17}$$

with

$$\begin{aligned} C_{j,\,1/2}=\bar{B}_{j,0}^\dagger\left[-\frac{1}{\sqrt{3}}\,B_{j,0}X_j^{0\uparrow}+\sqrt{\frac{2}{3}}\,B_{j,1}X_j^{0\downarrow}\right] \\ +B_{j,-1}^\dagger\left[-\sqrt{\frac{2}{3}}\,B_{j,-1}X_j^{0\uparrow}+\frac{1}{\sqrt{3}}\,B_{j,0}X_j^{0\downarrow}\right], \end{aligned} \tag{18}$$

where $\bar{B}_{j,0}^\dagger=(1/\sqrt{2})\,B_{j,0}^\dagger$. The first term on the right hand side of Eq. (17) describes the four hole transport processes which are connected with the transfer of the spin projection equal to 1/2. The second term in Eq. (17), comprising the remaining four hopping processes obtained from the previous ones by the time reversal operation, corresponds to the transfer of spin projection equal to $(-1/2)$.

Obviously, in $\mathcal{H}_t$ the Hubbard operators of holes are coupled to the Schwinger boson operators, showing thus a rather complicated dependence of the hole transport on the spin background. We can even go a step further by expressing the hole Hubbard operators in terms of decoupled charge (holon) and spin variables. Using a slightly modified treatment proposed recently for the mapping of the t-J model onto the tensor product space of holon and spin-1/2 states,[11] the Hubbard operators (14) are obtained in terms of independent holon (h_i) and pseudo-spin-1/2 ($\tilde{s}_i$) operators as

$$X_i^{0\uparrow}=h_i(\tilde{s}_i^+\tilde{s}_i^-+e^{i\varphi}\tilde{s}_i^-)/\sqrt{2}, \tag{19}$$

$$X_i^{0\downarrow}=h_i(\tilde{s}_i^++e^{i\varphi}\tilde{s}_i^-\tilde{s}_i^+)/\sqrt{2}, \tag{20}$$

where the arbitrary phase factor φ has no effect on the matrix elements of physical variables. The local number operator of spinless fermionic holons,

$$h_i^\dagger h_i=\sum_\sigma X_i^{\sigma 0}X_i^{0\sigma}, \tag{21}$$

has eigenvalues $n_i^h=0,1$, and the spin operators of the physical hole spins are connected with the pseudospin operators by

$$s_i^{\pm}=h_i^{\dagger}h_i\tilde{s}_i^{\pm}, \quad s_i^z=h_i^{\dagger}h_i\tilde{s}_i^z. \tag{22}$$

The corresponding representation of the operators $C_{j,\pm 1/2}$ defined by Eq. (18) is given by

$$C_{j,1/2}=\frac{1}{\sqrt{6}}\,h_j[(\sqrt{2}\bar{B}_{j,0}^{\dagger}B_{j,1}+B_{j,-1}^{\dagger}B_{j,0})(\tilde{s}_j^{+}+e^{i\varphi}\tilde{s}_j^{-}\tilde{s}_j^{+}) - (\bar{B}_{j,0}^{\dagger}B_{j,0}+\sqrt{2}B_{j,-1}^{\dagger}B_{j,-1})(\tilde{s}_j^{+}\tilde{s}_j^{-}+e^{i\varphi}\tilde{s}_j^{-})], \tag{23}$$

and the effective transport Hamiltonian (17) becomes

$$\mathcal{H}_t=\sum_{\langle i,j\rangle}\hat{t}_{ij}h_i^{\dagger}h_j. \tag{24}$$

At this point we should stress that a comprehensive study of the propagation of carriers (holes) with an internal spin degree of freedom in both high-spin and low-spin backgrounds was performed in the context of doped Mott-Hubbard insulators by Zaanen and Oleś.[7] In the low-high spin situation their effective Hamiltonian describes the transport of LSS using auxiliary fermion operators *ignoring* the internal structure of LSS. In our treatment, consistent with the deduction of the spin-dependent transport matrix elements, the interior structure of the LSS (composite holes) is incorporated in $\mathcal{H}_t$ by the products of Hubbard and Schwinger boson operators referring to doped holes and spin background, respectively. As a consequence, the exclusion of doubly occupancy of doped holes may be explicitly assured in the hopping part (17) of our generalized one-band t-J Hamiltonian by expressing the Hubbard operators in terms of holon and spin-1/2 operators. Moreover, the occurrence of B operators in the creation and annihilation operators of LSS leads to products of B operators at the same site, which may be replaced by a spin-1 operators if nearly AF ordering takes place.

To demonstrate more explicitly the dependence of the charge transport on the spin background we shall consider the strong AF correlations of the Ni^{2+} spins at low hole concentrations, which enables us to use the spin wave approximation (SWA). Accordingly, separating the lattice sites into two AF sublattices $\{k\},\{l\}$ characterized by $S_k^z=S$, $S_l^z=-S$, respectively, the states $|k,-1\rangle,|l,1\rangle$ of Ni^{2+} ions will be excluded. Then the representation of spin operators (10), (11) may be approximated by

$$S_k^{+}\simeq\sqrt{2}B_{k,1}^{\dagger}B_{k,0}, \quad S_k^z\simeq B_{k,1}^{\dagger}B_{k,1}, \tag{25}$$

$$S_l^{+}\simeq\sqrt{2}B_{l,0}^{\dagger}B_{l,-1}, \quad S_l^z\simeq -B_{l,-1}^{\dagger}B_{l,-1}, \tag{26}$$

which makes it possible to express the transport Hamiltonian given by Eqs. (17), (18) by means of $S^{\pm}$ (spin wave) operators, up to quadratic terms, as follows:

$$\mathcal{H}_t^{\mathrm{SWA}}=\frac{t}{6}\sum_{\langle kl\rangle}[(S_k^{-}S_k^{+}+S_l^{-}S_k^{+})X_l^{\uparrow 0}X_k^{0\uparrow}+(S_l^{+}S_l^{-}+S_l^{+}S_k^{-}) \times X_l^{\downarrow 0}X_k^{0\downarrow}-2(S_k^{-}+S_l^{-})X_l^{\uparrow 0}X_k^{0\downarrow}+\mathrm{H.c.}]. \tag{27}$$

A closer resemblance of the t-J model is obtained if the transport Hamiltonian (27) is averaged with respect to the ground state of AF magnons. Following the procedure outlined for the t-J model in Ref. 11, we get the mean-field Hamiltonian

$$\mathcal{H}_t^{\mathrm{SWA}}=t_{\mathrm{eff}}\sum_{\langle i,j\rangle}h_i^{\dagger}h_j(g_{ij}+\vec{\tilde{s}}_i\vec{\tilde{s}}_j+\tfrac{1}{4}), \tag{28}$$

with

$$t_{\mathrm{eff}}=\frac{t}{3}(\langle\delta S_k^z\rangle+\tfrac{1}{2}\,\langle S_k^{+}S_l^{-}\rangle), \tag{29}$$

$$g_{ij}=\{e^{i\varphi}[(\tfrac{1}{2}-\tilde{s}_j^z)\tilde{s}_i^{-}+\tilde{s}_j^{-}(\tfrac{1}{2}+\tilde{s}_i^z)]+e^{-i\varphi}[(\tfrac{1}{2}+\tilde{s}_j^z)\tilde{s}_i^{+} +\tilde{s}_j^{+}(\tfrac{1}{2}-\tilde{s}_i^z)]\}/2. \tag{30}$$

Here $\langle\delta S_k^z\rangle$ is the reduction of the local $|S_i^z|$ from the classical value S in the ground state of AF magnons. The expectation values in Eq. (29) vanish in the classical AF Néel ground state. Supposing the quantum antiferromagnet, t_{eff} is nonzero owing to the zero-point fluctuations.

In a next step we consider the spin interactions. Here we have to take into account the strong effective on-site interaction, leading to the formation of LSS at the hole occupied sites and the (much weaker) superexchange interaction of the NN spins. Thus we get

$$\mathcal{H}_{\mathcal{J}}=\mathcal{J}_0\sum_i h_i^{\dagger}h_i\vec{\tilde{s}}_i\vec{S}_i+\sum_{\langle i,j\rangle}\mathcal{J}_{ij}\vec{J}_i\vec{J}_j, \tag{31}$$

where

$$\vec{J}_i=(1-h_i^{\dagger}h_i)\vec{S}_i+h_i^{\dagger}h_i(\vec{S}_i+\vec{\tilde{s}}_i). \tag{32}$$

The effective on-site coupling constant $\mathcal{J}_0$ is given by the energy difference between the $J=1/2$ (LSS) and $J=3/2$ states of the Ni ion occupied by an additional hole. Dagotto's estimate[12] of the latter difference is ~ 1.3 eV, so that the on-site interaction is much stronger than than all the intersite ones. Most notably, recent experiments[3] show that the intersite spin interactions play a secondary role in formation the charge-spin stripe structure as the charge ordering occurs always at higher temperatures as the ordering of spins.

We now turn to a qualitative discussion of the electron-lattice coupling effects in $La_{2-x}Sr_xNiO_4$. For the Sr-doped nickelates there is both experimental[4,13] and theoretical[14,15] evidence for a strong coupling of the additional holes to the in-plane oxygen phonon modes. Obviously a small oxygen shift along the Ni-O bonding direction leads to a significant change in the $Ni_{3d_{x^2-y^2}}$-$O_{2p_{x,y}}$ hybridization, which, in the framework of a three-band model, results in a bond-length dependence of the transfer integrals t_{pd}.[15,16] To model this situation within an effective single-band description, we assume a short-ranged Holstein-type hole-phonon interaction term, $\mathcal{H}_{h-p}=g\Sigma_{i,\vec{\delta}}(u_{i,\vec{\delta}}-u_{i-\vec{\delta},\vec{\delta}})h_i^{\dagger}h_i$, where $u_{i,\vec{\delta}}$ and $u_{i-\vec{\delta},\vec{\delta}}$ denote the projections of the displacements of the four oxygens (surrounding a nickel ion) along the positive x and y directions (i.e., $\vec{\delta}=\hat{x},\hat{y}$).[17] That means, as a result of the hole-lattice interaction an extra hole, located at some Ni site i, causes a displacement of the oxygens towards nickel, thus

producing a potential well that will bind the hole itself by a nonlinear feedback mechanism. $\mathcal{H}_{h-p}$ can be cast into the form

$$\mathcal{H}_{h-p}=g\sum_{i,\vec{\delta}} u_{i,\vec{\delta}}(h_i^{\dagger}h_i-h_{i+\vec{\delta}}^{\dagger}h_{i+\vec{\delta}}). \tag{33}$$

We note that such a *nonlocal* Holstein hole-phonon coupling has been used in combination with the usual t-J model to investigate the interaction between optical phonons and charge carriers in the copper oxides as well.[17,18] Recent exact diagonalization studies of such modified Holstein t-J models on *finite* lattices show that, if the density of holes is low, isolated local lattice distortions associated with self-trapped hole polarons are formed in the adiabatic strong-coupling regime.[17,18] At and near quarter filling, the calculated charge structure factor indicates a type of polaronic superlattice solidification reminiscent of those observed in $La_{1.5}Sr_{0.5}NiO_4$.[19] In the intermediate doping regime, the lattice distortion can be regarded as (diagonal) arrays of quasilocalized polarons, however the charge modulation could not be compared quantitatively with the experimental data due to the smallness of the lattices one could calculate.[19] On the other hand, three-band mean-field calculations performed for the *infinite* system suggest that the observed charge and spin modulations are driven by a charge segregation in stripelike structures, i.e., by phase separation on a mesoscopic length scale, connected with breathing-mode polaron formation.[15] From our considerations the mechanism for such polaron ordering is expected to be based on (i) the nonlocal character of the electron-phonon interaction determining the energy gain caused by the bond deformation to be proportional to the hole population difference of the NN Ni sites, and (ii) on the Coulomb polaron interaction. Once the ordering of polarons is established, the distribution of LSS and HSS in the lattice is fixed and at a sufficiently low temperature the stripe spin-ordering arises.

Based on these findings we argue that the hole-phonon coupling term (33) is able to describe at least qualitatively correct the relevant lattice degrees of freedom in the nickelates. Therefore we propose as an effective Hamiltonian for the layered nickel perovskites the following generalized Holstein t-J model:

$$\mathcal{H}=\mathcal{H}_t+\mathcal{H}_{\mathcal{J}}+\mathcal{H}_{h-p}+\mathcal{H}_p\,, \tag{34}$$

where $\mathcal{H}_p$ refers to the bare phonon part given in the harmonic approximation.

In summary, we have derived the hopping transport Hamiltonian of spin-1/2 composite holes in the background of spin-1 Ni^{2+} ions using Serber's results for the transition matrix elements between different electron configurations. The suppression of the spin-dependent transport was explicitly demonstrated for the case where the Ni^{2+} spins are strongly AF correlated. The experimentally observed stripe structures appear to be comprehensible on the basis of the strong coupling of doped holes to the in-plane oxygen lattice modes, incorporated in the effective one-band Hamiltonian (34) by a nonlocal Holstein-type interaction.

Finally, we would like to emphasize that applying the approach described above to the electronic transport in the ferromagnetic (colossal magnetoresistance) manganites, e.g., $La_{1-x}Ca_xMnO_3$,[20] shows the two essential differences between the doped Ni and Mn oxides. First, the itinerant electron of Mn^{3+} couples to the three t_{2g} electrons according to Hund's rule forming a *high-spin state* with total $S=2$. In contrast the crystal field splitting is dominant for Ni^{3+} ions leading to a *low-spin state* with total spin 1/2. Second, whereas the e_g electrons of Mn ions are separated from the spin background, determined by the localized t_{2g} electrons, the holes in the $d_{x^2-y^2}$ orbitals of Ni ions take part in the hopping, as well as in the formation of spin background.

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