Jahn-Teller effect in the augmented Hubbard model

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We investigate the effects induced by the interplay of microscopic degrees of freedom. In many cases, one has to consider spin and orbital degeneracy to explain complex structures of magnetic and orbital order. Frequently, attention is focused on electronic correlations. We study how the interaction of electrons with lattice degrees of freedom modifies the pure electronic case. Because of orbital degeneracy we have to deal with the Jahn-Teller effect. In particular, the $E \otimes \beta$ Jahn-Teller effect allows a perturbative approach. Assuming that the excitation energies dominate the hopping rate, we derive an effective model and analyze the interaction-induced symmetry breaking. The additional orbital degree of freedom results in a spin-orbital model and phonons are taken into account as modified coupling parameters. A quantum mechanical treatment of phonons results in an exponentially quenched orbital exchange coupling. Furthermore, by considering electronic symmetry one obtains symmetry breaking in the orbital sector. This was also found when Hund's rule coupling was taken into account, but in this case higher symmetry can be restored by proper choice of parameters, which is not the case for Jahn-Teller coupling. Surprisingly, adiabatic treatment shows neither exponential damping nor nonrestorable symmetry breaking in the orbital sector.

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I. INTRODUCTION

The interplay of microscopic degrees of freedom, such as spin, orbitals, and charge, plays an essential role in the description of a rich variety of physical phenomena in new and rediscovered materials.[1] Over the last years, most research activities have been based either on purely electronic pictures or on electronic models, which include coupling of the electrons to the static lattice degrees of freedom, to understand the peculiar features and exotic orders of strongly correlated many-body systems, such as, e.g., manganites and various spinel compounds.[2–5] Less is known about the dynamical effects on the properties, due to the interplay between electron-electron and electron-phonon interactions, of strongly correlated materials. In this context, a large amount of work has been devoted to the study of the Holstein-Hubbard model within the dynamical mean field theory (DMFT).[6] In this highly simplified model, electronic states from a nondegenerate band are considered and electron-electron as well as electron-phonon interactions are assumed to act locally only. It has been shown, for example, that the presence of electron-phonon interaction may give rise to polaronic bands at finite electron density near the Fermi level.[7] Most strongly correlated systems of interest to condensed matter physicists, however, require extensions that take into account orbital degeneracy in addition to spin degeneracy. In general, degenerate orbital states couple to degenerate vibrational modes, such that the electronic and vibrational motion cannot be simply decoupled by a canonical transformation due to the breakdown of the Born-Oppenheimer approximation.[8] In this paper, we consider an analytically treatable minimal model in which this type of decoupling is possible and the local problem can be treated exactly. In this regard, we are interested mainly in the influence of the electron-phonon interaction on orbital and spin exchange processes, which are treated in a spin-orbital model of the Kugel-Khomskii type.[9,10] In this paper, we consider a two-band Hubbard model at quarter filling and analyze the dynamical consequences due to the Jahn-Teller effect of local, tetragonal E-doublets,[11] but the approach also generalizes to other electron-phonon interacting systems, such as, e.g., $T \otimes \epsilon$ Jahn-Teller coupling[12] in cubic systems. Strictly speaking, our model is directly applicable for rare earth (R) compounds, like $R\mathrm{VO}_4$ and $R\mathrm{AsO}_4$ with, for example, $R=\mathrm{Dy}^{3+}$, Tb^{3+}, etc.[13]

The paper is organized as follows. The model is introduced in Sec. II. In Sec. III the interaction-induced symmetry breaking is discussed. We derive an effective Hamiltonian in Sec. IV. Its limits and symmetries are studied and compared with the microscopic Hamiltonian in Sec. V.

II. MODEL

We consider ions with an E-doublet electronic ground state at lattice sites of tetragonal point group symmetry. The interaction of the electronic orbitals with ligand displacements has a destabilizing effect on the ionic configuration. In the above case, symmetry allows a local coupling of the doubly degenerate electronic state to a nondegenerate vibrational mode: the $E \otimes \beta$ Jahn-Teller (JT) effect.[12–14] We shall be particularly concerned with ^2E states having electronic spin 1/2 in addition to orbital degeneracy. The highest local symmetry of the problem is given by the group SU(4) whose defining representation is spanned by $|\gamma\sigma\rangle_{\mathbf{i}}=c^{\dagger}_{\mathbf{i}\gamma\sigma}|0\rangle$ on each lattice site where the orbital label $\gamma=\theta,\epsilon$ (refers to the orbitals yz and zx) and the spin index $\sigma=\uparrow,\downarrow$. Ionic displacements break the fourfold symmetry and stabilize a distorted configuration with orthorhombic point group symmetry, shown in Fig. 1. The energy minimum is given by $E_{\min}=-(n_{\mathbf{i}\theta}-n_{\mathbf{i}\epsilon})^2E_p$, where $n_{\mathbf{i}\gamma}$ is the occupation number on site $\mathbf{i}$ in the orbital γ. The Jahn-Teller stabilization energy E_p, in units of the excitation energy of the harmonic oscillator, is

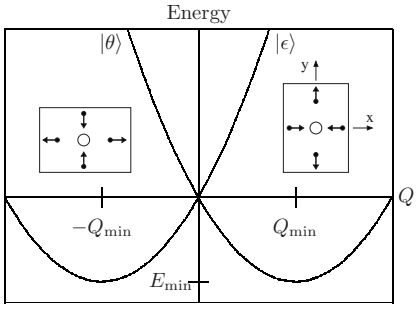

FIG. 1. On-site energy splitting of a doubly degenerate electronic state under a nondegenerate distortion Q that lifts the electronic degeneracy in first order and gives rise to a twofold degeneracy of the coupled electronic-ionic (vibronic) system: $E\otimes\beta$ instability of the symmetric configuration $Q=0$.

the squared dimensionless JT coupling g. The associated distortion is $Q_{\min}=2g(n_{\mathbf{i}\theta}-n_{\mathbf{i}\epsilon})$.

The Hamiltonian of the coupled electron-phonon system, including electronic correlations and electronic and vibrational motion, reads $H=H_t+H_{\rm ph}+H_{\rm JT}+H_{ee}$, where

$$H_t=-t\sum_{\langle\mathbf{ij}\rangle\gamma\sigma}c^{\dagger}_{\mathbf{i}\gamma\sigma}c_{\mathbf{j}\gamma\sigma}, \tag{1a}$$

$$H_{\rm ph}=\sum_{\mathbf{i}}b^{\dagger}_{\mathbf{i}}b_{\mathbf{i}}, \tag{1b}$$

$$H_{\rm JT}=-g\sum_{\mathbf{i}}(b^{\dagger}_{\mathbf{i}}+b_{\mathbf{i}})(n_{\mathbf{i}\theta}-n_{\mathbf{i}\epsilon}), \tag{1c}$$

$$H_{ee}=U\sum_{\mathbf{i}\gamma=\theta,\epsilon}n_{\mathbf{i}\gamma\uparrow}n_{\mathbf{i}\gamma\downarrow}+U_o\sum_{\mathbf{i}}n_{\mathbf{i}\theta}n_{\mathbf{i}\epsilon}+\frac{J}{2}\sum_{\mathbf{i}\sigma\sigma'}\sum_{\gamma\neq\gamma'}c^{\dagger}_{\mathbf{i}\gamma\sigma}c^{\dagger}_{\mathbf{i}\gamma'\sigma'}c_{\mathbf{i}\gamma\sigma'}c_{\mathbf{i}\gamma'\sigma}. \tag{1d}$$

$\langle\mathbf{ij}\rangle$ denotes nearest neighbors. $c^{(\dagger)}_{\mathbf{i}\gamma\sigma}$ is the annihilation (creation) operator for an electron on site $\mathbf{i}$ in the orbital γ with spin σ. $b^{(\dagger)}_{\mathbf{i}}$ are bosonic annihilation (creation) operators for phonons on site $\mathbf{i}$. The orbital occupation operator is given by $n_{\mathbf{i}\gamma}=n_{\mathbf{i}\gamma\uparrow}+n_{\mathbf{i}\gamma\downarrow}$.

The dynamics of the electrons is modeled within H_t [Eq. (1a)], which describes an orbital-conserving hopping between nearest-neighbor JT ions with isotropic hopping rate t. The decoupled motion of the vibrational β mode in terms of a harmonic oscillator on each site is governed by $H_{\rm ph}$ [Eq. (1b)]. $H_{\rm JT}$ [Eq. (1c)] is the bilinear JT coupling.[12] The electronic correlations are modeled by a two-band Hubbard model. The electron-electron interaction is expressed as H_{ee} [Eq. (1d)].[15] Double occupancy requires an energy U (U_o) for electrons in the same (different) orbital(s). Furthermore, we deal with Hund's rule coupling J that favors spin triplets compared to singlets. The energies are given in units of $\hbar\omega_0$ and the parameters are assumed to be positive. Correlations and JT coupling are treated as on-site interactions and nonlocal interactions, such as nearest-neighbor Coulomb repulsion or phonon-phonon coupling as well as on-site pair hopping, are disregarded.

In the following section, we analyze the symmetry properties of the Hamiltonian (1a)–(1d) depending on the choice of interaction parameters. The aim is the identification of conserved quantities which can be used to reduce the dimension of the Hilbert space and to characterize the eigensystem.

III. SYMMETRY AND CONSERVED QUANTITIES

We investigate symmetries related to electronic and phononic degrees of freedom. It is assumed that the lattice symmetry is tetragonal. Below we study the interaction-induced symmetry breaking of the Hamiltonian (1a)–(1d). The aim is the classification of symmetry breaking caused by on-site interactions and comparison with various models in the current literature. Furthermore, symmetry analysis allows the identification of conserved quantities. Utilizing these quantities enables a decomposition of the electronic Hilbert space.

To discuss electronic symmetry properties, it is convenient to introduce electronic spin-1/2 and orbital spin-1/2 (pseudospin) operators. These operators are defined in terms of the Pauli matrices $\boldsymbol{\sigma}^{\lambda}$ for $\lambda=x,y,z$,

$$S^{\lambda}_{\mathbf{i}\gamma}=\frac{1}{2}\sum_{\sigma\sigma'}c^{\dagger}_{\mathbf{i}\gamma\sigma}\boldsymbol{\sigma}^{\lambda}_{\sigma\sigma'}c_{\mathbf{i}\gamma\sigma'}, \tag{2a}$$

$$T^{\lambda}_{\mathbf{i}\sigma}=\frac{1}{2}\sum_{\gamma\gamma'}c^{\dagger}_{\mathbf{i}\gamma\sigma}\boldsymbol{\sigma}^{\lambda}_{\gamma\gamma'}c_{\mathbf{i}\gamma'\sigma}, \tag{2b}$$

$$\mathbf{S}_{\mathbf{i}}=\mathbf{S}_{\mathbf{i}\theta}+\mathbf{S}_{\mathbf{i}\epsilon},\quad \mathbf{T}_{\mathbf{i}}=\mathbf{T}_{\mathbf{i}\uparrow}+\mathbf{T}_{\mathbf{i}\downarrow}. \tag{2c}$$

It is easily verified that the angular momentum operators defined in this way satisfy the standard SU(2) commutation relations

$$[S^{\lambda}_{\mathbf{i}},S^{\mu}_{\mathbf{j}}]=\delta_{\mathbf{ij}}\mathrm{i}\epsilon_{\lambda\mu\nu}S^{\nu}_{\mathbf{i}}, \tag{3a}$$

$$[T^{\lambda}_{\mathbf{i}},T^{\mu}_{\mathbf{j}}]=\delta_{\mathbf{ij}}\mathrm{i}\epsilon_{\lambda\mu\nu}T^{\nu}_{\mathbf{i}}, \tag{3b}$$

and in addition

$$[S^{\lambda}_{\mathbf{i}},T^{\mu}_{\mathbf{i}}]=0. \tag{3c}$$

The same relations hold true for the global operators $S^{\lambda}=\Sigma_{\mathbf{i}}S^{\lambda}_{\mathbf{i}}$ and $T^{\lambda}=\Sigma_{\mathbf{i}}T^{\lambda}_{\mathbf{i}}$. The total site spin $\mathbf{S}_{\mathbf{i}}$ generates SU(2) rotations in the spin sector, whereas total pseudospin $\mathbf{T}_{\mathbf{i}}$ generates SU(2) rotations in the orbital sector and they satisfy $(S^{\lambda}_{\mathbf{i}})^2=(T^{\lambda}_{\mathbf{i}})^2=\frac{1}{4}\mathbb{1}$ in the single-particle representation. Equation (3c) shows that the local site spin and pseudospin algebras are decoupled, which in general does not hold for the components $S^{\lambda}_{\mathbf{i}\gamma}$ and $T^{\lambda}_{\mathbf{i}\sigma}$, respectively.

Explicit calculations establish the following relations that are useful for making the symmetry of the Hamiltonian (1a)–(1d) particularly transparent:

$$\mathbf{S}^2_{\mathbf{i}}+\mathbf{T}^2_{\mathbf{i}}=\tfrac{1}{2}n_{\mathbf{i}}(4-n_{\mathbf{i}}), \tag{4a}$$

$$\mathbf{S}^2_{\mathbf{i}}+\mathbf{T}^2_{\mathbf{i}}+2(T^{z}_{\mathbf{i}})^2=2n_{\mathbf{i}}-2n_{\mathbf{i}\theta}n_{\mathbf{i}\epsilon}, \tag{4b}$$

$$\mathbf{S}^2_{\mathbf{i}}+\mathbf{T}^2_{\mathbf{i}}-2(T^{z}_{\mathbf{i}})^2=n_{\mathbf{i}}-2\sum_{\gamma}n_{\mathbf{i}\gamma\uparrow}n_{\mathbf{i}\gamma\downarrow}, \tag{4c}$$

$$(T_{\mathbf{i}}^{\zeta})^2 = \frac{1}{2}(\mathbf{S}_{\mathbf{i}}^2 + \mathbf{T}_{\mathbf{i}}^2) - \frac{2}{3}\sum_{\gamma} \mathbf{S}_{\mathbf{i}\gamma}^2, \tag{4d}$$

where the on-site occupation operator is given by $n_{\mathbf{i}} = \Sigma_{\gamma\sigma} n_{\mathbf{i}\gamma\sigma}$. At a first glance, Eqs. (3a)–(3c) suggest that the identity (4a) is $SO(4) \cong SU(2) \times SU(2)$ invariant, but a closer inspection reveals that Eq. (4a) is actually SU(4) invariant.[16]

Furthermore, Hund's rule coupling can be expressed in terms of either spin or pseudospin operators,

$$H_J = -J\sum_{\mathbf{i}} \left(2\mathbf{S}_{\mathbf{i}\theta} \cdot \mathbf{S}_{\mathbf{i}\epsilon} + \frac{n_{\mathbf{i}\theta} n_{\mathbf{i}\epsilon}}{2} \right) \tag{5a}$$

$$= J\sum_{\mathbf{i}} [\mathbf{T}_{\mathbf{i}}^2 - (T_{\mathbf{i}}^{\zeta})^2] - \frac{J}{2} N_e, \tag{5b}$$

where $N_e = \Sigma_{\mathbf{i}} n_{\mathbf{i}}$ is the total number of electrons.

In the following sections we point out symmetry properties of the Hamiltonian (1a)–(1d) concerning phononic and electronic degrees of freedom.

A. Electronic symmetry

Due to particle conservation, one finds $U(1)_{\gamma}$ symmetry generated by $\Sigma_{\mathbf{i}} n_{\mathbf{i}\gamma}$. This symmetry holds as long as the hopping is considered as orbital conserving and on-site pair hopping is neglected. Otherwise only the total particle number N_e is conserved.

To discuss the electronic symmetry of the Hamiltonian (1a)–(1d), we take advantage of the fermion realization of angular momentum algebras, Eqs. (2a)–(2c) and (3a)–(3c), as well as of the identities (4a)–(4d), (5a), and (5b). Neglecting a constant, this yields

$$H_{ee} + H_{\mathrm{JT}} = -\sum_{\mathbf{i}} [b_S \mathbf{S}_{\mathbf{i}}^2 + b_T \mathbf{T}_{\mathbf{i}}^2 + b_z (T_{\mathbf{i}}^{\zeta})^2 + 2g(b_{\mathbf{i}}^{\dagger} + b_{\mathbf{i}}) T_{\mathbf{i}}^{\zeta}], \tag{6}$$

where $b_S = \frac{1}{2}(U + U_o)$, $b_T = \frac{1}{2}(U + U_o - 2J)$, and $b_z = -U + U_o + J$.

1. SU(4) and $SU(2)_{spin} \times SU(2)_{orb}$ symmetry

The highest symmetry in the electronic sector, i.e., the largest number of conserved quantities, is SU(4), which can be obtained by setting $U = U_o$ and $J = g = 0$. The defining representation is spanned by the four states $|\theta\uparrow\rangle_{\mathbf{i}}$, $|\theta\downarrow\rangle_{\mathbf{i}}$, $|\epsilon\uparrow\rangle_{\mathbf{i}}$, and $|\epsilon\downarrow\rangle_{\mathbf{i}}$ at each site. H_{ee} in Eq. (6) can be rewritten in the form

$$H_{ee}^{\mathrm{SU(4)}} = -U\sum_{\mathbf{i}} (\mathbf{T}_{\mathbf{i}}^2 + \mathbf{S}_{\mathbf{i}}^2) = \frac{U}{2}\sum_{\mathbf{i}} n_{\mathbf{i}}(n_{\mathbf{i}} - 4), \tag{7}$$

where we have neglected a constant. Since the particle number is conserved, the Hamiltonian (7) has SU(4) symmetry. Even when hopping is taken into account the Hamiltonian has global SU(4) symmetry.

Including Hund's rule coupling and assuming $U = U_o + J$, but neglecting JT coupling, leads to a rotational invariance in spin and orbital space. The resulting symmetry is $SU(2)_{\mathrm{spin}} \times SU(2)_{\mathrm{orb}}$. The generators are S^{λ} and T^{λ}. Equation (6) shows that b_z vanishes and the Hamiltonian is isotropic in the spin and orbital sectors. The electron-electron interaction term can be rewritten as a sum of the SU(4)-invariant form given in Eq. (7) and a $T_{\mathbf{i}}^2$ term that breaks this symmetry.

2. Jahn-Teller and Hund's rule coupling

Both JT and arbitrary ($U \neq U_o + J$) Hund's rule couplings break the symmetry only in the orbital sector, whereas the spin sector stays isotropic. These interactions yield a linear and a quadratic term in $T_{\mathbf{i}}^{\zeta}$, respectively. Hund's rule coupling reduces $SU(2)_{\mathrm{orb}}$ to $U(1)_{\mathrm{orb}}$ with generator T^{z}.[17] Setting $J = 0$ and analyzing the symmetry breaking of the JT term, one has to take into account that $T_{\mathbf{i}}^{\zeta}$ commutes also with the spin operators with orbital index S_{γ}^{λ}. These commutating operators yield an enlarged symmetry in the spin sector $U(1)_{\mathrm{orb}} \times SU(2)_{\theta} \times SU(2)_{\epsilon}$ which can also be interpreted as $U(1)_{\mathrm{orb}} \times SO(4)$.[16] The significance of this augmented spin symmetry is the rotational invariance in the spin space for each orbital. Rewriting of the Hamiltonian $H_{ee} + H_{\mathrm{JT}}$ (6) illustrates that symmetry. One finds

$$(H_{ee} + H_{\mathrm{JT}})_{J=0} = -\sum_{\mathbf{i}} \left[\left(b_s + \frac{1}{2} b_z \right) (\mathbf{S}_{\mathbf{i}}^2 + \mathbf{T}_{\mathbf{i}}^2) - \frac{2}{3} b_z \sum_{\gamma} \mathbf{S}_{\mathbf{i}\gamma}^2 + 2g(b_{\mathbf{i}}^{\dagger} + b_{\mathbf{i}}) T_{\mathbf{i}}^{\zeta} \right]. \tag{8}$$

The first contribution of Eq. (8) is SU(4) invariant while the remaining terms reduce the symmetry to $U(1)_{\mathrm{orb}} \times SU(2)_{\theta} \times SU(2)_{\epsilon}$. Arbitrary J results in a $\mathbf{T}_{\mathbf{i}}^2$ contribution with independent coupling parameter and leads to reduction from $SU(2)_{\theta} \times SU(2)_{\epsilon}$ to $SU(2)_{\mathrm{spin}}$.

The electronic symmetries are summarized in Table I.

B. Vibronic symmetry

So far we have been concerned with continuous electronic symmetries. We now consider the influence of the lattice and in particular the symmetry of the coupled vibronic system, giving rise to discrete space group symmetries.

The β mode, shown in Fig. 1, transforms according to the B_{1g} representation of the point group D_{4h}. The associated matrix group is Z_2, i.e., elements of D_{4h} are mapped onto ± 1 in the B_{1g} representation. Elements with +1 form the subgroup D_{2h}. H_{ph} is written as the sum of the squares of the distortion and the momentum and hence is invariant with respect to D_{4h}. The electronic operator has the same transformation properties as the coordinates. Hence H_{JT} is invariant with respect to D_{4h}. In Sec. III A it was shown that T^{z} is a conserved quantity, and therefore a rotation with arbitrary angle about this axis leaves the Hamiltonian invariant. However, due to the coupling term H_{JT}, we have to consider symmetry elements of the vibronic system, i.e., take both electronic and phononic degrees of freedom into account. The appropriate on-site operators $\mathcal{P}_{\mathbf{i}}^{\lambda}$, $\lambda = x, y$, consist of phononic and electronic parts $\mathcal{R}_{\mathbf{i}}$ and $\mathcal{F}_{\mathbf{i}}^{\lambda}$ and are given by[8]

$$\mathcal{P}_{\mathbf{i}}^{\lambda} = \mathcal{R}_{\mathbf{i}} \mathcal{F}_{\mathbf{i}}^{\lambda}$$

where

TABLE I. Electronic symmetries of the microscopic Hamiltonian (1a)–(1d) and the effective Hamiltonian (16), respectively.

Parameters	Coupling	Symmetry
$U=U_o$ and $J,g=0$	$\alpha^+=\alpha^-=\beta^+=\beta^-=\gamma$	SU(4)
Adiabatic, $E_p=(1/4)(U-U_o)$and $J=0$	$\alpha^+=\alpha^-=\beta^+=\beta^-=\gamma$	SU(4)
Arbitrary U,U_o,g, and $J=0$	$\alpha^+=\alpha^-$, $\beta^+=\beta^-$, γ given by $\bar{\Gamma}$	$U(1)_{orb}\times SU(2)_\theta\times SU(2)_\epsilon$
$U=U_o+J$ and $g=0$	$\alpha^+=\beta^+=\gamma$ and $\alpha^-=\beta^-$	$SU(2)_{orb}\times SU(2)_{spin}$
Adiabatic, $E_p=(1/4)(U-U_o-J)$	$\alpha^+=\beta^+=\gamma$ and $\alpha^-=\beta^-$	$SU(2)_{orb}\times SU(2)_{spin}$
Adiabatic	$\alpha^+=\beta^+$ and $\alpha^-=\beta^-$	$U(1)_{orb}\times SU(2)_{spin}$
Arbitrary U,U_o,g,J	α^+, α^-, β^+, β^-, γ given by $\bar{\Gamma}$	$U(1)_{orb}\times SU(2)_{spin}$

$$\mathcal{R}_\mathbf{i}=\exp(i\pi b_\mathbf{i}^\dagger b_\mathbf{i}) \quad \text{and} \quad \mathcal{F}_\mathbf{i}^\lambda=\exp(i\pi T_\mathbf{i}^\lambda). \tag{9}$$

$\mathcal{R}_\mathbf{i}$ changes the sign of the distortion and the momentum while $\mathcal{F}_\mathbf{i}^\lambda$ describes π rotations about the $T_\mathbf{i}^\lambda$ axis. For the electronic and bosonic operators, it follows that

$$\mathcal{R}_\mathbf{i}^\dagger b_\mathbf{i}^{(\dagger)}\mathcal{R}_\mathbf{i}=-b_\mathbf{i}^{(\dagger)}, \tag{10a}$$

$$(\mathcal{F}_\mathbf{i}^\lambda)^\dagger \mathbf{c}_{\mathbf{i}\sigma}\mathcal{F}_\mathbf{i}^\lambda=i\boldsymbol{\sigma}^\lambda\mathbf{c}_{\mathbf{i}\sigma} \quad \text{where} \quad \mathbf{c}_{\mathbf{i}\sigma}=\begin{pmatrix} c_{\mathbf{i}\theta\sigma} \\ c_{\mathbf{i}\epsilon\sigma}\end{pmatrix}. \tag{10b}$$

The identities (10a) and (10b) imply the invariance of the Hamiltonian under $\mathcal{P}^\lambda$. Hence, to describe symmetry properties of the coupled electron-phonon system, we must use vibronic operators.

IV. EFFECTIVE HAMILTONIAN

In this section we derive an effective Hamiltonian, which describes the ground state properties and low-lying excitations. We consider excitations from the quarter-filled ground state without phonons and consider hopping processes to second order. The quantum mechanical nature of phonons is included, and one obtains a spin-orbital model of the Kugel-Khomskii type[9,10] with modified coupling parameters compared with the pure electronic case. The dimension of the Hilbert space of such a model is given by the electronic degrees of freedom while JT coupling (1c) gives rise to an infinite-dimensional Hilbert space due to phononic excitations. In the effective model, the couplings are modified by the phononic excitations and appear in the form of infinite series.

We start by applying the Lang-Firsov (LF) transformation[18] $U_{LF}=\Pi_\mathbf{i}U_\mathbf{i}$ to the Hamiltonian (1a)–(1d), where

$$U_\mathbf{i}=\exp[g(b_\mathbf{i}^\dagger-b_\mathbf{i})(n_{\mathbf{i}\theta}-n_{\mathbf{i}\epsilon})], \tag{11a}$$

$$U_{LF}^\dagger b_\mathbf{i}^{(\dagger)}U_{LF}=b_\mathbf{i}^{(\dagger)}+g(n_{\mathbf{i}\theta}-n_{\mathbf{i}\epsilon}), \tag{11b}$$

$$U_{LF}^\dagger c_{\mathbf{i}\gamma\sigma}^{(\dagger)}U_{LF}=c_{\mathbf{i}\gamma\sigma}^{(\dagger)}X_{\mathbf{i}\gamma}^{(\dagger)}, \tag{11c}$$

and $X_{\mathbf{i}\theta}^\dagger=X_{\mathbf{i}\epsilon}=\exp[-g(b_\mathbf{i}^\dagger-b_\mathbf{i})]$ are shift operators that change the electronic to polaronic operators. The transformed Hamiltonian is given by $\tilde{H}=U_{LF}^\dagger HU_{LF}=\tilde{H}_0+\tilde{H}_t$ with the on-site interaction

$$\tilde{H}_0=(U-2E_p)\sum_{\mathbf{i}\gamma}n_{\mathbf{i}\gamma\uparrow}n_{\mathbf{i}\gamma\downarrow}+(U_o+2E_p)\sum_\mathbf{i}n_{\mathbf{i}\theta}n_{\mathbf{i}\epsilon}$$
$$+\frac{J}{2}\sum_{\mathbf{i}\sigma\sigma'}\sum_{\gamma\neq\gamma'}c_{\mathbf{i}\gamma\sigma}^\dagger c_{\mathbf{i}\gamma'\sigma'}^\dagger c_{\mathbf{i}\gamma\sigma'}c_{\mathbf{i}\gamma'\sigma}+\sum_\mathbf{i}b_\mathbf{i}^\dagger b_\mathbf{i}-E_pN_e \tag{12}$$

and the hopping term

$$\tilde{H}_t=-t\sum_{\langle\mathbf{ij}\rangle\gamma\sigma}c_{\mathbf{i}\gamma\sigma}^\dagger c_{\mathbf{j}\gamma\sigma}X_{\mathbf{i}\gamma}^\dagger X_{\mathbf{j}\gamma}. \tag{13}$$

$E_p=g^2$ is the energy gain due to JT coupling and N_e is the total number of electrons. The inter- and intraorbital Coulomb interaction is modified in such a way that U is reduced by $2E_p$ while U_o is increased by a similar contribution. The reason is that the JT term vanishes for double occupancy of different orbitals (JT inactive) while the energy is further reduced by the double occupancy of the same orbital (JT active). The local states for single and double occupancy and the related energies are shown in Fig. 2.

The transformed Hamiltonian $\tilde{H}$, Eqs. (12) and (13), serves as a starting point to derive the effective model. We study the low-energy properties of $\tilde{H}$ by perturbation theory.

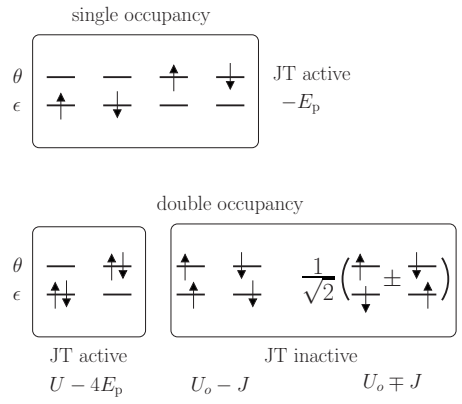

FIG. 2. Local states with single and double occupancy without excited phonons.

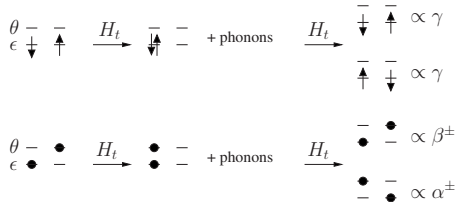

FIG. 3. Hopping processes of second order. The dots stand for electrons. The label ± indicates whether the intermediate state is a spin singlet or triplet. The coefficients $\alpha^{\pm}$, $\beta^{\pm}$, and γ are given in Eq. (17).

$\tilde{H}_0$ is taken as the zeroth-order Hamiltonian while $\tilde{H}_t$ is regarded as a perturbation. To evaluate H_{eff}, we consider a quarter-filled lattice with single occupancy and no excited phonons. Excitations from the ground state are given via six possible doubly occupied states labeled with $|\beta_{\mathbf{j}\lambda}\rangle$, shown in Fig. 2, plus phononic excitations relative to shifted harmonic oscillators caused by the LF transformation. To ensure the singly occupied ground state for a system without hopping we have to assume $U-2E_p>0$ and $U_o-J+2E_p>0$. Up to second order, we obtain the effective Hamiltonian

$$H_{\text{eff}} = {}_{\text{ph}}\langle 0|\tilde{H}_t A \tilde{H}_t|0\rangle_{\text{ph}} \quad \text{with} \quad A = \sum_{\mathbf{j}} A_{\mathbf{j}}$$

and

$$A_{\mathbf{j}} = \sum_{\{n\}=0}^{\infty} \sum_{\lambda=1}^{6} \frac{|\beta_{\mathbf{j}\lambda}\rangle|\{n\}\rangle\langle\{n\}|\langle\beta_{\mathbf{j}\lambda}|}{-N_e E_p - E_\beta}, \tag{14}$$

where $|0\rangle_{\text{ph}}$ is the phononic vacuum and $|\{n\}\rangle$ is the phononic configuration associated with the energy n. The zeroth-order Hamiltonian is given by $-N_e E_p$ and is neglected. Contributions from the first-order perturbation vanish. The excitations consist of a doubly occupied and a nearest-neighbor empty site and phononic excitations. The ground state energy is $-N_e E_p$. The excitation energies E_β are $U-4E_p-(N_e-2)E_p$ and $U_o \pm J-(N_e-2)E_p$ for intra- and interorbital doubly occupied sites, respectively (left and right lower panels in Fig. 2). Additional phonon excitations entail a nonzero n.

To derive an effective model we have to take into account the hopping processes shown in Fig. 3. Processes for nearest-neighbor electrons in the same orbital (upper panel) lead to the same energy gain, independent of whether spin exchange occurs or not. These processes and the role of changing the lattice configuration have been discussed in the context of bipolaron formation in the Holstein-Hubbard model.[19,20] The situation differs for processes with nearest-neighbor electrons in different orbitals (lower panel). The energy gain of such processes, caused by Hund's rule coupling, depends on whether the doubly occupied state is a spin singlet or triplet state. We distinguish these situations with the label ±. Processes conserving the orbital occupancy relative to the initial state are preferred compared with processes that change the orbital configuration. This last conclusion was also found from studies of the bipolaron problem of the model.[21] In other words, changing the orbital configuration reduces the energy gain. The different contributions from the hopping processes yield a symmetry breaking in the orbital sector and $\text{SU}(2)_{\text{orb}}$ cannot be restored by a special choice of parameters. This is in contrast to the case without electron-phonon interaction or in the adiabatic limit. We will discuss this point later on. The isotropy in the spin sector results in $\text{SU}(2)_{\text{spin}}$.

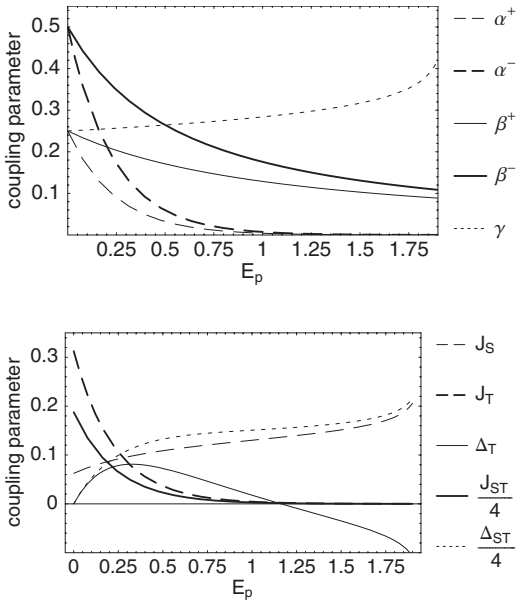

FIG. 4. Coupling parameters in units of $2t^2$ versus the JT stabilization energy $E_p=g^2$ for $U=4$, $U_0=3$, and $J=1$.

Evaluation of Eq. (14) results in products of an electronic creation and annihilation operator on sites $\mathbf{i}$ and $\mathbf{j}$. These fourfold products can be rewritten in terms of spin and pseudospin operators in the following way. One considers the action of $c^{\dagger}_{\mathbf{j}\gamma\sigma}c_{\mathbf{j}\gamma'\sigma'}$ on a state with quarter filling $\Pi_{\mathbf{i}}c^{\dagger}_{\mathbf{i}\gamma_{\mathbf{i}}\sigma_{\mathbf{i}}}|0\rangle_{\text{el}}$ and finds the translation rules[15]

$$\begin{array}{ll} \gamma\gamma' & \sigma\sigma' \\ \theta\theta \to \frac{1}{2}+T^z & \uparrow\uparrow \to \frac{1}{2}+S^z \\ \epsilon\epsilon \to \frac{1}{2}-T^z & \downarrow\downarrow \to \frac{1}{2}-S^z . \\ \theta\epsilon \to T^+ & \uparrow\downarrow \to S^+ \\ \epsilon\theta \to T^- & \downarrow\uparrow \to S^- \end{array} \tag{15}$$

For instance, the operator $c^{\dagger}_{\mathbf{j}\theta\downarrow}c_{\mathbf{j}\epsilon\downarrow}$ can be expressed as $T^+_{\mathbf{j}}(\frac{1}{2}-S^z_{\mathbf{j}})$. One finds the effective Hamiltonian

$$H_{\text{eff}} = \sum_{\langle\mathbf{ij}\rangle} \left(-\alpha^+ \mathbf{T_i}\cdot\mathbf{T_j} + (\beta^+ + \alpha^+ - 2\gamma) T^z_{\mathbf{i}} T^z_{\mathbf{j}} - \frac{\gamma}{2} - \frac{\beta^+}{4} \right) P^{S=0}_{\mathbf{ij}}$$
$$+ \left(\alpha^- \mathbf{T_i}\cdot\mathbf{T_j} + (\beta^- - \alpha^-) T^z_{\mathbf{i}} T^z_{\mathbf{j}} - \frac{\beta^-}{4} \right) P^{S=1}_{\mathbf{ij}}, \tag{16}$$

where the coupling parameters, shown in Fig. 4, are

$$\alpha^{\pm} = \bar{\Gamma}(U_o \pm J + 2E_p, 2E_p),$$

$$\beta^{\pm} = \bar{\Gamma}(U_o \pm J + 2E_p, -2E_p),$$

$$\gamma = \bar{\Gamma}(U - 2E_p, -2E_p), \tag{17}$$

where

$$\bar{\Gamma}(\Delta,y) = 2t^2 e^{-2E_p} \sum_{n=0}^{\infty} \frac{(-y)^n}{n!\,(n+\Delta)}.$$

The spin singlet and triplet operators on a bond are given by

$$P_{\mathbf{ij}}^{S=0} = \tfrac{1}{4} - \mathbf{S_i}\cdot\mathbf{S_j} \quad \text{and} \quad P_{\mathbf{ij}}^{S=1} = \mathbf{S_i}\cdot\mathbf{S_j} + \tfrac{3}{4}. \tag{18}$$

Interorbital processes differ in intermediate spin singlet (α^+, β^+) and triplet (α^-,β^-) states. Due to their lower excitation energy the triplet states lead to an enhanced energy gain. In the following, α und β without the label $\pm$ indicate coupling parameters for $J=0$. Moreover, one has to distinguish between changed ($\alpha^{\pm}$) and conserved ($\beta^{\pm}$) orbital configurations. The former results in an alternating series and leads to exponential quenching for increasing E_p, while the latter behaves algebraically as shown in Fig. 4. In the limit of strong JT coupling, i.e., $E_p \gg 1$, one obtains the approximation

$$\alpha^{\pm} \approx \frac{2t^2 e^{-4E_p}}{U_o \pm J}, \quad \beta^{\pm} \approx \frac{2t^2}{U_o \pm J + 4E_p}, \quad \gamma \approx \frac{2t^2}{U}. \tag{19}$$

Without JT coupling one finds the parameters known from the two-band Hubbard model

$$\alpha^{\pm} = \beta^{\pm} = \frac{2t^2}{U_o \pm J}, \quad \gamma = \frac{2t^2}{U}. \tag{20}$$

To discuss spin-orbital models of terms of the Kugel-Khomskii type, it is useful to rewrite H_{eff} in isotropic spin, orbital, and mixed coupling and anisotropic contributions. This yields

$$H_{\text{eff}} = \sum_{\langle \mathbf{ij}\rangle} J_S \mathbf{S_i}\cdot\mathbf{S_j} + J_T \mathbf{T_i}\cdot\mathbf{T_j} + J_{ST}(\mathbf{T_i}\cdot\mathbf{T_j})(\mathbf{S_i}\cdot\mathbf{S_j}) + \Delta_T T_{\mathbf{i}}^{\zeta} T_{\mathbf{j}}^{\zeta} + \Delta_{ST} T_{\mathbf{i}}^{\zeta} T_{\mathbf{j}}^{\zeta} (\mathbf{S_i}\cdot\mathbf{S_j}) + C. \tag{21}$$

The coupling parameters, also shown in Fig. 4, are determined from Eq. (16). Starting from $\mathrm{SU(2)_{spin}}\times\mathrm{SU(2)_{orb}}$ for $g=0$, one finds vanishing anisotropy coefficients Δ_T and Δ_{ST}. J_S varies smoothly while the orbital exchange parameters J_T and J_{ST} are exponentially damped with E_p. It is remarkable that Δ_T changes sign. This anisotropic orbital coupling alters from antiferro-orbital to ferro-orbital.

V. LIMITS AND SYMMETRY

It is instructive for later discussions to briefly summarize some results of bare electronic models available in the current literature to point out the potential significance of electron-phonon interaction in strongly correlated materials. In this context, particular emphasis is set on symmetry aspects associated with electron-phonon coupling.

A. Symmetries of the isotropic model

We start from the case of highest symmetry SU(4) which is obtained for $U=U_o$ and $J=g=0$. The coupling parameters of the effective model (21) achieve $J_S=J_T=\frac{1}{4}J_{ST}$ and $\Delta_T=\Delta_{ST}=0$.[22,23] One obtains

$$H^{\mathrm{SU(4)}} = J_{ST} \sum_{\langle \mathbf{ij}\rangle} \left(\mathbf{S_i}\cdot\mathbf{S_j} + \frac{1}{4}\right)\left(\mathbf{T_i}\cdot\mathbf{T_j} + \frac{1}{4}\right), \tag{22}$$

where we have neglected a constant. This model, also with additional interaction terms and in higher dimensions, has been intensively studied.[22,24–30] In one dimension, SU(N) models are integrable.[31] It is known that, in the thermodynamic limit[32] and if the number of sites is a multiple of 4,[33] the ground state of the SU(4) symmetric model is a SU(4) singlet.

The isotropic model ($\Delta_T=\Delta_{ST}=0$) with free parameters $x=J_S/J_{ST}$ and $y=J_T/J_{ST}$, respectively, was found to be $\mathrm{SU(2)_{spin}}\times\mathrm{SU(2)_{orb}}$ invariant, and a rich phase diagram and points with exact solutions were discussed[34–43] and the analogy to spin ladders was studied.[44–46] To achieve this symmetry we have to take $U=U_o+J$ and $g=0$, which produces a line in the (x,y) diagram from the SU(4) point for $J=0$ to $(-1/4,3/4)$ for the maximum value of $J=U/2$.

B. Pure electronic case

The frequently studied spin-orbital models with electronic correlations are given by setting $g=0$.[15,33,40,47–49] Although the lattice symmetry considered in these references differs from our case, the structure of the effective model is the same because of the high symmetry of H_{ee}. In the underlying model (1a)–(1d) with isotropic orbital-conserving hopping and without on-site pair hopping, one finds $\mathrm{U(1)_{orb}}\times\mathrm{SU(2)_{spin}}$ symmetry with generators T^{ζ} and S^{λ}. The effective Hamiltonian written in these operators, neglecting a constant, is given by

$$H_{\text{eff}}^{g=0} = H^{\mathrm{SU(4)}} + \left(J_T - \frac{J_{ST}}{4}\right)\sum_{\langle \mathbf{ij}\rangle} (\mathbf{T_i}\cdot\mathbf{T_j} - \mathbf{S_i}\cdot\mathbf{S_j}) - 4\Delta_T \sum_{\langle \mathbf{ij}\rangle} \left(T_{\mathbf{i}}^{\zeta} T_{\mathbf{j}}^{\zeta} + \frac{1}{4}\right)\left(\mathbf{S_i}\cdot\mathbf{S_j} - \frac{1}{4}\right). \tag{23}$$

The dot products of spin and pseudospin operators lower the SU(4) symmetry to $\mathrm{SU(2)_{orb}}\times\mathrm{SU(2)_{spin}}$. The last term reduces the symmetry further to $\mathrm{U(1)_{orb}}\times\mathrm{SU(2)_{spin}}$ and vanishes for $U=U_o+J$.

The limits and symmetries above are well-known properties of spin-orbital models that take solely electron-electron interaction into account. Let us now consider the limits including JT coupling and investigate their effects on magnetic and orbital order. Finally, we discuss the consequences of an adiabatic treatment and show that the anisotropy caused by different contributions from changed and conserved orbital configurations is missing.

C. Ferro-orbital and ferromagnetic case

The restriction to single-orbital occupation results in a Heisenberg model with an antiferromagnetic coupling constant γ. Neglect of the electron-phonon interaction yields the well-known $t \ll U$ limit of the Hubbard model with the Heisenberg coupling $2t^2/U$. This model belongs to the class of SU(N) models and is solvable in one dimension,[31,50] too.

Neglecting the spin degree of freedom and taking only ferromagnetic configurations into account, one ends up with a model describing orbital degrees of freedom in terms of spinless fermions. This formulation results in an XXZ pseudospin model[51] with an anisotropy parameter $\Delta = \beta/\alpha \geq 1$. The XXZ model is solvable, e.g., via the Bethe ansatz.[52–54] In the limit $g=0$ or within the adiabatic treatment the XXZ model becomes isotropic ($\Delta=1$). $\Delta > 1$ corresponds to the quantum mechanical picture of the JT problem. One obtains exponential increase of the anisotropy parameter caused by E_p and the nature of the model shifts from Heisenberg to Ising type. Hence the coupling to phonons favors antiferro-orbital order. This cooperative effect is induced by hopping of electrons, in contrast to the cooperative JT effect mediated by phonon-phonon coupling.

D. Hund's rule coupling $J=0$

Vanishing Hund's rule coupling results in $\mathrm{U}(1)_{\mathrm{orb}} \times \mathrm{SU}(2)_\theta \times \mathrm{SU}(2)_\epsilon$ symmetry. Hence, one finds five conserved quantities compared to three in the case with Hund's rule coupling and without JT coupling. Furthermore, the symmetry breaking caused by J can be extenuated through particular choice of the parameters $U=U_o+J$, while this is not possible in terms of JT coupling. The symmetry properties for $J=0$ can be seen by rewriting the effective Hamiltonian (16) in terms of generators of the group $\mathrm{U}(1)_{\mathrm{orb}} \times \mathrm{SU}(2)_\theta \times \mathrm{SU}(2)_\epsilon$, which means T^ζ and S^λ_γ. One finds

$$H^{J=0}_{\mathrm{eff}} = H^{\mathrm{SU}(4)} + \frac{\Delta_{ST}}{2} \sum_{\langle \mathbf{ij} \rangle \gamma} \mathbf{S}_{\mathbf{i}\gamma} \cdot \mathbf{S}_{\mathbf{j}\gamma} + \Delta_T \sum_{\langle \mathbf{ij} \rangle} T^\zeta_{\mathbf{i}} T^\zeta_{\mathbf{j}}, \qquad (24)$$

where we have neglected a constant. Here we take advantage of the fact that, at quarter filling, the two-particle operators $T^\zeta_{\mathbf{i}} S^\lambda_{\mathbf{i}}$ can be replaced by $\frac{1}{2}(S^\lambda_{\mathbf{i}\theta} - S^\lambda_{\mathbf{i}\epsilon})$.

The Heisenberg coupling $\Delta_{ST}/2$ for the spin in each orbital changes sign for $U > U_o$. Weak JT coupling favors ferromagnetic (FM) order and the system switches to antiferromagnetic (AFM) coupling with increasing values of the coupling. Analogously the Ising coupling Δ_T changes from antiferro-orbital to ferro-orbital (FO). Hence, in the strong coupling limit $E_p \gg 1$, one expects an AFM-FO ground state. Hund's rule coupling favors FM order and, therefore, competes with JT coupling.

E. Adiabatic limit

Let us consider the adiabatic limit. One finds that the shift operators in Eq. (13) vanish in that limit, and therefore the coupling constants are the same as in the purely electronic case apart from a renormalization of the Coulomb interactions. Hence, the intraorbital (interorbital) repulsion U (U_o) is converted to an effective repulsion $U-2E_p$ (U_o+2E_p) and the anisotropy and the exponential behavior of the orbital exchange processes vanish. One obtains

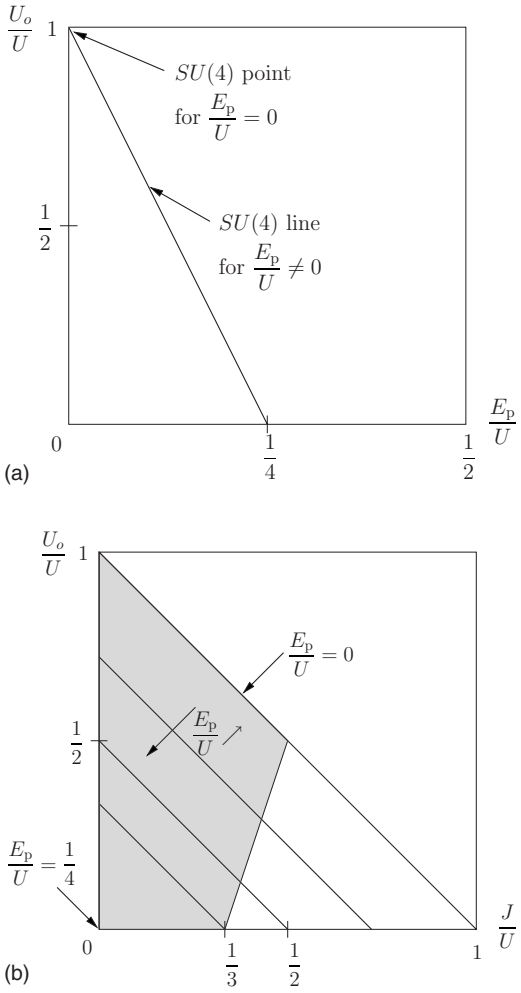

FIG. 5. Symmetry in the adiabatic limit. (a) Possible values for SU(4) symmetry given by $E_p=(1/4)(U-U_o)$ and $J=0$. (b) The shaded area shows values of U_o/U and J/U, where SU(2) $\times$ SU(2) symmetry is possible without violating $E_p>0$ and $U_0-J+2E_p>0$. Points on lines satisfy the SU(2) $\times$ SU(2) condition $E_p=(1/4)(U-U_o-J)$ for constant values of E_p/U.

$$\alpha^{\pm}_{\mathrm{ad}} = \beta^{\pm}_{\mathrm{ad}} = \frac{2t^2}{U_o \pm J + 2E_p} \quad \text{and} \quad \gamma_{\mathrm{ad}} = \frac{2t^2}{U - 2E_p}. \qquad (25)$$

Hence the SU(4) condition $U=U_o$ and $J=0$ without JT coupling changes in the adiabatic limit to $E_p=\frac{1}{4}(U-U_o)$ and $J=0$. The SU(4) point expands to a line shown in Fig. 5(a). Alternatively, it is possible to restore $\mathrm{SU}(2)_{\mathrm{spin}} \times \mathrm{SU}(2)_{\mathrm{orb}}$ by setting $E_p=\frac{1}{4}(U-U_o-J)$ instead of $U=U_o+J$ and $g=0$. The restrictions $U_o > 3J-U$ and $U_o+J<U$ ensure positive excitation energy U_o-J+2E_p and JT energy E_p. These inequalities are satisfied within the shaded area in Fig. 5(b). The lines satisfy the $\mathrm{SU}(2)_{\mathrm{spin}} \times \mathrm{SU}(2)_{\mathrm{orb}}$ condition $E_p=\frac{1}{4}(U-U_o-J)$ for constant values of E_p/U. The restoration of these high symmetries is solely possible in the adiabatic limit. Taking phononic excitations into account results in anisotropic behavior and one finds $\alpha < \beta$ and hence $\mathrm{U}(1)_{\mathrm{orb}}$ symmetry.

The relations between coupling coefficients for special choices of parameters and related symmetries are given in Table I.

VI. CONCLUSION

In this paper, we have considered a two-band Hubbard model including both on-site Coulomb interactions and Hund's rule coupling as well as the local $E\otimes\beta$ Jahn-Teller effect.

Treating delocalization of the electrons within the framework of degenerate perturbation theory and taking into account the quantum nature of the Jahn-Teller effect yields an effective spin-orbital model for the description of electronic and lattice degrees of freedom. In this effective model, the coupling parameters are strongly modified in comparison to pure electronic models, owing to phononic Jahn-Teller excitations. Additionally, the occupancy of the initial and final orbitals involved in the various virtual hopping processes plays an important role. In particular, we find that orbital exchange ($\propto\alpha^{\pm}$) due to virtual nearest-neighbor hopping is exponentially suppressed with the strength of the Jahn-Teller coupling and even completely quenched in the limit $E_p\gg 1$. This is in contrast to orbital-conserving processes ($\propto\beta^{\pm}$), which show algebraic renormalization of the bare electronic coupling constants. Spin exchange processes ($\propto\gamma$) are basically proportional to the value of systems without phonons. If we treat the lattice as static, the exponential quenching is absent. Instead, we find algebraic contributions for all exchange processes. Particularly in this limit, orbital-changing and -conserving processes of neighboring electrons in different orbitals result in the same contribution ($\alpha^{\pm}=\beta^{\pm}$). The same holds true for the effective model without Jahn-Teller coupling.

Hence, the main features that arise for the quantum mechanical but not for the adiabatic treatment are the dependence of the energy gain due to virtual hopping processes on the orbital occupancy and the exponential damping for orbital exchange processes. This considerations result in an anisotropic effective spin-orbital model, which means an *XXZ* type of orbital. Since the spin sector is isotropic, one obtains a Heisenberg-type result for the spin degree of freedom. In the limit of strong electron-phonon coupling ($E_p\gg 1$), the Ising term dominates the orbital part, because the contributions from orbital exchange processes are exponentially suppressed. Note that this damping is caused by the quantum mechanical treatment of the Jahn-Teller coupling.

In addition, the facts mentioned above produce remarkable results for consideration of the symmetry properties. We studied the interaction-induced symmetry breaking for both the microscopic and the effective Hamiltonian. The rotational invariance of the spin in each orbital appears as $\mathrm{SU}(2)_{\theta}\times\mathrm{SU}(2)_{\epsilon}$. This symmetry is not affected by the Jahn-Teller effect but is broken to $\mathrm{SU}(2)_{\mathrm{spin}}$ through Hund's rule coupling. That the $\mathrm{SU}(2)_{\mathrm{spin}}$ symmetry is not affected by the couplings we considered can be seen by the formulation of the interaction contributions in terms of $\mathbf{S}_{\mathbf{i}}^2$ and the local pseudospin operators, given in Eq. (6). Referring to the symmetry breaking in the orbital sector, one finds for the adiabatic limit, just as in the case without Jahn-Teller coupling, that both SU(4) and $\mathrm{SU}(2)_{\mathrm{spin}}\times\mathrm{SU}(2)_{\mathrm{orb}}$ symmetry are restorable through proper choice of parameters. However, including phononic excitations breaks SU(2) symmetry in the orbital sector down to U(1).

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