# Jahn-Teller systems at half filling: Crossover from Heisenberg to Ising behavior

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The Jahn-Teller model with $E\otimes\beta$ electron-phonon coupling and local (Hubbard-like) Coulomb interaction is considered to describe a lattice system with two orbitals per site at half filling. Starting from a state with one electron per site, we follow the tunneling of the electrons and the associated creation of an arbitrary number of phonons due to electron-phonon interaction. For this purpose we apply a recursive method which allows us to organize systematically the number of pairs of empty/doubly occupied sites and to include infinitely many phonons which are induced by electronic hopping. In lowest order of the recursion (i.e., for all processes with only one pair of empty/doubly occupied sites) we obtain an effective anisotropic pseudospin 1/2 Heisenberg Hamiltonian $H_{eff}$ as a description of the orbital degrees of freedom. The pseudospin coupling depends on the physical parameters and the energy. This implies that the resulting resolvent $[E-H_{eff}(E)]^{-1}$ has an infinite number of poles, even for a single site. $H_{eff}$ is subject to a crossover from an isotropic Heisenberg model (weak electron-phonon coupling and isotropic hopping) to an Ising model (strong electron-phonon coupling).

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## I. INTRODUCTION

It has been known for a long time that orbital degrees of freedom in systems with Jahn-Teller coupling can be described by an effective pseudospin Hamiltonian.[1–4] The coupling parameter of the pseudospin interaction is $t^2/U$, where $t$ is the orbital hopping rate and $U$ is the strength of the onsite Coulomb interaction. This description is of great interest because it provides a model to study orbital ordering and the possibility of orbital liquids in terms of conventional spin theories.

The main problem of treating electrons that couple to phonons is that even for small systems with one or a few electrons the Hilbert space is infinite dimensional. This implies a complex spectrum with level crossing and avoided level crossing.[5] There are various treatments of small Jahn-Teller systems, e.g., exact numerical diagonalization with truncated phonon spectrum,[6–8] Monte Carlo simulations[9] or variational methods.[10]

In this paper the influence of the electron-phonon coupling strength on the effective pseudospin Hamiltonian will be studied in detail for electrons on a lattice. In order to keep the calculations simple only the case of a system with $E\otimes\beta$ Jahn-Teller coupling[11] is considered, and the electron spin is neglected. A recursive projection formalism[12,13] is applied to derive the effective pseudospin Hamiltonian. This approach provides pseudospin coupling parameters that depend on the electron-phonon coupling strength.

The paper is organized as follows. In Sec. II the model is defined. As a physical quantity the resolvent, related to the electron-phonon Hamiltonian, is considered. Its relation with physical quantities is discussed in Sec. II A. The recursive projection method is briefly described in Sec. III and the effective pseudospin Hamiltonian, obtained from this method, is presented in Sec. IV. Finally, the crossover from weak to strong electron-phonon coupling is studied in Sec. IV A.

## II. THE $E\otimes\beta$ JAHN-TELLER MODEL

The Jahn-Teller model describes fermions with pseudospin $\sigma=\uparrow,\downarrow$, coupled to phonons. It is defined by the Hamiltonian $H=H_t+H_0$, where $H_t$ is the hopping term of the fermions between nearest-neighbor sites $\mathbf{j}$ and $\mathbf{j}'$,

$$H_t=-\sum_{\langle \mathbf{j},\mathbf{j}'\rangle}\sum_{\sigma=\uparrow,\downarrow} t_{\sigma,\mathbf{j}\mathbf{j}'}c^\dagger_{\mathbf{j}\sigma}c_{\mathbf{j}'\sigma}+\text{H.c.} \tag{1}$$

and $H_0$ is a local (Hubbard-like) interaction and a phonon term:

$$H_0=\sum_{\mathbf{j}}\left[\omega_0 b^\dagger_{\mathbf{j}}b_{\mathbf{j}}+g(b^\dagger_{\mathbf{j}}+b_{\mathbf{j}})(n_{\mathbf{j}\uparrow}-n_{\mathbf{j}\downarrow})+Un_{\mathbf{j}\uparrow}n_{\mathbf{j}\downarrow}\right] \tag{2}$$

for dispersionless phonons with energy $\omega_0$. The hopping rate $t_{\sigma,\mathbf{j}\mathbf{j}'}$ from orbital $\sigma$ at site $\mathbf{j}$ to orbital $\sigma$ at site $\mathbf{j}'$ depends on $\sigma$ such that in general $t_\uparrow\neq t_\downarrow$. Moreover, it is assumed that hopping between different orbitals is very weak such that $t_{\uparrow\downarrow}=0$, similar to the model considered in Ref. 4. For the subsequent study it is not crucial that the hopping rate depends on the sites. Therefore, it will not be explicitly written.

For a given ensemble of fermions, represented by integer numbers $n_{\mathbf{j}\sigma}=0,1$, the Hamiltonian $H_0$ can be diagonalized with product states

$$\prod_{\mathbf{j}}|N_{\mathbf{j}},n_{\mathbf{j}\uparrow},n_{\mathbf{j}\downarrow}\rangle \quad (N_{\mathbf{j}}\geqslant 0). \tag{3}$$

For $n_{\mathbf{j}\uparrow}=n_{\mathbf{j}\downarrow}=0$ (no fermions) $N_{\mathbf{j}}=0,1,\ldots$ is the number of phonons at site $\mathbf{j}$. That is $|N_{\mathbf{j}},0,0\rangle$ is an eigenstate of the phonon-number operator $b^\dagger_{\mathbf{j}}b_{\mathbf{j}}$:

$$b^\dagger_{\mathbf{j}}b_{\mathbf{j}}|N_{\mathbf{j}},0,0\rangle=N_{\mathbf{j}}|N_{\mathbf{j}},0,0\rangle.$$

The corresponding states with a single fermion at $\mathbf{j}$ are obtained from $|N_{\mathbf{j}},0,0\rangle$ as

$$|N_{\mathbf{j}},1,0\rangle=c^\dagger_{\mathbf{j}\uparrow}\exp\left[-\frac{g}{\omega_0}(b^\dagger_{\mathbf{j}}-b_{\mathbf{j}})\right]|N_{\mathbf{j}},0,0\rangle,$$

$$|N_{\mathbf{j}},0,1\rangle=c^\dagger_{\mathbf{j}\downarrow}\exp\left[\frac{g}{\omega_0}(b^\dagger_{\mathbf{j}}-b_{\mathbf{j}})\right]|N_{\mathbf{j}},0,0\rangle \tag{4}$$

and a state with two fermions as

 

$$|N_{\mathbf{j}},1,1\rangle = c^{\dagger}_{\mathbf{j}\uparrow}c^{\dagger}_{\mathbf{j}\downarrow}|N_{\mathbf{j}},0,0\rangle.$$

$\Pi_{\mathbf{j}}|N_{\mathbf{j}},n_{\mathbf{j}\uparrow},n_{\mathbf{j}\downarrow}\rangle$ is an eigenstate of $H_0$ with energies

$$E_0(\{N_{\mathbf{j}},n_{\mathbf{j}\uparrow},n_{\mathbf{j}\downarrow}\}) = \sum_{\mathbf{j}}\left[\omega_0 N_{\mathbf{j}} - \frac{g^2}{\omega_0}(n_{\mathbf{j}\uparrow}-n_{\mathbf{j}\downarrow})^2 + U n_{\mathbf{j}\uparrow}n_{\mathbf{j}\downarrow}\right]. \tag{5}$$

The groundstate of $H_0$ is a product of singly occupied states from Eq. (4) with $N_{\mathbf{j}}=0$. The groundstate energy per lattice site is $-g^2/\omega_0$.

### A. The resolvent

In the following the resolvent

$$(z-H)^{-1}$$

shall be studied. It is directly related to a number of physical quantities. One is linked with the thermodynamic properties of a statistical ensemble governed by the Hamiltonian $H$ through the Boltzmann weight at inverse temperature $\beta$:

$$e^{-\beta H} = \int_{\Gamma}(z-H)^{-1}e^{-\beta z}\frac{dz}{2\pi}. \tag{6}$$

$\Gamma$ is a closed contour that encloses all eigenvalues of $H$. Another connection is with the dynamics of quantum states in a system which is characterized by the Hamiltonian $H$: The evolution of a state $|\Psi_0\rangle$ at time 0 to the state $|\Psi_t\rangle$ a later time $t>0$ is given by

$$|\Psi_t\rangle = e^{iHt}|\Psi_0\rangle.$$

A Laplace transformation for positive time gives with $\mathrm{Im}z<0$ the resolvent that acts on the initial state:

$$\int_0^{\infty} e^{-izt}|\Psi_t\rangle dt = \int_0^{\infty} e^{-izt}e^{iHt}dt|\Psi_0\rangle = (z-H)^{-1}|\Psi_0\rangle. \tag{7}$$

The return probability to the initial state is obtained from the inverse Laplace transform and reads

$$\langle\Psi_0|\Psi_t\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{izt}\langle\Psi_0|(z-H)^{-1}|\Psi_0\rangle dz. \tag{8}$$

Using the spectral representation of $H$ with eigenvalues $E_j$, the expectation value in the integrand reads

$$\langle\Psi_0|(z-H)^{-1}|\Psi_0\rangle = \sum_j \frac{|\langle E_j|\Psi_0\rangle|^2}{z-E_j}.$$

Inserting this into Eq. (8) allows us to apply Cauchy's Theorem to perform the integration.

In order to evaluate the resolvent a standard procedure is to expand it in terms of $H_t$ in a Neumann series

$$(z-H)^{-1} = (z-H_0-H_t)^{-1} = (z-H_0)^{-1}\sum_{l\geq 0}[H_t(z-H_0)^{-1}]^l,$$

and to truncate this series after a finite number of terms. The poles of any finite truncation are the eigenvalues of the unperturbed Hamiltonian $H_0$. This may be insufficient for a good approximation of $(z-H)^{-1}$. In the next section a recursive approach is applied that avoids this limitation.

## III. RECURSIVE PROJECTION FORMALISM

Considering a restricted Hilbert space for states $|\Psi_0\rangle$, the projected resolvent $P_0(z-H)^{-1}P_0$ must be evaluated. It is assumed that $P_0$ projects the states of the entire Hilbert space $\mathcal{H}$ to the subspace $\mathcal{H}_0$. The projected resolvent satisfies the identity

$$P_0(z-H)^{-1}P_0 = [P_0(z-H)P_0 - P_0HP_1(z-H)_1^{-1}P_1HP_0]_0^{-1}, \tag{9}$$

where $P_1=\mathbf{1}-P_0$ projects onto the Hilbert space $\mathcal{H}_1$ that is complementary to $\mathcal{H}_0$. $(z-H)_1^{-1}$ is the inverse of $z-H$ on the $P_1$-projected Hilbert space $\mathcal{H}_1$, i.e.,

$$(z-H)_1^{-1} \equiv P_1(P_1(z-H)P_1)^{-1}P_1.$$

If $H$ obeys the relations

$$P_0HP_1 = P_0HP_2, \quad P_1HP_0 = P_2HP_0 \quad (P_2 \neq P_1) \tag{10}$$

(i.e., matrix elements of $H$ connect only states in $\mathcal{H}_0$ with states in $\mathcal{H}_2$, where the latter is a subspace of $\mathcal{H}_1$), Eq. (9) can also be written

$$P_0(z-H)^{-1}P_0 = [P_0(z-H)P_0 - P_0HP_2(z-H)_1^{-1}P_2HP_0]_0^{-1}. \tag{11}$$

The identity used in Eq. (9) can be applied again to $P_2(z-H)_1^{-1}P_2$ on the right-hand side:

$$P_2(z-H)_1^{-1}P_2 = [P_2(z-H)P_2 - P_2HP_3(z-H)_3^{-1}P_3HP_2]_2^{-1}, \tag{12}$$

where $P_3$ projects onto the complement of $\mathcal{H}_2$ on $\mathcal{H}_1$. A typical Hamiltonian obeys relations analogous to those in Eq. (10) with the replacements $P_0\rightarrow P_2$ and $P_1\rightarrow P_3$.

This procedure can be applied iteratively, as shown in Fig. 1. It creates a hierarchy of projectors $P_k$ onto Hilbert spaces $\mathcal{H}_k$: $\mathcal{H}_{2j+2}$ is defined as a subspace of $\mathcal{H}_{2j+1}$ by the properties of the Hamiltonian:

$$P_{2j}HP_{2j+1} = P_{2j}HP_{2j+2} \equiv H_{j,j+1}$$

and

$$P_{2j+1}HP_{2j} = P_{2j+2}HP_{2j} \equiv H_{j+1,j}, \tag{13}$$

and $\mathcal{H}_{2j+1}$ is the complement of $\mathcal{H}_{2j}$ with respect to $\mathcal{H}_{2j-1}$. In terms of the projected resolvents this construction implies a recursion relation. Using the notation

$$G_{2j} = P_{2j}(z-H)_{2j-1}^{-1}P_{2j},$$

the recursion relation reads

$$G_{2j} = [z - P_{2j}HP_{2j} - H_{j,j+1}G_{2j+2}H_{j+1,j}]_{2j}^{-1}. \tag{14}$$

The recursion terminates for $j=j_t$ if $P_{2j_t}HP_{2j_t+1}=0$. This is the case when $H$ is diagonal on $\mathcal{H}_{2j_t+1}$.

The special form of the Hamiltonian $H$ in Sec. II as the sum of two Hamiltonians $H=H_0+H_t$ can be used to obtain projections with the following properties:

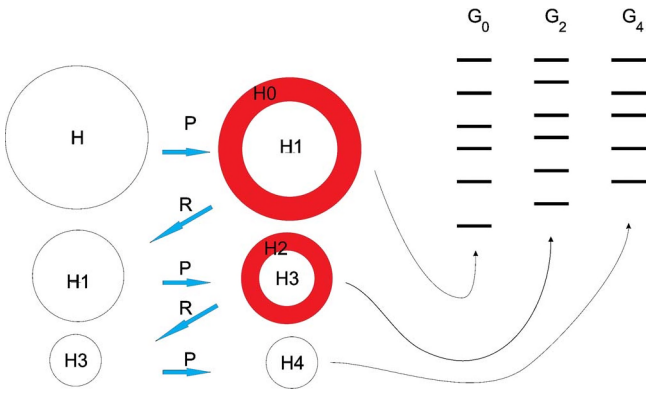


FIG. 1. (Color online) The schematic structure of the recursive projection method that reduces the Hilbert space (Russian doll approach). The actual reduction is due to the recursion relation ($R$), whereas the projection ($P$) separates a part of the Hilbert space through the Hamiltonian $H_{j+1,j}$. The low-lying poles of the resolvent $G_{2j}$ (indicated by the levels) are removed recursively by the method.

(i) $H_0$ stays inside the projected Hilbert space:

$$H_0P_0 = P_0H_0 = P_0H_0P_0.$$

(ii) $H_t$ maps from $\mathcal{H}_{2j}$ to $\mathcal{H}_{2j+2}$:

$$H_t:\mathcal{H}_{2j} \to \mathcal{H}_{2j+2},$$

where $\mathcal{H}_{2j}$ is orthogonal to $\mathcal{H}_{2j+2}$. In the next section these properties will be used to construct an effective Hamiltonian.

## IV. THE EFFECTIVE HAMILTONIAN

The projection formalism is now applied to the Hamiltonian $H=H_0+H_t$ of Sec. II. The Hilbert space separates subspaces with a fixed number of fermions with pseudospin $\uparrow$ and a fixed number with pseudospin $\downarrow$ because $H$ cannot change it with a diagonal pseudospin term. The case is considered here where $P_0$ projects onto singly occupied sites with $N_{\mathbf{j}}=0$. $H_t$ is off diagonal with respect to the phonons and changes the number of pairs of empty/doubly-occupied sites (PEDS) by one. Therefore, $P_{2j}$ $(j \geqslant 1)$ projects onto states with $j$ PEDS and $N_{\mathbf{j}} \geqslant 0$. According to this construction, the matrix elements of $P_{2j}HP_{2j+2}=P_{2j}H_tP_{2j+2}$ and $P_{2j+2}HP_{2j}=P_{2j+2}H_tP_{2j}$ are all nonzero with respect to different phonon numbers. $P_{2j}H_0P_{2j}$ is diagonal in the basis (4) with matrix elements:

$$\omega_0 \sum_{\mathbf{j}} N_{\mathbf{j}} - 2(M-j)g^2/\omega_0 + Uj,$$

where $2(M-j)$ counts the number of singly-occupied sites and $j$ the number of doubly-occupied sites on a lattice with $2M$ sites. Thus the recursion relation of Eq. (14) becomes

$$G_{2j} = \left[ z - \omega_0 \sum_{\mathbf{j}} b_{\mathbf{j}}^\dagger b_{\mathbf{j}} + 2(M-j)g^2/\omega_0 - Uj - H_{j,j+1}G_{2j+2}H_{j+1,j} \right]_{2j}^{-1} \tag{15}$$

with $H_{j,j+1}$ defined in Eq. (13). The recursion terminates on a finite lattice $(M<\infty)$ if $j=M$, since at most $M$ PEDS can be created and, therefore, $P_{2M+1}$ is a projection onto the empty space. $G_{2M}$ is diagonal with matrix elements

$$\frac{1}{z - \omega_0 \sum_{\mathbf{j}} N_{\mathbf{j}} - UM}.$$

This can serve as a starting point for the iterative approximation of $G_0$. The poles of $G_{2M}$ are

$$z_N = \omega_0 \sum_{\mathbf{j}} N_{\mathbf{j}} + UM = \omega_0 N + UM \quad \left( N = \sum_{\mathbf{j}} N_{\mathbf{j}} = 0,1,\ldots \right).$$

They are very large in comparison with the groundstate energy $-2Mg^2/\omega_0$ of Eq. (5) due to the doubly occupied sites that contribute the interaction energy $U$ per site. The main interest is in the low-lying states (i.e., in states near the groundstate). Then $z$ is restricted to values close to $-2Mg^2/\omega_0$. It is convenient to introduce the energy $E$ that measures the excitation energy with respect to the groundstate energy of the system with Hamiltonian $H_0$:

$$E = z + 2Mg^2/\omega_0. \tag{16}$$

In terms of $E$ the recursion relation reads

$$G_{2j} = \left[ E - \omega_0 \sum_{\mathbf{j}} b_{\mathbf{j}}^\dagger b_{\mathbf{j}} - (2g^2/\omega_0 + U)j - H_{j,j+1}G_{2j+2}H_{j+1,j} \right]_{2j}^{-1}. \tag{17}$$

On the right-hand side the diagonal term,

$$-E + \omega_0 \sum_{\mathbf{j}} b_{\mathbf{j}}^\dagger b_{\mathbf{j}} + (2g^2/\omega_0 + U)j,$$

can be compared with the off-diagonal term,

$$H_{j,j+1}G_{2j+2}H_{j+1,j}.$$

For $j=M-1$ the diagonal term is of order $-E+(2g^2/\omega_0+U)(M-1)$ and the off-diagonal term is of order $[-E+(2g^2/\omega_0+U)M]^{-1}$. It is assumed that $2g^2/\omega_0+U$ is sufficiently large, i.e., either the electron-phonon or the Hubbard interaction is strong. In this case the off-diagonal term can be neglected in comparison with the diagonal term. Consequently, $G_{2M-2}$ is diagonal in this approximation. This type of approximation can be repeated for each recursion step $j=M-2,M-3,\ldots,1$, always leading to a diagonal resolvent $G_{2j}$, because the diagonal term is of the order $-E+(2g^2/\omega_0+U)(j-1)$ and the off-diagonal term is of order $[-E+(2g^2/\omega_0+U)j]^{-1}$. Finally, the approximated $G_2$ reads

$$G_2 \approx \left( E - \omega_0 \sum_{\mathbf{j}} b_{\mathbf{j}}^\dagger b_{\mathbf{j}} - 2g^2/\omega_0 - U \right)_2^{-1}. \tag{18}$$

This approximation corresponds with a truncation of all scattering processes with more than one PEDS. It is valid for weak hopping, i.e., for $t_\sigma$ small in comparison with $2g^2/\omega_0+U$. Subsequently, it will turn out that an effective expansion parameter for the truncation is $t_\sigma t_{\sigma'}/(U/\omega_0+2g^2/\omega_0^2)$.

Equations (17) and (18) give for $G_0$ the expression

$$G_0 = \left[ E - H_{0,1} \left( E - \omega_0 \sum_{\mathbf{j}} b_{\mathbf{j}}^\dagger b_{\mathbf{j}} - 2g^2/\omega_0 - U \right)_2^{-1} H_{1,0} \right]_0^{-1}. \tag{19}$$

$H_{0,1}(\cdots)_2^{-1}H_{1,0}$ is a matrix in a Hilbert space with $N_{\mathbf{j}}=0$ according to the definition of $P_0$. $H_{1,0}$ creates phonons as well as a PEDS. This will be picked up by the diagonal matrix $(\cdots)_2^{-1}$. Finally, $H_{0,1}$ annihilates the phonons and the PEDS. Consequently, the entire expression is either diagonal or has off-diagonal elements with nearest-neighbor pseudospin exchanges. Such a matrix can be expressed by an (anisotropic) pseudospin-1/2 Hamiltonian. A detailed calculation gives an anisotropic Heisenberg Hamiltonian

$$\begin{aligned} H_{\text{eff}} &\equiv H_{0,1} \left[ E - \omega_0 \sum_{\mathbf{j}} b_{\mathbf{j}}^\dagger b_{\mathbf{j}} - 2g^2/\omega_0 - U \right]_2^{-1} H_{1,0} \\ &= \sum_{\mathbf{j},\mathbf{j}'} \left[ a_{\uparrow\uparrow} \left( S_{\mathbf{j}}^z S_{\mathbf{j}'}^z - \frac{1}{4} \right) + a_{\uparrow\downarrow} (S_{\mathbf{j}}^x S_{\mathbf{j}'}^x + S_{\mathbf{j}}^y S_{\mathbf{j}'}^y) \right] \end{aligned} \tag{20}$$

with the pseudospin-1/2 operators $S^x$, $S^y$, $S^z$, and $E$-dependent coupling coefficients (cf. the Appendix)

$$\begin{aligned} a_{\uparrow\uparrow} &= (t_\uparrow^2 + t_\downarrow^2) \frac{e^{-2g^2/\omega_0^2}}{\omega_0} \gamma^* \left( \frac{U + 2g^2/\omega_0 - E}{\omega_0}, -2g^2/\omega_0^2 \right), \\ a_{\uparrow\downarrow} &= 2t_\uparrow t_\downarrow \frac{e^{-2g^2/\omega_0^2}}{\omega_0} \gamma^* \left( \frac{U + 2g^2/\omega_0 - E}{\omega_0}, 2g^2/\omega_0^2 \right). \end{aligned} \tag{21}$$

$\gamma^*$ is related to the incomplete gamma function (Ref. 16):

$$\gamma^*(a,y) = \sum_{m \geqslant 0} \frac{1}{m!} \frac{(-y)^m}{a+m}.$$

It should be noticed that the coupling coefficients depend on the pair of neighboring sites $(\mathbf{j},\mathbf{j}')$ through the hopping rates:

$$a_{\sigma\sigma',\mathbf{j}\mathbf{j}'} = a_{\sigma\sigma'}(t_{\uparrow,\mathbf{j}\mathbf{j}'}, t_{\downarrow,\mathbf{j}\mathbf{j}'}).$$

The parameter $U+2g^2/\omega_0$ as well as the parameter $2g^2/\omega_0^2$ appear separately in the coupling coefficients. The former parameter is assumed to be large, whereas the latter can be tuned independently without leaving the region of validity of the approximations. It will be discussed in the next section that this provides a tool to describe a crossover of the model between two qualitatively different regimes by changing the electron-phonon coupling constant $g$.

### A. Crossover from weak to strong electron-phonon coupling

The $E$-dependent coefficients in $H_{\text{eff}}$ simplify substantially for the asymptotic regimes of weak and strong electron-phonon coupling $g$. Relevant are low energies $E$ which represent the poles of the resolvent in Eq. (6). To avoid the poles of the incomplete gamma function, the following discussion is restricted to energies:

$$E \leqslant U + 2g^2/\omega_0. \tag{22}$$

It will be shown that in this case there exist poles of the projected resolvent with $E_j \leqslant 0$. The restriction (22) implies that the approximated diagonal resolvent $G_2$ in Eq. (18) has only negative matrix elements:

$$G_2 = \left( E - 2g^2/\omega_0 - U - \sum_{\mathbf{j}} N_{\mathbf{j}} \right)_2^{-1} < 0.$$

Thus $H_{0,1}G_2H_{1,0}$ is a negative matrix and the projected resolvent,

$$(E - H_{0,1}G_2H_{1,0})_0^{-1},$$

has all poles $E_j$ on the negative real axis. The relevant parameter in our truncated recursive projection formalism is $U/\omega_0 + 2g^2/\omega_0^2 \gg 1$. This allows a free tuning of the electron-phonon coupling $g$, as long as $U$ is sufficiently large.

The weak-coupling limit of the isotropic case $t_\downarrow = t_\uparrow \equiv t$ corresponds with the Hubbard model. For the latter (i.e., for $g=0$) it is known that a $1/U$ expansion at half filling gives in leading order an isotropic Heisenberg model with coupling coefficients (Ref. 14)

$$a_{\uparrow\uparrow} = a_{\uparrow\downarrow} = 2t^2/U.$$

A similar result was obtained for the strong-coupling perturbation theory of the Holstein model.[15] The main difference between the strong-coupling perturbation theory and the recursive projection method is the energy dependence of the coupling constants in the latter. The result of the recursive projection method can be understood as a partial summation of the strong-coupling expansion. For nonzero but small $g$ $(g/\omega_0 \ll 1)$ the coupling coefficients of Eq. (21) have the asymptotic behavior

$$a_{\uparrow\uparrow} \sim \frac{t_\uparrow^2 + t_\downarrow^2}{2g^2/\omega_0 + U - E}, \quad a_{\uparrow\downarrow} \sim \frac{2t_\uparrow t_\downarrow}{2g^2/\omega_0 + U - E}.$$

Thus, the coupling of the $S^z$ component dominates in the anisotropic case since $a_{\uparrow\uparrow} \geqslant a_{\uparrow\downarrow}$.

In the opposite regime, where the electron-phonon coupling is strong (i.e. $g/\omega_0 \gg 1$), the incomplete gamma function is approximated by

$$\begin{aligned} &\gamma^* \left( \frac{U + 2g^2/\omega_0 - E}{\omega_0}, \mp 2g^2/\omega_0^2 \right) \\ &\sim \frac{\omega_0}{U + 2g^2/\omega_0 - E} \sum_{m \geqslant 0} \frac{1}{m!} (\pm 2g^2/\omega_0^2)^m = \frac{\omega_0 e^{\pm 2g^2/\omega_0^2}}{U + 2g^2/\omega_0 - E}. \end{aligned}$$

Thus the coupling coefficients of the pseudospin-1/2 Hamiltonian are

$$a_{\uparrow\uparrow} \sim \frac{t_\uparrow^2 + t_\downarrow^2}{2g^2/\omega_0 + U - E}, \quad a_{\uparrow\downarrow} \sim 0.$$

The crossover regime, within the restriction of Eq. (22), is plotted in Fig. 2 for isotropic hopping. It indicates that at weak electron-phonon coupling there is a strong isotropic pseudospin-pseudospin coupling, whereas a strong electron-phonon coupling implies a strong pseudospin-pseudospin coupling only for the $S^z$ component but a weak one for $S^x$ and $S^y$. Thus the tuning of the electron-phonon interaction is

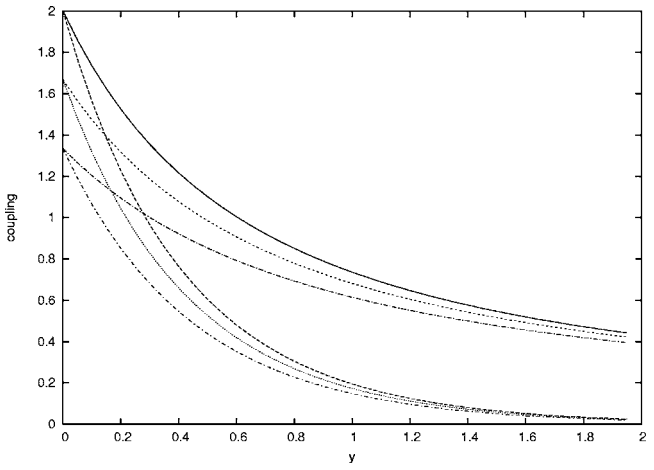


FIG. 2. Coupling coefficients of the effective pseudospin-1/2 Hamiltonian of Eq. (21) for isotropic hopping $t_\downarrow = t_\uparrow \equiv t$ as a function of $y = 2g^2/\omega_0^2$: $a_{\uparrow\uparrow}$ (upper set of curves) and $a_{\uparrow\downarrow}$ (lower set of curves) in units of $t^2/\omega_0$ for $(U-E)/\omega_0 = 1.0, 1.2, 1.5$ (from top to bottom in each set of curves).

given by a crossover from an isotropic Heisenberg to an Ising model. This may be accompanied by a sequence of crossovers and/or phase transitions.

The pole from the groundstate of the projected resolvent $(E-H_{\text{eff}})^{-1}$ is easily evaluated in the asymptotic regimes. For the weak-coupling regime it is

$$E_H = g^2/\omega_0 + U/2 - \sqrt{(g^2/\omega_0 + U/2)^2 - \lambda_H},$$

and for the strong-coupling regime

$$E_I = g^2/\omega_0 + U/2 - \sqrt{(g^2/\omega_0 + U/2)^2 - \lambda_I},$$

where $\lambda_H$ ($\lambda_I$) is the lowest eigenvalue of the Heisenberg (Ising) Hamiltonian with coupling constants $J^x = J^y = 2t_\uparrow t_\downarrow$, $J^z = t_\uparrow^2 + t_\downarrow^2$ ($J^x = J^y = 0$, $J^z = t_\uparrow^2 + t_\downarrow^2$), respectively.

These results imply that the anisotropy of the electronic hopping with respect to the orbitals is created or enhanced by the electron-phonon interaction. The exponential suppression of the $S^x - S^y$ coupling by the latter strongly supports an Ising-like interaction of the orbital degrees of freedom. This may be crucial in two-dimensional systems, where an Ising-like interaction can lead to orbital order, in contrast to a Heisenberg interaction.

An experimental consequence of the crossover to the Ising-like behavior should be observed in layered materials (e.g., $La_{1-x}Sr_{1+x}MnO_4$ or $La_4Ru_2O_{10}$). To separate the spin degrees of freedom, a spin-polarized state can be created by a weak magnetic field. Then, in the presence of a strong electron-phonon interaction, the material undergoes an Ising-like phase transition to a state with orbital order. For $La_4Ru_2O_{10}$ a two-dimensional transition to orbital ordering with an opening of a spin gap was reported in Ref. 17. Whether or not the spin gap is related to a anisotropic interaction of the orbital degrees of freedom is not clear in this case.

## V. CONCLUSIONS

Starting from a Hamiltonian with short-range Coulomb and $E \otimes \beta$ Jahn-Teller interaction, a system of spinless fermions was studied at half filling. An effective Hamiltonian $H_{eff}$ was derived under the assumption that the kinetic energy (i.e., the hopping term) is always dominated by the local interaction energy. In the absence of the electron-phonon interaction this leads to the well-known isotropic pseudospin-1/2 Heisenberg Hamiltonian for $H_{eff}$. A weak electron-phonon interaction suppresses the pseudospin-1/2 interaction of the effective Hamiltonian, and an increasing electron-phonon interaction develops an anisotropy, where the pseudospin-pseudospin interaction in the $xy$ plane decreases as $\exp(-4g^2/\omega_0^2)$ with the electron-phonon coupling constant $g$ and the pseudospin-pseudospin interaction in the $z$ direction decreases like $1/g^2$.

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## APPENDIX

Using the shorthand notation

$$|0,\uparrow\rangle = |0,1,0\rangle \quad |0,\downarrow\rangle = |0,0,1\rangle$$

one can write for the coupling coefficients of the effective Hamiltonian

$$a_{\uparrow\uparrow} := -(t_\uparrow^2 + t_\downarrow^2) \sum_{m,m' \geq 0} \frac{\langle 0,\uparrow|m,0,0\rangle\langle m,0,0|0,\uparrow\rangle\langle 0,\downarrow|m',0,0\rangle\langle m',0,0|0,\downarrow\rangle}{E - [\omega_0(m+m') + 2g^2/\omega_0 + U]}$$

$$= -(t_\uparrow^2 + t_\downarrow^2) e^{-2g^2/\omega_0^2} \sum_{m,m' \geq 0} \frac{1}{m!m'!} \frac{(g^2/\omega_0^2)^{m+m'}}{E - [\omega_0(m+m') + 2g^2/\omega_0 + U]}.$$

The double sum is reduced to a single sum

$$= -(t_\uparrow^2 + t_\downarrow^2) e^{-2g^2/\omega_0^2} \sum_{m \geq 0} \frac{1}{m!} \frac{(2g^2/\omega_0^2)^m}{E - \omega_0 m - 2g^2/\omega_0 - U}$$

and

$$a_{\uparrow\downarrow} := -2t_\uparrow t_\downarrow \sum_{m,m' \geqslant 0} \frac{\langle 0,\uparrow|m,0,0\rangle\langle m,0,0|0,\downarrow\rangle\langle 0,\downarrow|m',0,0\rangle\langle m',0,0|0,\uparrow\rangle}{E-[\omega_0(m+m')+2g^2/\omega_0+U]}$$

$$= -2t_\uparrow t_\downarrow e^{-2g^2/\omega_0^2} \sum_{m,m' \geqslant 0} \frac{1}{m!m'!} \frac{(-g^2/\omega_0^2)^{m+m'}}{E-[\omega_0(m+m')+2g^2/\omega_0+U]}.$$

The double sum is again reduced to a single sum

$$= -2t_\uparrow t_\downarrow e^{-2g^2/\omega_0^2} \sum_{m \geqslant 0} \frac{1}{m!} \frac{(-2g^2/\omega_0^2)^m}{E-\omega_0 m-2g^2/\omega_0-U}.$$

These expressions are related to the incomplete gamma function (Ref. 16)

$$\gamma^*(a,y) = \sum_{m \geqslant 0} \frac{1}{m!} \frac{(-y)^m}{a+m}$$

such that

$$a_{\uparrow\uparrow} = (t_\uparrow^2 + t_\downarrow^2) \frac{e^{-2g^2/\omega_0^2}}{\omega_0} \gamma^*\left(\frac{U-E+2g^2/\omega_0}{\omega_0}, -2g^2/\omega_0^2\right),$$

$$a_{\uparrow\downarrow} = 2t_\uparrow t_\downarrow \frac{e^{-2g^2/\omega_0^2}}{\omega_0} \gamma^*\left(\frac{U-E+2g^2/\omega_0}{\omega_0}, 2g^2/\omega_0^2\right).$$


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