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An analytic study of the E ⊗ e Jahn-Teller polaron

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Abstract. An analytic study is presented of the $E \otimes e$ Jahn-Teller (JT) polaron, consisting of a mobile e_g electron linearly coupled to the local e_g normal vibrations of a periodic array of octahedral complexes. Due to the linear coupling, the parity operator $\mathcal{K}$ and the angular momentum operator $\mathcal{J}$ commute with the JT part and cause a twofold degeneracy of each JT eigenvalue. This degeneracy is lifted by the anisotropic hopping term. The Hamiltonian is then mapped onto a new Hilbert space, which is isomorphic to an eigenspace of $\mathcal{J}$ belonging to a fixed angular momentum eigenvalue $j > 0$. In this representation, the Hamiltonian depends explicitly on j and decomposes into a Holstein term and a residual JT interaction. While the ground state of the JT polaron is shown to belong to the sector $j = 1/2$, the Holstein polaron is obtained for the "unphysical" value $j = 0$. The new Hamiltonian is then subjected to a variational treatment, yielding the dispersion relations and effective masses for both kinds of polarons. The calculated polaron masses are in remarkably good agreement with recent quantum Monte Carlo data. The possible relevance of our results to the magnetoresistive manganite perovskites is briefly discussed.

PACS. 71.38.-k Polarons and electron-phonon interactions – 63.20.Pw Localized modes – 72.80.Ga Transition-metal compounds

1 Introduction

The Jahn-Teller (JT) effect describes the interaction of lattice vibrational modes with orbitally degenerate electronic states and thus refers to a particular type of electron-phonon coupling [1]. Although this effect has proved indispensable for a proper understanding of the physics of a variety of systems, ranging from paramagnetic ions in nonmagnetic crystals [2] to structural phase transitions [3], it is fair to say that its role in condensed-matter physics has been marginal for a long time.

For nearly a decade, however, the significance of the JT effect is undergoing a profound change, triggered by the discovery of superconductivity in the fullerides [4] and of very large ("colossal") magnetoresistance (CMR) in the manganite perovskites [5]. Because of their high symmetry, both classes of compounds fulfil the requirement for a JT interaction to occur, and numerous experiments seem to indicate that this is, in fact, the case. Manifestations of the JT effect in the fullerides have been reviewed by O'Brien and Chancey [6], those in the manganites by Millis [7]. So far, however, there is no consensus as to the relative importance of the JT coupling in these materials. In their search of the origin of the CMR effect [5], *e.g.*, Millis *et al.* [8] argued that double exchange [9], designed as a mechanism to induce ferromagnetic order in doped manganites, is not sufficient to account for the resistivity data and suggested that JT polaron formation is essential, whereas other authors [10] invoke ferromagnetic spin polarons to explain the effect. Problems of this kind could possibly be resolved by means of a detailed analytic theory of the JT polaron, yielding the (approximate) ground-state energy together with the corresponding eigenvector. Since the eigenstates of JT systems are *vibronic* in nature [1], they may give rise to unexpected results for expectation values and correlation functions.

As a first step in this direction, we study the JT polaron of symmetry type $E \otimes e$, which is most conveniently introduced by recalling some basic properties of $La_{1-x}Ca_xMnO_3$, a representative of the manganite family [7]. Each unit cell of the crystal contains an octahedral MnO_6 complex and an average number of $4 - x$ d electrons. Since the Hund's rule coupling is believed to be very strong, the spins of all the d electrons are ferromagnetically aligned. Due to the crystal field produced by the oxygen ligands (point group O_h) the D state of the free Mn ion splits into a threefold degenerate t_{2g} and a twofold degenerate e_g level. Three of the electrons go into the tightly bound t_{2g} orbitals forming a core spin of magnitude 3/2, while the remaining $1-x$ d electrons occupy the e_g orbitals and are mobile. To study the formation of the polaron we start with pure $CaMnO_3$ ($x = 1$), where only the t_{2g} orbitals are filled, and imagine that *one* additional electron is injected into the system (*e.g.*, by replacing one Ca ion by La). The extra electron must go into the e_g levels and, by virtue of symmetry, may couple to the e_g normal vibrations of the octahedral complex. This type of vibronic

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interaction, where both the electron and the vibrational modes are of e_g symmetry, is referred to as $E \bigotimes e$ JT coupling. In addition, the electron is allowed to move in a band composed of the local e_g doublets. The resulting quasiparticle, consisting of the mobile e_g electron and the concomitant e_g distortion of the MnO_6 octahedra, is designated as $E \bigotimes e$ JT polaron. A somewhat simpler system, the $E \bigotimes b$ JT polaron, where b denotes a non-degenerate representation of the tetragonal site group, has already been treated by Höck, Nickisch and Thomas [11] nearly two decades ago.

In Section 2 we introduce our model, together with the angular momentum operator $\mathcal{J}$ and the parity operator $\mathcal{K}$. Since only linear JT coupling is considered, these operators commute with the JT Hamiltonian, but not with the (anisotropic) hopping term. In Section 3 we show that $\mathcal{K}$ generates new fermion operators such that both $\mathcal{J}$ and the JT term assume diagonal form with respect to the new fermionic basis. The spectrum of $\mathcal{J}$ is determined in Section 4, where we recover the well-known result that all eigenvalues of $\mathcal{J}$ are half-integral. We also show by rather general arguments that each eigenvalue of the JT Hamiltonian is still twofold degenerate. This degeneracy will be lifted by the hopping term. In Section 5 we construct a representation of the original Hamiltonian on a new Hilbert space, which is isomorphic to an eigenspace of $\mathcal{J}$ belonging to a fixed angular momentum eigenvalue $j > 0$. The new Hamiltonian depends explicitly on this quantum number and decomposes into a quasi-Holstein term and a residual JT interaction. This is the optimal form, which can be reached by purely analytic means, and elucidates the close relationship between the JT and the Holstein polaron. While the latter is obtained for the "unphysical" value $j = 0$, the ground state of the JT polaron is shown to belong to the sector $j = 1/2$. A variational treatment of the new Hamiltonian is outlined in Section 6, where also some ground-state properties like the dispersion relations and effective masses for both kinds of polarons are presented. Our results are summarized in Section 7.

2 The model Hamiltonian

In the $E \bigotimes e$ JT polaron the state of the electron is completely specified by the vectors $|i\gamma\rangle$, where i denotes the cell index and $\gamma = x, z$ the components of the e_g doublet (spin indices are omitted since only a single e_g electron is considered). The wave functions $\langle \boldsymbol{r}|ix\rangle$ and $\langle \boldsymbol{r}|iz\rangle$ transform like the orbitals $d_{x^2-y^2}$ and $d_{3z^2-r^2}$, respectively, forming a local basis of the E_g representation associated with each unit cell. The state of the electron may be more conveniently specified by the operators $e^\dagger_{i\gamma}$ and $e_{i\gamma}$, where $e^\dagger_{i\gamma}$ ($e_{i\gamma}$) creates (annihilates) an e_g electron in the orbital state $\gamma = x$ or z at lattice site i. Similarly, the e_g distortions of the MnO_6 octahedra may be described either in terms of the local normal coordinates $Q_{i\gamma}$ or, more conveniently, by the bosonic creation and annihilation operators $a^\dagger_{i\gamma}$ and $a_{i\gamma}$, respectively, where the indices have the same meaning as above. The Hamiltonian used for the description of the $E \bigotimes e$ JT polaron reads

$$\mathcal{H} = \mathcal{H}_t + \mathcal{H}_v + \mathcal{H}_{\mathrm{JT}}, \tag{1}$$

where

$$\mathcal{H}_t = -t \sum_{ia} \boldsymbol{e}_i{}^\dagger \cdot \mathbf{h}_a \cdot \boldsymbol{e}_{i+a} \tag{2a}$$

is the transfer or hopping term to be discussed below,

$$\mathcal{H}_v = \hbar\Omega \sum_i \boldsymbol{a}_i{}^\dagger \cdot \boldsymbol{a}_i \tag{2b}$$

describes the e_g normal vibrations of frequency Ω, while

$$\mathcal{H}_{JT} = g\hbar\Omega \sum_i \boldsymbol{e}_i{}^\dagger \left[(a^\dagger_{ix} + a_{ix})\sigma^x - (a^\dagger_{iz} + a_{iz})\sigma^z \right] \boldsymbol{e}_i \tag{2c}$$

represents the $E \bigotimes e$ JT coupling, where σ^a $(a = x, y, z)$ are the Pauli matrices and the coupling strength is expressed by the dimensionless parameter g. The column vectors

$$\boldsymbol{e}_i = \begin{pmatrix} e_{iz} \\ e_{ix} \end{pmatrix} \quad \text{and} \quad \boldsymbol{a}_i = \begin{pmatrix} a_{iz} \\ a_{ix} \end{pmatrix}, \tag{3}$$

as well as their associated row vectors $\boldsymbol{e}_i{}^\dagger$ and $\boldsymbol{a}_i{}^\dagger$, have been introduced for convenience and to avoid an accumulation of indices.

The somewhat unusual form of the hopping term (2a), where the summation over a runs over the six nearest neighbors of site i, originates from the orbital degeneracy of the electronic states. In orbitally degenerate systems the transfer of electrons between neighboring sites depends on the orientation of the orbitals and the direction of the transfer. The matrix elements $h_a^{\gamma\gamma'}$ of the matrices $\mathbf{h}_a$ are entirely determined by symmetry. Their numerical values along the three cubic axes are tabulated in reference [12], where the interatomic matrix element $V_{dd\sigma}$ is related to our hopping integral t. In the electronic basis defined by the vector $\boldsymbol{e}_i$ in equations (3), the matrices $\mathbf{h}_a$ take the explicit form

$$\begin{aligned} \mathbf{h}_{\pm x} &= (2\sigma^0 - \sqrt{3}\sigma^x - \sigma^z)/4, \\ \mathbf{h}_{\pm y} &= (2\sigma^0 + \sqrt{3}\sigma^x - \sigma^z)/4, \\ \mathbf{h}_{\pm z} &= (\sigma^0 + \sigma^z)/2, \end{aligned} \tag{4}$$

where σ^0 denotes the 2×2 unit matrix.

In equation (2c) we have restricted ourselves to linear JT coupling, adopted by the majority of authors [13,14]. Moreover, our model does not contain the intersite coupling of the normal modes, which one intuitively expects since oxygens are shared between adjacent MnO_6 octahedra. These coupling terms will give rise to optical phonon branches and, as was recently pointed out by Hotta *et al.* [15] and Popovic and Satpathy [16], to collective effects such as orbital ordering. Other terms like, *e.g.*, the Hund's rule coupling should also be included in

a more rigorous treatment. Hence, our model is probably too simplistic for a fair description of the manganites; we hope to include the neglected terms in future work.

Since $\mathcal{H}$ is invariant under lattice translations, the total crystal momentum $\mathbf{P} = \mathbf{K} + \mathbf{Q}$ is a conserved quantity. Here the operators $\mathbf{K} = \sum_{\mathbf{k}} \mathbf{k}\, \boldsymbol{e}_{\mathbf{k}}{}^{\dagger} \cdot \boldsymbol{e}_{\mathbf{k}}$ and $\mathbf{Q} = \sum_{\mathbf{q}} \mathbf{q}\, \boldsymbol{a}_{\mathbf{q}}{}^{\dagger} \cdot \boldsymbol{a}_{\mathbf{q}}$ denote the crystal momenta of the electron and the e_g vibrational modes, respectively, where $\boldsymbol{e}_{\mathbf{k}}$ and $\boldsymbol{a}_{\mathbf{q}}$ are the Fourier transforms of $\boldsymbol{e}_i$ and $\boldsymbol{a}_i$. In addition to $\mathbf{P}$, there are operators which commute with $\mathcal{H}_v$ and $\mathcal{H}_{JT}$, but not with the hopping term (unless $\mathcal{H}_t$ is assumed to be isotropic). Although these operators are not strictly conserved, they often greatly facilitate the diagonalization of $\mathcal{H}$, as we shall see below. There are two operators of this kind which prove particularly useful:
(i) the *parity operator*

$$\mathcal{K} = \mathcal{G}\mathcal{R}, \tag{5a}$$

where

$$\mathcal{G} = \exp\left(\mathrm{i}\pi \sum_i \boldsymbol{a}_i{}^{\dagger} \cdot \boldsymbol{a}_i\right) \tag{5b}$$

and

$$\mathcal{R} = \exp\left[i(\pi/2) \sum_i \boldsymbol{e}_i{}^{\dagger} \cdot (\sigma^y - \sigma^0) \cdot \boldsymbol{e}_i\right]; \tag{5c}$$

(ii) the *angular momentum operator*

$$\mathcal{J} = \mathcal{M} - \frac{1}{2} \sum_i \boldsymbol{e}_i{}^{\dagger} \cdot \sigma^y \cdot \boldsymbol{e}_i, \tag{6a}$$

where

$$\mathcal{M} = \sum_i \boldsymbol{a}_i{}^{\dagger} \cdot \sigma^y \cdot \boldsymbol{a}_i \tag{6b}$$

is referred to as vibrational angular momentum. The spectral properties of these operators will be discussed in the following sections. Here it suffices to mention that quantities similar to $\mathcal{K}$ and $\mathcal{J}$ also play an important role in isolated $E \bigotimes e$ JT centers, provided the JT coupling is *linear* [17]. In such systems the only eigenvalues of $\mathcal{K}$ are 1 and -1, whereas those of $\mathcal{J}$ range over all half-odd integers. The most important properties of the operator $\mathcal{K}$ may be summarized by the equations

$$\mathcal{K}^{\dagger} \boldsymbol{e}_i \mathcal{K} = \sigma^y \cdot \boldsymbol{e}_i, \quad \mathcal{K}^{\dagger} \boldsymbol{a}_i \mathcal{K} = -\boldsymbol{a}_i, \tag{7}$$

whose derivation rests on the well-known commutator expansion

$$\mathrm{e}^{S} A \mathrm{e}^{-S} = A + [S, A] + (2!)^{-1}[S, [S, A]] + \cdots$$

Using (7) we see that both $\mathcal{H}_v + \mathcal{H}_{JT}$ and $\mathcal{J}$ are left invariant by $\mathcal{K}$, *i.e.*, $\mathcal{H}_v + \mathcal{H}_{JT}$, $\mathcal{K}$ and $\mathcal{J}$ form a complete set of commuting operators:

$$[\mathcal{H}_v + \mathcal{H}_{JT}, \mathcal{K}] = [\mathcal{H}_v + \mathcal{H}_{JT}, \mathcal{J}] = [\mathcal{K}, \mathcal{J}] = 0. \tag{8}$$

3 Generation of new fermion operators

In this section we shall exploit the properties of the parity operator $\mathcal{K}$ to generate new fermionic creation and annihilation operators such that $\mathcal{H}_{JT}$ and $\mathcal{J}$ take diagonal form with respect to these operators. To this end we need another property of $\mathcal{K}$, which reads

$$\mathcal{K}^2 = 1 \tag{9}$$

and readily follows from equations (7) and the relation $(\sigma^a)^2 = \sigma^0$ valid for all Pauli matrices. Hence, as in an isolated JT center, the only eigenvalues of $\mathcal{K}$ are $\kappa = \pm 1$. Moreover, since $\mathcal{K}$ is also unitary, we have the additional relations $\mathcal{K} = \mathcal{K}^{-1} = \mathcal{K}^{\dagger}$.

As the next step, we need the projection operator $\mathcal{P}_\kappa$ for selecting the subspace associated with the eigenvalue κ of $\mathcal{K}$. According to Löwdin [18], $\mathcal{P}_\kappa$ is given by the expression

$$\mathcal{P}_\kappa = \frac{1}{2}(1 + \kappa\mathcal{K}) \quad (\kappa = \pm 1), \tag{10}$$

which, apart from being Hermitian, has the properties

$$\sum_\kappa \mathcal{P}_\kappa = 1, \tag{11a}$$

$$\mathcal{P}_\kappa \mathcal{P}_{\kappa'} = \delta_{\kappa\kappa'} \mathcal{P}_\kappa. \tag{11b}$$

We also have the obvious relation $\mathcal{K}\mathcal{P}_\kappa = \kappa\mathcal{P}_\kappa$, implying that the subspace projected out by $\mathcal{P}_\kappa$ is an eigenspace of $\mathcal{K}$ to the eigenvalue κ. Property (11a) allows us to decompose the Hamiltonian and the angular momentum operator $\mathcal{J}$ into components acting on the eigenspaces of $\mathcal{K}$ as follows

$$\mathcal{H} = \sum_{\kappa\kappa'} \mathcal{P}_\kappa \mathcal{H}_t \mathcal{P}_{\kappa'} + \mathcal{H}_v + \sum_\kappa \mathcal{P}_\kappa \mathcal{H}_{JT} \mathcal{P}_\kappa, \tag{12a}$$

$$\mathcal{J} = \sum_\kappa \mathcal{P}_\kappa \mathcal{J} \mathcal{P}_\kappa, \tag{12b}$$

where we have used equation (11b) and the fact that $\mathcal{H}_v$, $\mathcal{H}_{JT}$, and $\mathcal{J}$ commute with $\mathcal{P}_\kappa$. Since the hopping term does not commute with $\mathcal{K}$, the eigenspaces of the latter are mixed by $\mathcal{H}_t$, as was to be expected.

To obtain equations (12) in explicit form, we need to calculate the operators $\boldsymbol{e}_i \mathcal{P}_\kappa$. Using (7) and (10) we find

$$\boldsymbol{e}_i \mathcal{P}_\kappa = \frac{1}{2}(\sigma^0 + \kappa\sigma^y\mathcal{K}) \cdot \boldsymbol{e}_i = \frac{1}{2}\begin{pmatrix} e_{iz} - i\kappa\mathcal{K}e_{ix} \\ e_{ix} + i\kappa\mathcal{K}e_{iz} \end{pmatrix}, \tag{13}$$

and we shall now prove that the products $\mathcal{K}e_{i\gamma}$ ($\gamma = x, z$) on the right side of equation (13) may be replaced by $\mathcal{G}e_{i\gamma}$, where $\mathcal{G}$ is defined by equation (5b). To show this, let $|\Psi\rangle$ be an arbitrary vector of the underlying *single-particle* Hilbert space,

$$|\Psi\rangle = \sum_{i\gamma} \Psi_{i\gamma} e^{\dagger}_{i\gamma} |0\rangle, \tag{14}$$

where $\Psi_{i\gamma}$ are pure functions of the Bose operators $a_{i\gamma}$, $a_{i\gamma}^\dagger$ and $|0\rangle$ denotes the common vacuum for all particles. If $\mathcal{K}e_{i\gamma}$ is now applied to $|\Psi\rangle$ and use is made of the fact that $\mathcal{R}$ of equation (5c) commutes with $\Psi_{i\gamma}$ ($\gamma = x, z$), the result is

$$\mathcal{K}e_{i\gamma}|\Psi\rangle = \mathcal{K}\Psi_{i\gamma}|0\rangle = \mathcal{G}\Psi_{i\gamma}|0\rangle = \mathcal{G}e_{i\gamma}|\Psi\rangle\cdot$$

Hence, $\mathcal{K}e_{i\gamma} = \mathcal{G}e_{i\gamma}$ on the entire Hilbert space, which proves our claim. Expression (13) may thus be rewritten as

$$\boldsymbol{e}_i\mathcal{P}_\kappa = \frac{1}{2}\begin{pmatrix} e_{iz} - i\kappa\mathcal{G}e_{ix} \\ e_{ix} + i\kappa\mathcal{G}e_{iz}\end{pmatrix} = \boldsymbol{u}_\kappa d_{i\kappa}, \tag{15a}$$

where

$$\boldsymbol{u}_\kappa = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i\kappa\mathcal{G}\end{pmatrix} \tag{15b}$$

is a normalized vector (*i.e.*, $\boldsymbol{u}_\kappa{}^\dagger \cdot \boldsymbol{u}_\kappa = 1$), while the quantities

$$d_{i\kappa} = \frac{1}{\sqrt{2}}(e_{iz} - i\kappa\mathcal{G}e_{ix}) \tag{15c}$$

behave like ordinary fermion operators, *i.e.*,

$$[d_{i\kappa}, d_{j\kappa'}^\dagger]_+ = \delta_{ij}\delta_{\kappa\kappa'}, \quad [d_{i\kappa}, d_{j\kappa'}]_+ = 0. \tag{16}$$

However, due to the presence of the operator $\mathcal{G}$ in equation (15c), the $d_{i\kappa}$, $d_{i\kappa}^\dagger$ *cease to commute* with the Bose operators $a_{i\gamma}$ and $a_{i\gamma}^\dagger$, but continue to commute with quadratic forms like $\mathcal{G}$ and the vibrational angular momentum $\mathcal{M}$ of equation (6b).

With the help of equations (15), the various parts of the Hamiltonian (12a) may now be expressed in terms of the new fermion operators $d_{i\kappa}$ and $d_{i\kappa}^\dagger$ ($\kappa = \pm 1$). We start with the hopping term $\mathcal{H}_t$, which is transformed into

$$\mathcal{H}_t = -t\sum_{ia}\sum_{\kappa\kappa'} d_{i\kappa}^\dagger \tau_a^{\kappa\kappa'} d_{i+a,\kappa'}, \tag{17a}$$

$$\tau_a^{\kappa\kappa'} = \boldsymbol{u}_\kappa{}^\dagger \cdot \mathbf{h}_a \cdot \boldsymbol{u}_{\kappa'}, \tag{17b}$$

where the matrices $\mathbf{h}_a$ are given by equations (4). In the basis defined by the vector $\boldsymbol{d}_i = \binom{d_{i+}}{d_{i-}}$, equations (17) may also be written as

$$\mathcal{H}_t = -t\sum_{ia} \boldsymbol{d}_i{}^\dagger \cdot \boldsymbol{\tau}_a \cdot \boldsymbol{d}_{i+a}, \tag{18a}$$

where the new hopping matrices $\boldsymbol{\tau}_a$ read

$$\begin{aligned} \boldsymbol{\tau}_{\pm x} &= (2\sigma^0 - \sigma^x - \sqrt{3}\mathcal{G}\sigma^y)/4, \\ \boldsymbol{\tau}_{\pm y} &= (2\sigma^0 - \sigma^x + \sqrt{3}\mathcal{G}\sigma^y)/4, \\ \boldsymbol{\tau}_{\pm z} &= (\sigma^0 + \sigma^x)/2, \end{aligned} \tag{18b}$$

being now explicit functions of the operator $\mathcal{G}$. The vibrational part $\mathcal{H}_v$ remains unchanged, while the JT coupling takes the form

$$\mathcal{H}_{JT} = g\hbar\Omega\sum_{i\kappa} d_{i\kappa}^\dagger[i\kappa(a_{ix}^\dagger + a_{ix})\mathcal{G} - (a_{iz}^\dagger + a_{iz})]d_{i\kappa}. \tag{19}$$

In deriving this result we have used the relations $a_{i\gamma}\boldsymbol{u}_\kappa = \boldsymbol{u}_{-\kappa}a_{i\gamma}$, $\boldsymbol{u}_\kappa{}^\dagger \cdot \sigma^x \cdot \boldsymbol{u}_{-\kappa} = -i\kappa\mathcal{G}$, and $\boldsymbol{u}_\kappa{}^\dagger \cdot \sigma^z \cdot \boldsymbol{u}_{-\kappa} = 1$. Finally, the angular momentum operator $\mathcal{J}$ of equation (12b) is obtained as

$$\mathcal{J} = \mathcal{M} - (\mathcal{G}/2)\sum_{i\kappa}\kappa d_{i\kappa}^\dagger d_{i\kappa}, \tag{20a}$$

and we see that $\mathcal{H}_{JT}$ and $\mathcal{J}$ are now *diagonal* with respect to the new fermion operators. The vibrational part of $\mathcal{J}$ is, however, still nondiagonal. The diagonalization of $\mathcal{M}$ is readily accomplished by means of the substitutions

$$\begin{aligned} a_{iz} &\to \frac{1}{\sqrt{2}}(a_{iz} + a_{ix}), \\ a_{ix} &\to \frac{-i}{\sqrt{2}}(a_{iz} - a_{ix}), \end{aligned}$$

which leave $\mathcal{H}_t$ and $\mathcal{H}_v$ invariant, while $\mathcal{M}$ is brought to the diagonal form

$$\mathcal{M} = \sum_i (a_{ix}^\dagger a_{ix} - a_{iz}^\dagger a_{iz}) = \sum_i \mathcal{M}_i. \tag{20b}$$

The JT coupling is transformed into the expression

$$\mathcal{H}_{JT} = -\sqrt{2}g\hbar\Omega\sum_{i\kappa} d_{i\kappa}^\dagger(a_{ix}\Pi_\kappa + a_{iz}\Pi_{-\kappa} + \text{h.c.})d_{i\kappa}, \tag{21}$$

where the new projection operators

$$\Pi_\kappa = \frac{1}{2}(1 + \kappa\mathcal{G}) \quad (\kappa = \pm 1) \tag{22}$$

have been introduced. For later purposes we need the properties

$$\Pi_\kappa a_{i\gamma} = a_{i\gamma}\Pi_{-\kappa}, \tag{23a}$$

$$\Pi_\kappa\Pi_{\kappa'} = \delta_{\kappa\kappa'}\Pi_\kappa, \tag{23b}$$

$$\Pi_\kappa + \Pi_{-\kappa} = 1, \tag{23c}$$

$$\Pi_\kappa - \Pi_{-\kappa} = \kappa\mathcal{G}, \tag{23d}$$

which follow immediately from definition (22). Before we set out to develop strategies for dealing with the complicated vibrational terms in $\mathcal{H}_{JT}$, we shall first derive the spectrum of $\mathcal{J}$ and investigate the possible symmetries and degeneracies of the JT Hamiltonian.

4 Symmetries and degeneracies

In isolated JT centers there often exist "hidden" symmetries giving rise to unexpected degeneracies of the energy levels. In the linearly coupled $E \bigotimes e$ JT center, *e.g.*, all eigenvalues are twofold degenerate, and higher-order coupling terms are necessary to (partially) remove the degeneracy [1]. This section is devoted to a study of these degeneracies in JT crystals like the manganites.

To investigate the possible symmetries of our system, we first need the spectrum of the angular momentum operator $\mathcal{J}$, equations (20). Since $\mathcal{J}$, $\mathcal{K}$, and $\mathcal{H}_v$ commute with each other, these operators possess common eigenstates. The latter are of the form

$$|\Psi^0_{nj\kappa}\rangle = \sum_i C_{i\kappa} d^\dagger_{i\kappa} \prod_i |n_i, m_i\rangle \quad (\kappa = \pm 1), \tag{24a}$$

where $C_{i\kappa}$ are coefficients and the product extends over the local eigenstates of the isotropic oscillator in two dimensions [19]:

$$|n_i, m_i\rangle = \frac{(a^\dagger_{ix})^{(n_i+m_i)/2}(a^\dagger_{iz})^{(n_i-m_i)/2}}{\sqrt{(\frac{n_i+m_i}{2})!\,(\frac{n_i-m_i}{2})!}}|0\rangle, \tag{24b}$$

$$n_i = 0, 1, 2, \cdots;\ m_i = n_i, n_i - 2, \cdots, -n_i. \tag{24c}$$

In fact, a simple calculation shows that $|\Psi^0_{nj\kappa}\rangle$ is an eigenstate of $\mathcal{K}$, $\mathcal{J}$, and $\mathcal{H}_v$ with the respective eigenvalues κ, j_κ, and $E^0_{nj\kappa}$, where

$$E^0_{nj\kappa} = n\hbar\Omega, \quad j_\kappa = m - \frac{\kappa}{2}(-1)^n, \tag{25a}$$

$$n = \sum_i n_i, \quad m = \sum_i m_i. \tag{25b}$$

There are many other linearly independent eigenvectors of $\mathcal{K}$, $\mathcal{J}$, and $\mathcal{H}_v$ belonging to the same eigenvalues: all vectors of the form (24a), whose quantum numbers n_i and m_i satisfy the constraints (24c) and (25b), are also eigenstates with the required properties. Together they span a vector space $\mathcal{U}^0_j$, and we see that the energies $E^0_{nj\kappa}$ are highly degenerate [20].

For a single site we have the relation $m_i = n_i - 2p_i$ ($p_i = 0, 1, \cdots, n_i$) which, after summation over all cells, becomes $m = n - 2p$ ($p = 0, 1, \cdots, n$). Thus, for a given n, the quantum number m may take the $n+1$ integral values $m = n, n-2, \cdots, -n$, whence we conclude that the angular momentum quantum numbers j_κ must all be *half-integral*, as in an isolated $E \bigotimes e$ JT center with linear coupling [1]. A more detailed analysis of j_κ, equation (25a), requires a distinction between even and odd n (n and m always have the same parity, both being either even or odd). It is not difficult to verify that, for fixed κ, both cases yield the same eigenvalues j_κ so that we may restrict ourselves to even m (n). The angular momentum quantum numbers may thus also be written as

$$j_\kappa = m - \kappa/2 \quad (m = 0, \pm 2, \pm 4, \cdots)$$

or, explicitly:

$$j_\kappa = \begin{cases} \cdots, -5/2, -1/2, 3/2, 7/2, \cdots & \kappa = 1 \\ \cdots, -7/2, -3/2, 1/2, 5/2, \cdots & \kappa = -1. \end{cases} \tag{26}$$

We now set out to examine more closely the structure of $\mathcal{J}$ and $\mathcal{H}_{JT}$ which, for the present purpose, are written as $\mathcal{J} = \sum_\kappa \mathcal{J}^{(\kappa)}$ and $\mathcal{H}_{JT} = \sum_\kappa \mathcal{H}^{(\kappa)}_{JT}$. A glance at equations (20) and (21) then reveals that the substitution $d_{i\kappa} \to d_{i,-\kappa}$, combined with the interchange $a_{ix} \leftrightarrow a_{iz}$ (these operations correspond to canonical transformations and, hence, do not affect the eigenvalues), has the effect that $\mathcal{H}^{(\kappa)}_{JT} \to \mathcal{H}^{(-\kappa)}_{JT}$ and $\mathcal{J}^{(\kappa)} \to -\mathcal{J}^{(-\kappa)}$. Denoting the eigenvalues of $\mathcal{H}^{(\kappa)}_{JT}$ and $\mathcal{J}^{(\kappa)}$ by $E_{nj\kappa}$ and j_κ, respectively, and the common eigenvectors of these operators by $|\Psi_{nj\kappa}\rangle$, we may thus draw the following conclusions:

1. $\mathcal{H}^{(+)}_{JT}$ and $\mathcal{H}^{(-)}_{JT}$ have the same eigenvalues which must, therefore, be independent of κ: $E_{nj\kappa} = E_{nj}$. Since the corresponding eigenvectors $|\Psi_{nj+}\rangle$ and $|\Psi_{nj-}\rangle$ are orthogonal by virtue of equation (11b), each eigenvalue E_{nj} of $\mathcal{H}_{JT}$ is necessarily *twofold degenerate*.
2. The spectra of $\mathcal{J}^{(+)}$ and $\mathcal{J}^{(-)}$ have the property that to any positive eigenvalue j_+ of $\mathcal{J}^{(+)}$ there is always a negative eigenvalue $j_- = -j_+$ of $\mathcal{J}^{(-)}$ and *vice versa*. This property is most clearly reflected by equation (26). Since the eigenvalues of $\mathcal{H}_{JT}$ are independent of κ, they can only depend on $j \equiv |j_\kappa| = 1/2, 3/2, 5/2, \cdots$

Thus, we see that the huge degeneracy of the eigenvalues $E^0_{nj\kappa}$ of $\mathcal{H}_v$ (see Ref. [20]) is nearly completely lifted by the JT Hamiltonian. The remaining twofold degeneracy of $\mathcal{H}_{JT}$, which is of the same origin as that in the linearly coupled $E \bigotimes e$ JT center, will be removed by the hopping term $\mathcal{H}_t$ (apart from accidental degeneracy).

Only relatively few of the vectors contained in $\mathcal{U}^0_j$ are simultaneous eigenstates of $\mathcal{J}$ and $\mathcal{H}_{JT}$. To find these eigenvectors, we shall take advantage of the existence of a simple operator $\mathcal{C}$, which also commutes with $\mathcal{J}$ and is of help to select the proper candidates. This operator will be shown in Section 5 to emerge from the JT Hamiltonian and reads

$$\mathcal{C} = \sum_{i\kappa} d^\dagger_{i\kappa}(1 - \kappa\mathcal{G}\mathcal{M}_i)d_{i\kappa}. \tag{27}$$

There are, in fact, *two* orthogonal sets of eigenstates both belonging to the *same* quantum number j, but to *different* eigenvalues of $\mathcal{C}$. For *positive* j the two sets are represented by the vectors (similar vectors have been constructed in Ref. [21])

$$|\Psi^+_{nj\kappa}\rangle = \sum_i \sum_{n_i=0}^{\infty} C^+_{i\kappa}(n_i) d^\dagger_{i\kappa} |m + 2n_i, m\rangle \prod_{l\neq i} |0_l, 0_l\rangle, \tag{28a}$$

$$|\Psi^-_{nj\kappa}\rangle = \sum_i \sum_{n_i=0}^{\infty} C^-_{i\kappa}(n_i) d^\dagger_{i\kappa} |m+2n_i+1, m+1\rangle \prod_{l\neq i} |0_l, 0_l\rangle, \tag{28b}$$

where m is the *same* for all i and may assume the values

$$m = j - 1/2 = 0, 1, 2, \cdots \tag{28c}$$

It is then straightforward to verify the eigenvalue equations

$$\mathcal{J}|\Psi^\pm_{nj\kappa}\rangle = j|\Psi^\pm_{nj\kappa}\rangle, \tag{29a}$$

$$\mathcal{C}|\Psi^\pm_{nj\kappa}\rangle = (1/2 \pm j)|\Psi^\pm_{nj\kappa}\rangle, \tag{29b}$$

whose validity requires that

$$\kappa = -(-1)^m = (-1)^{j+1/2}. \tag{29c}$$

Common eigenstates of $\mathcal{J}$ and $\mathcal{C}$ for negative j also exist, but are not needed here.

Hence, the vectors $|\Psi^{\pm}_{nj\kappa}\rangle$ are common eigenstates of $\mathcal{J}$ and $\mathcal{C}$. Physically they represent *polaronic* states, where the electron is accompanied by an on-site distortion (vibrational excitation) of the molecular complex, all other complexes not coinciding with the location of the electron being left in their vibrational ground states. All vectors (28a), where m is given and κ is fixed by equation (29c), form a subspace $\mathcal{U}_j^+$, while those obtained from $|\Psi^-_{nj\kappa}\rangle$ span a subspace $\mathcal{U}_j^-$, which is orthogonal to $\mathcal{U}_j^+$. The direct sum of these spaces will be denoted as $\mathcal{U}_j$ to remind us that this is an eigenspace of $\mathcal{J}$ to the eigenvalue $j = m+1/2 > 0$. Since this is the most general eigenspace, which is compatible with the existence of the operator $\mathcal{C}$, the simultaneous eigenvectors $|\Psi_{nj\kappa}\rangle$ of $\mathcal{H}_{JT}$ and $\mathcal{J}$ are necessarily all contained in $\mathcal{U}_j$.

5 Representation of $\mathcal{H}$ for fixed quantum number j

Our main goal in this section is to construct a *representation* of the Hamiltonian on a subspace $\mathcal{V}_j$, which is defined to be isomorphic to the space $\mathcal{U}_j$ introduced at the end of the preceding section. We start with the JT term, whose representation rests on the operators

$$\mathcal{A} = \sqrt{2}\sum_{i\kappa} d^\dagger_{i\kappa}(a_{ix}\Pi_\kappa + a_{iz}\Pi_{-\kappa})d_{i\kappa}, \tag{30a}$$

$$\mathcal{A}^\dagger = \sqrt{2}\sum_{i\kappa} d^\dagger_{i\kappa}(a^\dagger_{ix}\Pi_{-\kappa} + a^\dagger_{iz}\Pi_\kappa)d_{i\kappa}, \tag{30b}$$

allowing the JT Hamiltonian (21) to be written in the simple form

$$\mathcal{H}_{\rm JT} = -g\hbar\Omega(\mathcal{A} + \mathcal{A}^\dagger). \tag{31}$$

The merits of this seemingly trivial reformulation will become obvious later on. As the next step, we calculate the products $\mathcal{A}\mathcal{A}^\dagger$ and $\mathcal{A}^\dagger\mathcal{A}$. Using properties (23a) and (23b) we find the expressions

$$\mathcal{A}\mathcal{A}^\dagger = 2\sum_{i\kappa} d^\dagger_{i\kappa}(1 + a^\dagger_{ix}a_{ix}\Pi_{-\kappa} + a^\dagger_{iz}a_{iz}\Pi_\kappa)d_{i\kappa}, \tag{32a}$$

$$\mathcal{A}^\dagger\mathcal{A} = 2\sum_{i\kappa} d^\dagger_{i\kappa}(a^\dagger_{ix}a_{ix}\Pi_\kappa + a^\dagger_{iz}a_{iz}\Pi_{-\kappa})d_{i\kappa}, \tag{32b}$$

which enable us to set up the commutator $[\mathcal{A}, \mathcal{A}^\dagger]$ and the anticommutator $[\mathcal{A}, \mathcal{A}^\dagger]_+$. Using properties (23c) and (23d) we obtain

$$\frac{1}{2}[\mathcal{A}, \mathcal{A}^\dagger] = \sum_{i\kappa} d^\dagger_{i\kappa}(1 - \kappa\mathcal{G}\mathcal{M}_i)d_{i\kappa} \equiv \mathcal{C}, \tag{33a}$$

$$\frac{1}{2}[\mathcal{A}, \mathcal{A}^\dagger]_+ = \sum_{i\kappa} d^\dagger_{i\kappa}(1 + \boldsymbol{a}_i{}^\dagger \cdot \boldsymbol{a}_i)d_{i\kappa} \equiv \mathcal{N}, \tag{33b}$$

where $\mathcal{C} = \frac{1}{2}[\mathcal{A}, \mathcal{A}^\dagger]$ is the operator (27), whose eigenvalue problem is given by equation (29b). The result may be restated as follows: on the subspace $\mathcal{U}_j^+$ the operator $\mathcal{C}$ reduces to a positive integer and takes the form

$$\frac{1}{2}[\mathcal{A}, \mathcal{A}^\dagger] = \mathcal{C} = m + 1 = j + 1/2 \quad (m \geq 0), \tag{34}$$

whereas on $\mathcal{U}_j^-$ it reduces to the number $1/2 - j$, which is negative for all $j > 1/2$. To appreciate this result, we now investigate the anticommutator $\mathcal{N}$, equation (33b). First of all one realizes that $\mathcal{N}$ is a *positive* operator. This property, together with the identity

$$\mathcal{N} = \mathcal{A}^\dagger\mathcal{A} + \mathcal{C}, \tag{35a}$$

imposes a constraint on $\mathcal{C}$ requiring that this must also be a positive operator. The only way to guarantee that $\mathcal{C}$ and, hence, $\mathcal{N}$ are positive for all $j \geq 1/2$ is to restrict the commutator to the subspace $\mathcal{U}_j^+$ as in equation (34).

Particularly interesting are the commutators $[\mathcal{N}, \mathcal{A}]$ and $[\mathcal{N}, \mathcal{A}^\dagger]$, since they agree with those of ordinary Bose operators [22]. In fact, using equations (30) and (33b) one obtains

$$[\mathcal{N}, \mathcal{A}] = -\mathcal{A}, \quad [\mathcal{N}, \mathcal{A}^\dagger] = \mathcal{A}^\dagger. \tag{35b}$$

We also need to express $\mathcal{H}_v$ in terms of the operators $\mathcal{A}$ and $\mathcal{A}^\dagger$. To this end we calculate the expectation value of $\mathcal{N}$ in the state $|i\kappa\rangle = d^\dagger_{i\kappa}|0\rangle_e$, where $|0\rangle_e$ denotes the *electronic* vacuum. The result is $\langle i\kappa|\mathcal{N}|i\kappa\rangle = 1 + \boldsymbol{a}_i{}^\dagger \cdot \boldsymbol{a}_i$ which, after summation over all sites, yields

$$\mathcal{H}_v = \hbar\Omega\sum_i(\langle i\kappa|\mathcal{N}|i\kappa\rangle - 1). \tag{36}$$

We are now in a position to construct the desired representation of the JT Hamiltonian, as defined at the beginning of this section. Our idea is to map the Hilbert space $\mathcal{U}_j$ onto a new space $\mathcal{V}_j$, isomorphic to $\mathcal{U}_j$, and to construct operators on the new space satisfying the same relations as $\mathcal{A}$ and $\mathcal{A}^\dagger$ on $\mathcal{U}_j$ (this procedure is closely related to that employed in the bosonization of spin operators). The new space $\mathcal{V}_j$ is spanned by all vectors of the form

$$|\Phi^+_{nj\kappa}) = \sum_i \sum_{n_i=0}^{\infty} C^+_{i\kappa}(n_i)c^\dagger_{i\kappa}\frac{(b_i^\dagger)^{2n_i}}{\sqrt{(2n_i)!}}|0), \tag{37a}$$

$$|\Phi^-_{nj\kappa}) = \sum_i \sum_{n_i=0}^{\infty} C^-_{i\kappa}(n_i)c^\dagger_{i\kappa}\frac{(b_i^\dagger)^{2n_i+1}}{\sqrt{(2n_i+1)!}}|0), \tag{37b}$$

where $b_i^\dagger$ and $c^\dagger_{i\kappa}$ create new bosons and fermions, respectively, and $|0)$ is the common vacuum of the new particles. The new fermion operators are similarly defined as our previous $d_{i\kappa}$ of equation (15c):

$$c_{i\kappa} = \frac{1}{\sqrt{2}}(e_{iz} - i\kappa G e_{ix}), \tag{38a}$$

$$G = \exp\left(\mathrm{i}\pi\sum_i b_i^\dagger b_i\right). \tag{38b}$$

The required isomorphism between $\mathcal{U}_j$ and $\mathcal{V}_j$ is achieved by the mapping prescription

$$|\Psi^{\pm}_{nj\kappa}\rangle \leftrightarrow |\Phi^{\pm}_{nj\kappa}), \tag{39}$$

which obviously establishes a one-to-one correspondence between all vectors of $\mathcal{U}_j$ and those of $\mathcal{V}_j$. As in our construction of the space $\mathcal{U}_j$, the new space may also be conceived as the direct sum of two orthogonal subspaces, $\mathcal{V}_j^+$ and $\mathcal{V}_j^-$, spanned by all vectors of the form (37a) and (37b), respectively. The quantum number κ in equations (37) may be assigned the value (29c), but we shall see below that the results are independent of this choice.

On the new space $\mathcal{V}_j$ we now define the operator

$$A_j = \sum_{i\kappa} c^{\dagger}_{i\kappa} A^{(j)}_i b_i c_{i\kappa}, \tag{40a}$$

where $A^{(j)}_i$ is self-adjoint and *explicitly* dependent on the quantum number j:

$$A^{(j)}_i = P_- + \left(1 + \frac{2j}{b_i^{\dagger} b_i + 1}\right)^{1/2} P_+, \tag{40b}$$

$$P_{\pm} = \frac{1}{2}(1 \pm G). \tag{40c}$$

The operators $P_{\pm}$, the analogues of our previous Π_{κ}, satisfy a set of relations differing from equations (23) only in notation (we have, *e.g.*, that $P_{\pm} b_i = b_i P_{\mp}$). We now set out to prove that A_j and $A_j^{\dagger}$ satisfy the same algebraic relations on $\mathcal{V}_j$ as $\mathcal{A}$ and $\mathcal{A}^{\dagger}$ on the space $\mathcal{U}_j$ (another proof of the equivalence of the operators $\mathcal{A}$ and A_j in terms of their matrix elements is given in Appendix A). To this end we start by calculating the products $A_j A_j^{\dagger}$ and $A_j^{\dagger} A_j$. Using the well-known relation $F(b_i^{\dagger} b_i) b_i = b_i F(b_i^{\dagger} b_i - 1)$, we find that

$$A_j A_j^{\dagger} = \sum_{i\kappa} c^{\dagger}_{i\kappa} (b_i^{\dagger} b_i + 2jP_+ + 1) c_{i\kappa}, \tag{41a}$$

$$A_j^{\dagger} A_j = \sum_{i\kappa} c^{\dagger}_{i\kappa} (b_i^{\dagger} b_i + 2jP_-) c_{i\kappa}. \tag{41b}$$

By means of these relations, we may now evaluate the commutator $[A_j, A_j^{\dagger}\,]$ and the anticommutator $[A_j, A_j^{\dagger}\,]_+$. A simple calculation gives

$$\frac{1}{2}[A_j, A_j^{\dagger}\,] = \sum_{i\kappa} c^{\dagger}_{i\kappa} (1/2 + jG) c_{i\kappa} \equiv C_j, \tag{42a}$$

$$\frac{1}{2}[A_j, A_j^{\dagger}\,]_+ = \sum_{i\kappa} c^{\dagger}_{i\kappa} (b_i^{\dagger} b_i + j + 1/2) c_{i\kappa} \equiv N_j, \tag{42b}$$

where C_j and N_j denote the analogues of our previous operators $\mathcal{C}$ and $\mathcal{N}$.

If our formalism is to be meaningful, we expect the commutators $[N_j, A_j\,]$ and $[N_j, A_j^{\dagger}\,]$ to be the same as in equations (35b), differing from the latter only in notation. This is in fact the case, for a straightforward calculation based on equations (40a) and (42b) shows that

$$[N_j, A_j\,] = -A_j, \quad [N_j, A_j^{\dagger}\,] = A_j^{\dagger}, \tag{43}$$

and we recover the Bose-like commutation relations (35b) [22]. It still remains to be verified that the commutator (42a) agrees with that of equation (34). This is readily shown and follows from the observation that on $\mathcal{V}_j^+$ the operator G acts like the unit operator, while on $\mathcal{V}_j^-$ it has the eigenvalue -1. Moreover, since N_j is again a *positive* operator, C_j must also be positive by the same arguments as those used in conjunction with equation (34). Hence, on the allowed subspace $\mathcal{V}_j^+$ the commutator reduces to the positive integer

$$\frac{1}{2}[A_j, A_j^{\dagger}\,] = C_j = j + 1/2, \tag{44}$$

exactly like $\mathcal{C}$ on $\mathcal{U}_j^+$ (see Eq. (34)). Thus, we have shown that the operators A_j, $A_j^{\dagger}$, N_j and $\mathcal{A}$, $\mathcal{A}^{\dagger}$, $\mathcal{N}$ are defined on isomorphic Hilbert spaces and satisfy the same algebra. The two sets are, therefore, physically indistinguishable from each other. In retrospect we realize that relations (43) and (44) do not depend on the sign of κ in equations (37). This independence is important, since it restores the twofold degeneracy of the eigenvalues of the JT Hamiltonian.

The equivalence of the sets $\{A_j,\ A_j^{\dagger},\ N_j\}$ and $\{\mathcal{A},\ \mathcal{A}^{\dagger},\ \mathcal{N}\}$ will now be exploited to construct the desired representation of the Hamiltonian on the space $\mathcal{V}_j$. Consider first the vibrational term $\mathcal{H}_v$, whose representation on $\mathcal{U}_j$ is given by equation (36). To represent $\mathcal{H}_v$ on $\mathcal{V}_j$, we start by using the correspondence $\mathcal{N} \sim N_j$ and $d_{i\kappa} \sim c_{i\kappa}$. Thereby the matrix element $\langle i\kappa|\mathcal{N}|i\kappa\rangle$ is mapped on $(i\kappa|N_j|i\kappa)$, where $|i\kappa) = c^{\dagger}_{i\kappa}|0)_e$ and $|0)_e$ denotes the *electronic* vacuum in $\mathcal{V}_j$. The representation of $\mathcal{H}_v$ on $\mathcal{V}_j$ is then obtained as

$$H_v^{(j)}/(\hbar\Omega) = \sum_i [(i\kappa|N_j|i\kappa) - 1] = \sum_i (b_i^{\dagger} b_i + j - 1/2), \tag{45}$$

where equation (42b) has been used. To find the representation of the JT term, we must go back to equation (31) and exploit the correspondence $\mathcal{A} \sim A_j$. In this way the representation of $\mathcal{H}_{\mathrm{JT}}$ on $\mathcal{V}_j$ is found to be given by the expression

$$H^{(j)}_{\mathrm{JT}}/(\hbar\Omega) = -g(A_j + A_j^{\dagger}) = -g \sum_{i\kappa} c^{\dagger}_{i\kappa} (A^{(j)}_i b_i + \mathrm{h.c.}) c_{i\kappa}, \tag{46}$$

where use has been made of equation (40a). For later purposes it proves more convenient to rewrite $H^{(j)}_{\mathrm{JT}}$ in the form

$$H^{(j)}_{\mathrm{JT}} = H^{(0)}_{\mathrm{JT}} - g\hbar\Omega \sum_{i\kappa} c^{\dagger}_{i\kappa} (P_+ B^{(j)}_i b_i + \mathrm{h.c.}) c_{i\kappa}, \tag{47}$$

where

$$H_{\rm JT}^{(0)} = -g\hbar\Omega \sum_{i\kappa} c_{i\kappa}^{\dagger}(b_i^{\dagger} + b_i)c_{i\kappa} \tag{48a}$$

and

$$B_i^{(j)} = \left(1 + \frac{2j}{b_i^{\dagger}b_i + 1}\right)^{1/2} - 1. \tag{48b}$$

We mention in passing that expressions quite similar to those in equations (45, 47, 48) have been derived for the isolated $E \bigotimes e$ JT center by means of a rather different approach [23]. In the *unphysical* limit $j = 0$ the JT interaction reduces to the displaced-oscillator term $H_{\rm JT}^{(0)}$, since $B_i^{(j)} = 0$ in this case [22]. The hopping term deserves some comment.

In Section 2 it was pointed out that $\mathcal{H}_t$ does *not*, in general, commute with $\mathcal{J}$ implying that $\mathcal{H}_t$ may induce transitions between subspaces belonging to different eigenvalues j of $\mathcal{J}$. However, from the vibrational term (45) it follows that the ground state belongs to $j = 1/2$ and is separated from the state with $j = 3/2$ by the energy $N\hbar\Omega$, which tends to infinity in the thermodynamic limit. This gives rise to a kind of selection rule, allowing transitions only within the ground-state manifold, and we may, therefore, regard $\mathcal{H}_t$ as being restricted to the subspace $\mathcal{U}_{j=1/2}$. Hence, its representation on $\mathcal{V}_{j=1/2}$ takes the form

$$H_t = -t \sum_{ia} \boldsymbol{c}_i{}^{\dagger} \cdot \mathbf{t}_a \cdot \boldsymbol{c}_{i+a}, \tag{49}$$

where the matrices $\mathbf{t}_a$ differ from the $\boldsymbol{\tau}_a$ in equations (18b) only in the replacement of $\mathcal{G}$ by G.

Putting together our findings, the representation of the total Hamiltonian can now be easily written down. For the ground state ($j = 1/2$), the result may be recast into the form

$$H = H_{\rm QH} - g\hbar\Omega \sum_{i\kappa} c_{i\kappa}^{\dagger} \left(P_+ B_i^{(j)} b_i + \text{h.c.}\right) c_{i\kappa}, \tag{50a}$$

where $B_i^{(j)}$ ($j = 1/2$) is defined by equation (48b) and

$$H_{\rm QH} = -t \sum_{ia} \boldsymbol{c}_i{}^{\dagger} \cdot \mathbf{t}_a \cdot \boldsymbol{c}_{i+a} + \hbar\Omega \sum_i b_i^{\dagger}b_i - g\hbar\Omega \sum_{i\kappa} c_{i\kappa}^{\dagger} \left(b_i^{\dagger} + b_i\right) c_{i\kappa} \tag{50b}$$

will be referred to as quasi-Holstein model. Although $H_{\rm QH}$ and the standard Holstein model [24] have the same formal appearance, they differ from each other in two respects. First of all they differ in the hopping term, which is isotropic in the standard model and anisotropic in our case. A more subtle difference lies in the properties of the fermion operators: while those of the standard model commute with the boson operators, this is not the case with the $c_{i\kappa}$, $c_{i\kappa}^{\dagger}$ in equations (50). The peculiar behavior of our fermion operators will, however, not entail any problems in the further analysis.

6 Variational treatment

The structure of the vibrational term (45) led us to conclude that the ground state of the $E \bigotimes e$ JT polaron belongs to $j = 1/2$ and thus agrees with the well-known fact that the lowest state of the isolated $E \bigotimes e$ JT center belongs to the same quantum number [1]. Subsequently our Hamiltonian H of equations (50) will be subjected to a variational treatment, yielding the (approximate) ground-state energy and the corresponding eigenvector for both the JT and the Holstein polaron. From equations (50) we see that the quasi-Holstein model results for $j = 0$, while the JT case is obtained for $j = 1/2$, allowing both types of polarons to be treated in a unified way. A substantial simplification of the Hamiltonian may be achieved by an expansion of the square root in equation (48b) which, for $j = 1/2$, converges for all eigenvalues of $b_i^{\dagger}b_i$. Keeping only terms linear in j, the expansion of $B_i^{(j)}$ becomes

$$B_i^{(j)} = j\left(b_i^{\dagger}b_i + 1\right)^{-1} + O(j^2). \tag{51}$$

Since $B_i^{(j)}$ vanishes for $j = 0$, we expect equation (51) to be reasonable for $j = 1/2$. Indeed, for the isolated $E \bigotimes e$ JT center this turns out to be an excellent approximation [23], and we shall use it in the subsequent analysis.

One of the main ingredients of our treatment is a unitary operator (Lee-Low-Pines or Jost transformation) having the property that the transformed Hamiltonian assumes diagonal form with respect to the fermion momenta. This transformation, which has already proved its utility in various other polaron problems [25], has the form

$$U = \exp\left(-\mathrm{i}\sum_{i\kappa} c_{i\kappa}^{\dagger}\mathbf{Q}\cdot\mathbf{R}_i c_{i\kappa}\right) = \sum_{i\kappa} c_{i\kappa}^{\dagger} U_i c_{i\kappa}, \tag{52}$$

where the last equality only holds on the single-particle Hilbert space. The operator

$$U_i = \exp(-\mathrm{i}\mathbf{Q}\cdot\mathbf{R}_i), \tag{53a}$$

where

$$\mathbf{Q} = \sum_{\mathbf{q}} \mathbf{q}\, b_{\mathbf{q}}^{\dagger}b_{\mathbf{q}} \tag{53b}$$

denotes the crystal momentum of the boson field, commutes with all $c_{i\kappa}$ and is a translation operator for the Bose particles:

$$U_i{}^{\dagger} b_l U_i = b_{l-i}. \tag{53c}$$

To better understand why the Jost transformation leads to a partial diagonalization of the Hamiltonian in momentum space, we recall from Section 2 that the total crystal momentum $\mathbf{P} = \mathbf{K} + \mathbf{Q}$, where $\mathbf{K} = \sum_{\mathbf{k}} \mathbf{k}\, \boldsymbol{c}_{\mathbf{k}}{}^{\dagger} \cdot \boldsymbol{c}_{\mathbf{k}}$ denotes the fermion momentum and $\mathbf{Q}$ is given by equation (53b), is a conserved quantity. Using the alternative form $U = \sum_{\mathbf{k}} \boldsymbol{c}_{\mathbf{k}}{}^{\dagger} \cdot \boldsymbol{c}_{\mathbf{k}+\mathbf{Q}}$, one readily establishes the relation $U^{\dagger}\mathbf{P}U = \mathbf{K}$, showing that in the transformed system $\mathbf{K}$ plays the role of the total crystal momentum. This

necessarily implies that the transformed Hamiltonian becomes diagonal in the fermion momenta $\mathbf{k}$, the eigenvalues of $\mathbf{K}$, whereas the indices κ remain unaffected.

To obtain the transformed Hamiltonian $U^\dagger HU$, we use the last equality in equation (52) and property (53c). The calculation is straightforward and leads to the result

$$U^\dagger HU = -t\sum_{ia} U_a \boldsymbol{c}_i{}^\dagger \cdot \mathbf{t}_a \cdot \boldsymbol{c}_{i+a} + \hbar\Omega \sum_i b_i^\dagger b_i - g\hbar\Omega \sum_{i\kappa} c_{i\kappa}^\dagger [(1 + P_+ B_0^{(j)})b_0 + \text{h.c.}] c_{i\kappa}, \quad (54)$$

where $b_0 \equiv b_{i=0}$ and $B_0^{(j)}$ is given by equation (51). After Fourier transformation of the fermion operators the Hamiltonian assumes the expected form

$$U^\dagger HU = \sum_{\mathbf{k}} \sum_{\kappa\kappa'} c_{\mathbf{k}\kappa}^\dagger H_{\mathbf{k}}^{\kappa\kappa'} c_{\mathbf{k}\kappa'}, \quad (55a)$$

where

$$H_{\mathbf{k}}^{\kappa\kappa'} = -T_{\mathbf{k}-\mathbf{Q}}^{\kappa\kappa'} + \delta_{\kappa\kappa'}\hbar\Omega \Big\{ \sum_i b_i^\dagger b_i - g[(1 + P_+ B_0^{(j)})b_0 + \text{h.c.}] \Big\} \quad (55b)$$

and

$$T_{\mathbf{k}-\mathbf{Q}}^{\kappa\kappa'} = t \sum_a t_a^{\kappa\kappa'} \exp[\mathrm{i}(\mathbf{k} - \mathbf{Q}) \cdot \mathbf{R}_a]. \quad (55c)$$

Our variational treatment is based on the displacement transformation

$$V = \sum_{\mathbf{k}\kappa} c_{\mathbf{k}\kappa}^\dagger V_{\mathbf{k}} c_{\mathbf{k}\kappa}, \quad (56a)$$

defined on the single-particle Hilbert space, where the operator [26]

$$V_{\mathbf{k}} = \exp\left[\frac{v_{\mathbf{k}}}{\sqrt{N}} \sum_{\mathbf{q}} (b_{\mathbf{q}}^\dagger - b_{\mathbf{q}}) \right] \quad (56b)$$

displaces the $b_{\mathbf{q}}$ according to the familiar formula $V_{\mathbf{k}}^\dagger b_{\mathbf{q}} V_{\mathbf{k}} = b_{\mathbf{q}} + v_{\mathbf{k}}/\sqrt{N}$ (N denotes the total number of sites). The unknown parameters $v_{\mathbf{k}}$ will be determined from the variational principle. The Hamiltonian then acquires the form

$$\tilde{H} \equiv (UV)^\dagger H (UV) = \sum_{\mathbf{k}} \sum_{\kappa\kappa'} c_{\mathbf{k}\kappa}^\dagger V_{\mathbf{k}}^\dagger H_{\mathbf{k}}^{\kappa\kappa'} V_{\mathbf{k}} c_{\mathbf{k}\kappa'}, \quad (57)$$

where $H_{\mathbf{k}}^{\kappa\kappa'}$ is given by equation (55b). Our further strategy may now be outlined as follows: as the first step, we introduce new fermion operators $f_{\mathbf{k}\kappa}$, $f_{\mathbf{k}\kappa}^\dagger$ by means of the relation

$$f_{\mathbf{k}\kappa}^\dagger |0) = (\boldsymbol{c}_{\mathbf{k}}{}^\dagger \cdot \mathbf{L}_{\mathbf{k}})_\kappa |0) = \sum_{\kappa'} L_{\mathbf{k}}^{\kappa'\kappa} c_{\mathbf{k}\kappa'}^\dagger |0), \quad (58)$$

where $\mathbf{L}_{\mathbf{k}}$ is a unitary 2×2 matrix, which will be specified below. In terms of the new fermionic basis the Hamiltonian (57) takes the form

$$\tilde{H} = \sum_{\mathbf{k}} \sum_{\kappa\kappa'} f_{\mathbf{k}\kappa}^\dagger (\mathbf{L}_{\mathbf{k}}^\dagger V_{\mathbf{k}}^\dagger \mathbf{H}_{\mathbf{k}} V_{\mathbf{k}} \mathbf{L}_{\mathbf{k}})_{\kappa\kappa'} f_{\mathbf{k}\kappa'} \quad (59)$$

and possesses the matrix elements

$$(0| f_{\mathbf{k}\kappa} \tilde{H} f_{\mathbf{k}\kappa'}^\dagger |0) = (\mathbf{L}_{\mathbf{k}}^\dagger \mathbf{M}_{\mathbf{k}} \mathbf{L}_{\mathbf{k}})_{\kappa\kappa'} = \sum_{\lambda\lambda'} (L_{\mathbf{k}}^{\lambda\kappa})^* M_{\mathbf{k}}^{\lambda\lambda'} L_{\mathbf{k}}^{\lambda'\kappa'}, \quad (60a)$$

where the expectation values

$$M_{\mathbf{k}}^{\lambda\lambda'} = (0| V_{\mathbf{k}}^\dagger H_{\mathbf{k}}^{\lambda\lambda'} V_{\mathbf{k}} |0) \quad (\lambda, \lambda' = \pm 1) \quad (60b)$$

will be functionals of $v_{\mathbf{k}}$. The matrix $\mathbf{L}_{\mathbf{k}}$ is now fixed by the requirement

$$(\mathbf{L}_{\mathbf{k}}^\dagger \mathbf{M}_{\mathbf{k}} \mathbf{L}_{\mathbf{k}})_{\kappa\kappa'} = \mathcal{E}_\kappa(\mathbf{k}) \delta_{\kappa\kappa'}, \quad (61)$$

which gives rise to two energy bands $\mathcal{E}_\kappa(\mathbf{k})$ ($\kappa = \pm 1$). The variational parameters $v_{\mathbf{k}}$ are then obtained from the condition $\delta\mathcal{E}_-(\mathbf{k})/\delta v_{\mathbf{k}} = 0$, where $\mathcal{E}_-(\mathbf{k})$ denotes the band with the *lowest* energy. The approximate, normalized ground-state eigenvector has the form

$$|\Phi_{\mathbf{k}-}) = UV f_{\mathbf{k}-}^\dagger |0) = Z_{\mathbf{k}} \sum_{i\kappa} \sum_{n_i=0}^{\infty} C_{i\kappa,\mathbf{k}}(n_i) c_{i\kappa}^\dagger \frac{(b_i^\dagger)^{n_i}}{\sqrt{n_i!}} |0), \quad (62a)$$

where $Z_{\mathbf{k}} = N^{-1/2} \exp(-v_{\mathbf{k}}^2/2)$ and the coefficients are given by

$$C_{i\kappa,\mathbf{k}}(n_i) = \frac{(v_{\mathbf{k}})^{n_i}}{\sqrt{n_i!}} L_{\mathbf{k}}^{\kappa-} \exp(\mathrm{i}\mathbf{k} \cdot \mathbf{R}_i). \quad (62b)$$

Thus, our first task is to evaluate the matrix elements (60b). A somewhat lengthy, but straightforward calculation gives the following results

$$M_{\mathbf{k}}^{++} = -t_{\mathbf{k}} \sum_{a=x}^{z} \cos k_a + \hbar\Omega v_{\mathbf{k}}(v_{\mathbf{k}} - 2g) - 2jg\hbar\Omega v_{\mathbf{k}}^{-1} \exp(-v_{\mathbf{k}}^2) \sinh v_{\mathbf{k}}^2, \quad (63a)$$

$$M_{\mathbf{k}}^{+-} = -t_{\mathbf{k}} \left(\mathrm{e}^{2\mathrm{i}\pi/3} \cos k_x + \mathrm{e}^{-2\mathrm{i}\pi/3} \cos k_y + \cos k_z \right), \quad (63b)$$

$$M_{\mathbf{k}}^{--} = M_{\mathbf{k}}^{++}, \quad M_{\mathbf{k}}^{-+} = (M_{\mathbf{k}}^{+-})^*, \quad (63c)$$

where $j = 0$ for the quasi-Holstein model, $j = 1/2$ for the $E \bigotimes e$ JT polaron, and

$$t_{\mathbf{k}} = t \exp(-v_{\mathbf{k}}^2). \quad (64)$$

Having obtained the matrix $\mathbf{M}_{\mathbf{k}}$, we readily find its eigenvalues $\mathcal{E}_\kappa(\mathbf{k})$,

$$\mathcal{E}_\kappa(\mathbf{k}) = -t_{\mathbf{k}} E_\kappa(\mathbf{k}) + \hbar\Omega v_{\mathbf{k}}(v_{\mathbf{k}} - 2g) - 2jg\hbar\Omega v_{\mathbf{k}}^{-1} \exp(-v_{\mathbf{k}}^2) \sinh v_{\mathbf{k}}^2, \quad (65)$$

where the quantities

$$E_\kappa(\mathbf{k}) = \epsilon_0(\mathbf{k}) - \kappa\sqrt{\epsilon_1^2(\mathbf{k}) + \epsilon_2^2(\mathbf{k})} \quad (\kappa = \pm 1) \tag{66}$$

denote the two e_g bands in the absence of the JT coupling [27] and

$$\epsilon_0(\mathbf{k}) = \cos k_x + \cos k_y + \cos k_z, \tag{67a}$$

$$\epsilon_1(\mathbf{k}) = \frac{1}{2}(\cos k_x + \cos k_y - 2\cos k_z), \tag{67b}$$

$$\epsilon_2(\mathbf{k}) = -\frac{\sqrt{3}}{2}(\cos k_x - \cos k_y). \tag{67c}$$

The condition $\delta\mathcal{E}_-(\mathbf{k})/\delta v_\mathbf{k} = 0$ then yields a transcendental equation for $v_\mathbf{k}$, which may be written as

$$v_\mathbf{k} = g\frac{1 + 2j\exp(-v_\mathbf{k}^2)F_\mathbf{k}}{1 + (t_\mathbf{k}/\hbar\Omega)E_\mathbf{k}}, \tag{68a}$$

where $E_\mathbf{k} \equiv E_-(\mathbf{k})$ and

$$F_\mathbf{k} = \exp(-v_\mathbf{k}^2) - (2v_\mathbf{k}^2)^{-1}\sinh v_\mathbf{k}^2. \tag{68b}$$

To assess the range of validity of our variational approach, we shall now first investigate the limiting cases of weak and strong coupling.

(i) *weak coupling*: $g \ll 1$

In this coupling range, equations (68) possess the solution

$$v_\mathbf{k} = \frac{(1+j)g}{1 + \gamma E_\mathbf{k}} + O(g^2), \tag{69a}$$

where the adiabaticity parameter

$$\gamma = t/\hbar\Omega. \tag{69b}$$

If this is inserted into the expression for $\mathcal{E}_-(\mathbf{k})$, equation (65), the result is

$$\mathcal{E}_-(\mathbf{k})/\hbar\Omega = -\gamma E_\mathbf{k} - g^2\frac{1+2j}{1+\gamma E_\mathbf{k}}, \tag{70}$$

where terms of $O(j^2)$ have been excluded because of the expansion (51). To compare our formula with exact analytical results for the Holstein polaron, we set $j = 0$ and restrict ourselves to one dimension. At the Γ point, equation (70) then reduces to

$$\mathcal{E}_-^{1D}(0)/\hbar\Omega = -\gamma - \frac{g^2}{1+\gamma}\cdot \tag{71a}$$

This may now be compared with the result of weak-coupling perturbation theory [28], which is valid for all γ:

$$\mathcal{E}_-^{1D}(0)/\hbar\Omega = -\gamma - \frac{g^2}{\sqrt{1+2\gamma}}\cdot \tag{71b}$$

While these two expressions agree for $\gamma \ll 1$, they start to diverge for larger γ, and our formula (71a) gradually ceases to be a reasonable upper bound [26]. For the pure JT case ($\gamma = 0$, $j = 1/2$), equation (70) reduces to

$$\mathcal{E}_-(\mathbf{k})/\hbar\Omega = -2g^2, \tag{72}$$

which agrees with the result of perturbation theory [21].

(ii) *strong coupling*: $g \gg 1$

In this case, equations (68) are solved by the expression

$$v_\mathbf{k} = g - \frac{j}{2g} + O(g^{-2}), \tag{73}$$

which, after substitution into equation (65), leads to

$$\mathcal{E}_-(\mathbf{k})/\hbar\Omega = -g^2 - j. \tag{74a}$$

For the Holstein polaron, strong-coupling perturbation theory [28] yields the result

$$\mathcal{E}_-(\mathbf{k})/\hbar\Omega = -g^2 - \left(\frac{\gamma}{2g}\right)^2, \tag{74b}$$

which agrees with our formula (74a) (for $j = 0$) in the nonadiabatic limit $\gamma \ll 1$. In the pure JT case ($j = 1/2$), equation (74a) agrees with the strong-coupling expression in reference [21].

This concludes our discussion of the weak and strong coupling limits. Summarizing we may state that our variational treatment seems to work reasonably well in the nonadiabatic regime $\gamma \ll 1$, but becomes less reliable for larger γ [26]. The nonadiabatic regime might be relevant to the manganites. For, in the doping region considered in this work, the t_{2g} core spins form an antiferromagnetic (G-type) spin background, leading to a strong suppression of hopping because of the double-exchange mechanism [9].

Important characteristics of a polaron are its dispersion relation and effective mass. Subsequently these properties will be examined for both the quasi-Holstein model ($j = 0$) and the $E\bigotimes e$ JT case ($j = 1/2$) by means of a numerical evaluation of equations (68). The result of such a calculation for $g = 1.5$ and $\gamma = 0.5$ is shown in Figure 1, where the polaron dispersion relations $\mathcal{E}_-(\mathbf{k})$ for $j = 0$ and $j = 1/2$ are depicted along a closed path of the cubic Brillouin zone (BZ). For comparison, the lower tight binding e_g band ($g = 0$) is also shown in Figure 1. Although the polaron bands are shifted to lower energies and have a smaller width in comparison with the e_g band, as expected, the shapes of all three bands are very similar. In particular, all extrema of the dispersion curves are located at the same positions. Other prominent features of the bands are the extended flat minima between Γ and X and the absolute maxima at the R point.

The polaron effective mass m^* is defined by the relation

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\left(\frac{\partial^2\mathcal{E}_-(\mathbf{k})}{\partial k^2}\right)_{\mathbf{k}=\mathbf{0}},$$

where k is the wave-vector component along some symmetry line of the BZ. Using equation (65) we obtain the simple result

$$m_0/m^* = \exp(-v_{\mathbf{k}=\mathbf{0}}^2), \tag{75}$$

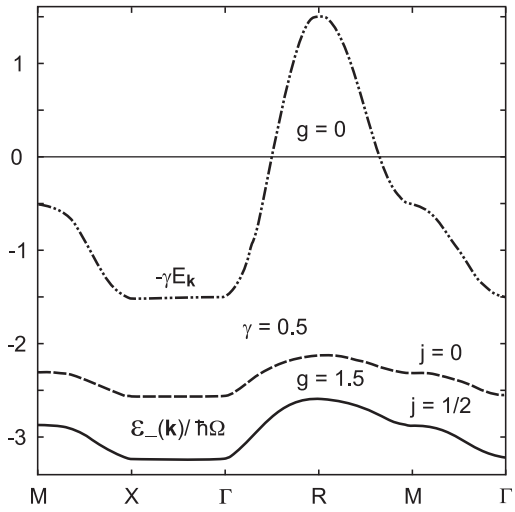

Fig. 1. Polaron dispersion curves $\mathcal{E}_{-}(\mathbf{k})/\hbar\Omega$, equation (65), for $j = 0$ (Holstein polaron) and $j = 1/2$ ($E \bigotimes e$ JT polaron). The lower tight binding e_g band ($g = 0$) is also shown for comparison. Symmetry points of the BZ are designated as in reference [27].

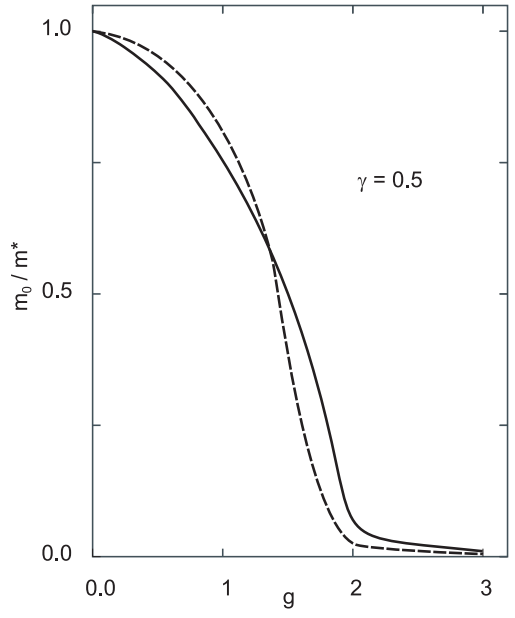

Fig. 2. Inverse effective masses of the Holstein polaron (dashed line) and the $E \bigotimes e$ JT polaron (solid line) as functions of the coupling strength g.

where

$$\frac{1}{m_0} = -\frac{t}{\hbar^2}\left(\frac{\partial^2 E_{\mathbf{k}}}{\partial k^2}\right)_{\mathbf{k}=\mathbf{0}}$$

denotes the inverse effective mass of the lower tight binding e_g band. We mention that in our derivation of equation (75) the $\mathbf{k}$ dependence of $v_{\mathbf{k}}$ has been properly taken into account, the simplicity of the result being due to a cancellation of all terms involving $\partial^2 v_{\mathbf{k}}/\partial k^2$.

In Figure 2 the mass ratio m_0/m^* is plotted as a function of the coupling strength g. Although both polaron masses behave similarly, there is an unexpected crossover where, for increasing g, the Holstein polaron starts to acquire a somewhat larger effective mass than the JT polaron. The effect is, however, not as dramatic as claimed by Takada [29]. For, in the strong-coupling limit, the polaron effective mass ratio $m^*_{\mathrm{JTP}}/m^*_{\mathrm{HP}}$ tends to the finite limit $\exp(-j) \approx 0.607$ for $j = 1/2$, as follows from equations (73) and (75). The results presented in Figure 2 are in remarkably good agreement with recent quantum Monte Carlo data [14], thus confirming our expectation that the proposed variational approach, restricted to the nonadiabatic regime, gives a fair account of polaronic properties over the whole coupling range.

7 Summary

In this work a detailed account has been given of the analytic properties of the $E \bigotimes e$ JT polaron, consisting of a mobile e_g electron linearly coupled to the local e_g normal vibrations of a periodic array of octahedral complexes. The linear JT coupling implies the existence of two operators, the angular momentum $\mathcal{J}$ and the parity $\mathcal{K}$, which commute with the JT part and are responsible for the twofold degeneracy of all JT eigenvalues. This degeneracy is lifted by the anisotropic hopping term, which does not commute with $\mathcal{J}$ and $\mathcal{K}$. The most interesting feature of our study is, however, the appearance of a close relationship between the JT problem and the Holstein model. Although such a connection has already been suspected to exist in the simpler $E \bigotimes b$ JT polaron [11], it has never been explicitly demonstrated. This connection only emerges in a particular representation of the original problem, in which the Hamiltonian acquires an explicit dependence on the half-integral angular momentum quantum number j and quite naturally decomposes into a Holstein term and a residual JT interaction. While the ground state of the JT polaron belongs to the sector $j = 1/2$, the Holstein polaron is formally obtained for the unphysical value $j = 0$. This is the optimal form of the Hamiltonian, which can be achieved by purely analytic means, allowing the JT and the Holstein polaron to be treated in a unified framework.

The Hamiltonian is then subjected to a variational treatment, yielding approximate ground-state energies and eigenvectors for both types of polarons. Although the ground-state eigenvector is explicitly given by equations (62), its application to the calculation of physical properties is relegated to future work. Here we have restricted ourselves to the polaron dispersion relations and effective masses. As expected, the polaron bands are shifted to lower energies and have a smaller width in comparison with the bare e_g band (see Fig. 1), but the shapes of all three bands are very similar. The dependence of the effective masses on the coupling strength g is also similar for both polarons (see Fig. 2). There is, however, an unexpected crossover where the Holstein polaron starts to acquire a somewhat bigger mass than the JT polaron with increasing g. These results are in remarkably good agreement with recent quantum Monte Carlo data [14].

This seems to indicate that our variational approach, restricted to the nonadiabatic regime for formal reasons, is fairly accurate. The nonadiabatic regime might be relevant to the manganites, for in the doping region considered in this work the core spins form an antiferromagnetic (G-type) spin background, leading to a strong suppression of hopping because of the double-exchange mechanism [9].

A more realistic model would have to include, at least, the intersite coupling of the normal vibrations. This coupling is expected to contribute to the splitting of the degenerate JT ground state and to turn the Einstein phonons of the present work into optical phonons. Whether these coupling terms will give rise to additional and unexpected effects, remains to be seen and will be investigated in future work.

Appendix A: Direct proof of equivalence

In Section 5 the equivalence of the operators $\mathcal{A}$ and A_j has been proven in terms of their algebraic properties. Here we intend to put forward a more direct proof by showing that the operators possess identical matrix elements, provided the states involved are related to each other by the mapping prescription (39). We start by defining the basis vectors

$$|i\kappa; m+2n_i, m\rangle \equiv d^\dagger_{i\kappa}|m+2n_i, m\rangle \prod_{l\neq i}|0_l, 0_l\rangle, \tag{A1a}$$

$$|i\kappa; m+2n_i+1, m+1\rangle \equiv d^\dagger_{i\kappa}|m+2n_i+1, m+1\rangle \times \prod_{l\neq i}|0_l, 0_l\rangle, \tag{A1b}$$

where the notation is the same as in equations (28) and κ is fixed by equation (29c). The vectors (A1a) and (A1b) are then eigenstates of the angular momentum operator $\mathcal{J}$ to the same eigenvalue $j = m + 1/2$ and belong to the subspaces $\mathcal{U}^+_j$ and $\mathcal{U}^-_j$, respectively, according to our definitions introduced at the end of Section 4. Given these basis states, the nonvanishing matrix elements of the operator $\mathcal{A}$, equation (30a), are readily evaluated by means of the easily proven relations

$$a_{ix}|m+2n_i, m\rangle = \sqrt{m+n_i}\,|m+2n_i-1, m-1\rangle, \tag{A2a}$$

$$a_{iz}|m+2n_i, m\rangle = \sqrt{n_i}\,|m+2n_i-1, m+1\rangle, \tag{A2b}$$

$$\Pi_\kappa|m+2n_i, m\rangle = 0, \quad \Pi_{-\kappa}|m+2n_i, m\rangle = |m+2n_i, m\rangle. \tag{A2c}$$

With the help of equations (A2) we then find the expressions

$$\mathcal{A}|i\kappa; m+2n_i, m\rangle = \sqrt{2n_i}\,|i\kappa; m+2n_i-1, m+1\rangle,$$
$$\mathcal{A}|i\kappa; m+2n_i+1, m+1\rangle = \sqrt{2j+2n_i+1}\,|i\kappa; m+2n_i, m\rangle,$$

and, hence, the only nonvanishing matrix elements of the operator $\mathcal{A}$ read:

$$\langle i\kappa; m+2n_i-1, m+1|\mathcal{A}|i\kappa; m+2n_i, m\rangle = \sqrt{2n_i}, \tag{A3a}$$

$$\langle i\kappa; m+2n_i, m|\mathcal{A}|i\kappa; m+2n_i+1, m+1\rangle = \sqrt{2j+2n_i+1}. \tag{A3b}$$

Our assertion is that the matrix elements of the operator A_j, defined by equations (40), are the same as those on the right side of equations (A3), provided the states are chosen as prescribed by equation (39). To prove our claim, we first introduce the new basis vectors

$$|i\kappa; 2n_i) \equiv c^\dagger_{i\kappa}\frac{(b^\dagger_i)^{2n_i}}{\sqrt{(2n_i)!}}|0), \tag{A4a}$$

$$|i\kappa; 2n_i+1) \equiv c^\dagger_{i\kappa}\frac{(b^\dagger_i)^{2n_i+1}}{\sqrt{(2n_i+1)!}}|0), \tag{A4b}$$

where we have adopted the notation of equations (37). Here, in contrast to the vectors (A1), the quantum number κ needs no longer to be fixed, but may be arbitrarily set equal to 1 or -1. Since, by definition, the vectors (A4a) and (A4b) are elements of the subspaces $\mathcal{V}^+_j$ and $\mathcal{V}^-_j$, respectively, the mapping prescription (39) requires the following one-to-one correspondence to exist between the vectors (A1) and (A4):

$$|i\kappa; m+2n_i, m\rangle \leftrightarrow |i\kappa; 2n_i), \tag{A5a}$$

$$|i\kappa; m+2n_i+1, m+1\rangle \leftrightarrow |i\kappa; 2n_i+1), \tag{A5b}$$

$$|i\kappa; m+2n_i-1, m+1\rangle \leftrightarrow |i\kappa; 2n_i-1). \tag{A5c}$$

By means of these relations the matrix elements (A3) are then mapped onto the following expressions

$$(i\kappa; 2n_i-1|A_j|i\kappa; 2n_i) = \sqrt{2n_i}, \tag{A6a}$$

$$(i\kappa; 2n_i|A_j|i\kappa; 2n_i+1) = \sqrt{2j+2n_i+1}, \tag{A6b}$$

whose validity is explicitly verified with the help of equations (A4) and (40). This proves the equivalence of the operators $\mathcal{A}$ and A_j, as far as the basis states are concerned. Owing to the completeness of these states, however, relations (A3) and (A6) suffice to extend the proof to arbitrary vectors of the spaces $\mathcal{U}_j$ and $\mathcal{V}_j$, provided these vectors are related to each other by equation (39). This completes our direct proof of the equivalence of the operators $\mathcal{A}$ and A_j.

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$$d_n = 2(n+1)\binom{n+N-1}{N-1},$$

where the factor $2(n+1)$ originates from the fact that κ ranges over two and j_κ over $n+1$ values, but $E^0_{nj\kappa}$ does not depend on these quantum numbers. The binomial coefficient gives the number of ways the relation $n = \sum_i n_i$ can be fulfilled in terms of the natural numbers n_i.
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