Simple accurate coupled cluster results for the linear $E \otimes e$ pseudo-Jahn–Teller effect

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Using the coupled cluster method (CCM), we present a simple accurate calculation for the energies of the ground- and first excited states of the linear $E \otimes e$ Jahn–Teller and pseudo-Jahn–Teller Hamiltonians. From the solution of a single transcendental equation, we obtain results with a maximal error of 1.2%. These results are notably better than previous results obtained both via the CCM and other many-body approximations. © 2000 American Institute of Physics.
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I. INTRODUCTION

The linear $E \otimes e$ Jahn–Teller (JT) and pseudo-Jahn–Teller (PJT) Hamiltonians describe a two-level fermionic system interacting with two independent modes of a quantized bosonic field. The JT Hamiltonian considers the case of degenerate fermionic levels, while the PJT Hamiltonian considers the case of nonzero fermionic level splitting. As such, these models serve as generic prototypes for a wide variety of physical systems. In quantum optics, models of this form are employed to describe the resonant or near-resonant interaction of a two-level atom with two perpendicularly polarized modes of a quantized electromagnetic field.^{1,2} In quantum chemistry, such models describe the vibronic coupling between two electronic levels (E) and two degenerate nuclear vibrational modes (e) in a molecule or crystal.³ Yet another realization of these models is provided by the two-site polaron in solid-state physics, describing the interaction of an electron confined to two sites in a crystal lattice with the quantized phononic field of the lattice.^{4,5} Besides their physical importance, these simple models also contain interesting symmetries, and as such are ideal testing grounds for approximate many-body methods.

Given their physical relevance, the linear $E \otimes e$ JT and PJT models have therefore been the subject of much theoretical investigation.^{6–9} Judd^{10,11} and subsequently Reik,¹² guided by the results of early numerical diagonalizations,^{13,14} proved the existence of analytic solutions for the linear $E \otimes e$ JT and PJT Hamiltonians at isolated values of the coupling between the fermionic and bosonic subsystems. However, no analytic solution is yet available for arbitrary fermionic level splitting ω_0 at all coupling strengths. There is an extremely rapidly convergent expansion in terms of generalized spheroidal wave functions¹⁵ but it is not exact, see Eq. (6.1) in Ref. 16. A complete analytic ground-state solution, valid for all couplings, does exist for the case of the linear

$E \otimes e$ resonant pseudo-Jahn–Teller (RPJT) model,¹² for which the fermionic level splitting ω_0 is equal to the bosonic excitation quantum ω . More recent many-body analyses include variational calculations, based on a correlated squeezed state, for the JT¹⁷ and PJT¹⁸ models, and several applications of the coupled cluster method (CCM) to the JT model.^{19,20}

The CCM, a nonperturbative method originally developed in nuclear physics by Coester and Kümmel,^{21,22} has been successfully applied in the analysis of the many-body groundstate in quantum chemistry,^{23,24} the electron gas,^{25,26} lattice gauge,^{27–29} latticized chiral meson,³⁰ and continuum field^{31,32} theories, and spin and electron lattice models.^{33,34} In previous applications of the CCM to the linear $E \otimes e$ JT Hamiltonian, the method was applied to a unitary-transformed Hamiltonian.^{19,20} Results for the ground-state energy were obtained which were in better agreement, over the full coupling spectrum, with the results of a large-scale numerical diagonalization than the results of previous non-CCM calculations.¹⁹ However, the unitary transformation employed in Ref. 19 destroys two important symmetries of the linear $E \otimes e$ JT Hamiltonian. Besides the resulting loss of accuracy in the ground-state energy results, this approach is therefore also not readily generalized either to the first excited state, or to the PJT case of nondegenerate fermionic levels ($\omega_0 > 0$).

We show here that it is possible to obtain extremely accurate CCM results for the ground- and first excited state energies of the linear $E \otimes e$ JT and linear $E \otimes e$ PJT systems in a straightforward manner, by maintaining the correct symmetries throughout the analysis. The key to our approach is the choice of the (analytic) linear $E \otimes e$ RPJT ground-state wave function as the model state for the CCM. We present the calculation in an operator-based form which is independent of the particular realization of the bosonic modes. This operator-based approach also reproduces the Juddian (isolated exact) solutions for these models, and leads to explicit expressions for the Juddian wave functions.

This paper is organized as follows: In Sec. II we intro-

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duce the linear $E \otimes e$ JT and PJT Hamiltonians, along with their symmetries. We rewrite these Hamiltonians in a representation-independent form in Sec. III, where we also present an explicit form for the analytic ground-state wave function of the linear $E \otimes e$ RPJT Hamiltonian. Section IV contains our CCM calculation and results, and in Sec. V we discuss these results and present our conclusions.

II. THE LINEAR $E \otimes e$ JT AND PJT HAMILTONIANS

The linear $E \otimes e$ PJT Hamiltonian is given by

$$H_{\text{PJT}} = \frac{1}{2}\omega_0\sigma^z + b_1^\dagger b_1 + b_2^\dagger b_2 + \eta(b_1^\dagger + b_1)\sigma^x - \eta(b_2^\dagger + b_2)\sigma^y, \quad (1)$$

where ω_0 is the fermionic level splitting, and η is the dipole coupling constant linking the bosonic modes to the fermionic level and thus indirectly to each other. The operators b_1, b_2 and $b_1^\dagger, b_2^\dagger$ are bosonic annihilation and creation operators, respectively, satisfying the standard bosonic commutation relations, and $\sigma^x, \sigma^y, \sigma^z$ are Pauli matrices. The origin of the fermionic energy scale has been chosen such that the lower (upper) fermionic state corresponds to energy $-\frac{1}{2}\omega_0$ ($\frac{1}{2}\omega_0$). For convenience, we have scaled out the dependence on the bosonic energy quantum ω , neglected the zero-point energy of the bosonic modes, and employed units such that $\hbar = 1$. The (pure) linear $E \otimes e$ JT Hamiltonian H_{JT} may formally be regarded as the special case of H_{PJT} where the two fermionic levels are degenerate ($\omega_0 = 0$).

The Hamiltonian (1) may also be written in the equivalent form

$$H_{\text{PJT}} = \frac{1}{2}\omega_0\sigma^z + a_1^\dagger a_1 + a_2^\dagger a_2 + \kappa(a_1 + a_2^\dagger)\sigma^+ + \kappa(a_1^\dagger + a_2)\sigma^- \quad \left(\kappa \equiv \frac{\eta}{\sqrt{2}} \right), \quad (2)$$

in terms of the spin-raising and spin-lowering operators $\sigma^\pm \equiv \sigma^x \pm i\sigma^y$, via the canonical transformation

$$\begin{aligned} a_1 &\equiv \frac{1}{\sqrt{2}}(b_1 + ib_2), & a_1^\dagger &\equiv \frac{1}{\sqrt{2}}(b_1^\dagger - ib_2^\dagger), \\ a_2 &\equiv \frac{1}{\sqrt{2}}(b_1 - ib_2), & a_2^\dagger &\equiv \frac{1}{\sqrt{2}}(b_1^\dagger + ib_2^\dagger), \end{aligned} \quad (3)$$

to modes of circular rather than linear polarization.

There are two important symmetries associated with the Hamiltonian H_{PJT} . The first is the parity symmetry

$$\Pi = \exp\{i\pi[N_b + \frac{1}{2}(\sigma^z + 1)]\}, \quad (4)$$

where the bosonic number operator N_b is defined by

$$N_b \equiv b_1^\dagger b_1 + b_2^\dagger b_2 = a_1^\dagger a_1 + a_2^\dagger a_2. \quad (5)$$

The second is the angular momentum component

$$J = i(b_1^\dagger b_2 - b_1 b_2^\dagger) + \frac{1}{2}\sigma^z = a_1^\dagger a_1 - a_2^\dagger a_2 + \frac{1}{2}\sigma^z, \quad (6)$$

with eigenvalues in the set $\{\dots, -\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots\}$ which also commutes with the parity operator Π (4).

III. AN OPERATOR-BASED APPROACH

It proves convenient to define the operator $c^\dagger$ and its Hermitian conjugate c via

$$c^\dagger \equiv \frac{1}{\sqrt{2}}(b_1^\dagger \sigma^x - b_2^\dagger \sigma^y) = \frac{1}{2}(a_2^\dagger \sigma^+ + a_1^\dagger \sigma^-), \quad (7)$$

$$c = \frac{1}{\sqrt{2}}(b_1 \sigma^x - b_2 \sigma^y) = \frac{1}{2}(a_2 \sigma^- + a_1 \sigma^+).$$

It is easily shown that

$$\begin{aligned} [c, J] &= [c^\dagger, J] = 0, \\ [c, \Pi] &= [c^\dagger, \Pi] = 0, \end{aligned} \quad (8)$$

and also that

$$(c^\dagger)^2 = \frac{1}{2}[(b_1^\dagger)^2 + (b_2^\dagger)^2] = a_1^\dagger a_2^\dagger. \quad (9)$$

The Hamiltonian H_{PJT} may, for arbitrary ω_0 , be rewritten as

$$H_{\text{PJT}} = \frac{1}{2}\omega_0\sigma^z + N_b + 2\kappa c^\dagger + 2\kappa c, \quad (10)$$

where the bosonic number operator N_b now assumes the form

$$N_b = 2c^\dagger c + J\sigma^z - \frac{1}{2}. \quad (11)$$

Here, $J\sigma^z = cc^\dagger - c^\dagger c - \frac{1}{2}$, and the parity operator Π retains the form (4). The operators $c, c^\dagger$, and σ^z obey the relations

$$\begin{aligned} [c, (c^\dagger)^{2n}] &= n(c^\dagger)^{2n-1}, \\ [c, (c^\dagger)^{2n+1}] &= (c^\dagger)^{2n}(J\sigma^z + n + \frac{1}{2}), \\ [\sigma^z, c^{2n}] &= [\sigma^z, (c^\dagger)^{2n}] = [\sigma^z, c^{2n+1}]_+ \\ &= [\sigma^z, (c^\dagger)^{2n+1}]_+ = 0, \end{aligned} \quad (12)$$

for $n = 0, 1, 2, \dots$, where the subscript $+$ denotes an anticommutator. It then follows that

$$[N_b, (c^\dagger)^n] = n(c^\dagger)^n, \quad [c, N_b] = c \quad (13)$$

and, as expected,

$$[J, \sigma^z] = [J, N_b] = 0. \quad (14)$$

Consider now the (infinite-dimensional) subspace of the full Hilbert space corresponding to an arbitrary eigenvalue j of J . Once can show that the requirement

$$c|\Psi\rangle_j^{\text{ref}} = 0, \quad (15)$$

uniquely determines the state $|\Psi\rangle_j^{\text{ref}}$,³⁵ which is a reference state of angular momentum component j which will be used as a starting vector for the construction of a suitable basis for this j sector. This reference state can also be shown³⁵ to be an eigenstate of σ_z with eigenvalue $s = 1$ for $j = p + \frac{1}{2} > 0$ and $s = -1$ for $j = -p - \frac{1}{2} < 0$ and of the parity operator Π with eigenvalue $\exp(i\pi(j + 1/2)s)$. In particular, in the occupation number representation of modes of circular polarization, the reference state for the $j = p + 1/2$ -sector is given by $|p\rangle|0\rangle|\uparrow\rangle$ and that for the $j = -p - 1/2$ -sector is $|0\rangle|p\rangle|\downarrow\rangle$, where the first (second) ket refers to a bosonic occupation number state for the first (second) bosonic mode, and the third ket denotes the lower ($|\downarrow\rangle$) or upper ($|\uparrow\rangle$) level of the fermionic mode.

The operator approach now allows for the construction of a suitable basis for this j sector, without the need to specify the explicit form of the basis states in terms of, e.g., linearly or circularly polarized bosonic modes. For an arbitrary j -sector eigenstate $|\Psi\rangle_j$ of H_{RPJT} , one may for instance construct the power series expansion

$$|\Psi\rangle_j = \sum_{n=0}^{\infty} X_n (c^\dagger)^n |\Psi\rangle_j^{\text{ref}}. \quad (16)$$

Since $c^\dagger$ commutes with both J and Π , it is clear that the state $|\Psi\rangle_j$ has the same J and Π quantum numbers as the reference state $|\Psi\rangle_j^{\text{ref}}$. Substituting the expansion (16) into the Schrödinger equation

$$H_{\text{PJT}}|\Psi\rangle_j = E|\Psi\rangle_j, \quad (17)$$

and using the relations (12), (13), and the condition (15), one obtains for the coefficients $\{X_i\}$ the recurrence relations

$$\begin{aligned} 0 &= 2\kappa X_{2n-1} + (p+2n+s\frac{1}{2}\omega_0 - E) \\ &\quad \times X_{2n} + 2\kappa(p+n+1)X_{2n+1}, \\ 0 &= 2\kappa X_{2n} + (p+2n+1-s\frac{1}{2}\omega_0 - E) \\ &\quad \times X_{2n+1} + 2\kappa(n+1)X_{2n+2}, \end{aligned} \quad (18)$$

where $s=1$ for $j=p+1/2$ and $s=-1$ for $j=-p-1/2$. These equations constitute a simple reformulation of the well-known Longuet–Higgins recurrence relations,^{10,13,36} generalized to incorporate the case $\omega_0 > 0$. It is clear that in general (i.e., arbitrary $\omega_0 > 0$), the solutions of (18) will be different for the cases $s = \pm 1$, and the eigenstates of H_{PJT} are thus singlet states of definite parity and angular momentum component j . In particular, the ground state of H_{PJT} is a unique positive-parity state, corresponding to $j = -1/2$ and $s = -1$, for all values of the coupling κ . Since the Longuet–Higgins relations (18) are invariant under the simultaneous replacements $\{\omega_0 \rightarrow -\omega_0, j \rightarrow -j, s \rightarrow -s\}$, it is clear that the first excited state of H_{PJT} , which is a unique negative-parity state corresponding to $j = 1/2$ and $s = 1$, may formally be obtained by making the replacement $\{\omega_0 \rightarrow -\omega_0\}$; we will use this fact in our CCM calculations.

For the linear $E \otimes e\text{JT}$ Hamiltonian H_{JT} , where $\omega_0 = 0$, the solution of (18) in the $j = p+1/2$ and $j = -p-1/2$ sectors (which are of opposite parity) are identical, which explains the twofold degeneracy of all energy levels in the spectrum of the linear $E \otimes e\text{JT}$ Hamiltonian. In particular, the solution of (18) for $\{\omega_0 = 0; p=0, j = -1/2\}$ and $\{\omega_0 = 0; p=0, j = 1/2\}$ yields the energy of the positive- and negative-parity ground states of H_{JT} , which are degenerate for all couplings. Thus, the inclusion of the (vibronic) interaction terms transforms the electronic degeneracy of the noninteracting ground state of H_{JT} into a parity degeneracy (which has previously been referred to as a vibronic degeneracy³) at finite coupling. In the H_{PJT} model, the finite fermionic level splitting ω_0 lifts the parity degeneracy of the ground state at all values of the coupling.

Juddian solutions

Reik *et al.*^{12,36–38} simplified the analysis of the Juddian (isolated exact) solutions for H_{PJT} by observing that, at the Juddian points, a Neumann expansion of the Bargmann space wave function in modified Bessel functions terminates after a finite number of terms. Here, we simply recover the results of Reik *et al.* using the operator approach given above and obtain explicit expressions (independent of the realization of the bosonic modes) for the Juddian wave functions in the Dirac rather than the Bargmann representation. In direct analogy with the approach in Ref. 12, we therefore construct the following (unnormalized) Neumann expansion for $|\Psi\rangle_j$:

$$\begin{aligned} |\Psi\rangle_j &= \sum_{n=0}^{\infty} \frac{x_n}{\kappa^{4n} n!} (\kappa c^\dagger)^{n-p} I_{n+p}(2\kappa c^\dagger) |\Psi\rangle_j^{\text{ref}} \\ &\quad + \sum_{n=0}^{\infty} \frac{y_n}{\kappa^{4n} n!} (\kappa c^\dagger)^{n-p} I_{n+p+1}(2\kappa c^\dagger) |\Psi\rangle_j^{\text{ref}}, \end{aligned} \quad (19)$$

where I_n is a modified Bessel function of the first kind of order n (see, e.g., Ref. 39), and as before $s=1$ ($s=-1$) for $j=p+1/2$ ($j=-p-1/2$). Substituting Eq. (19) into the Schrödinger equation (17) we obtain for $n=0,1,2,\dots$,

$$\begin{aligned} 0 &= \left\{ \frac{p}{2} + n + s \frac{\omega_0}{4} - \frac{E}{2} \right\} x_n + \kappa^2 y_n + n \kappa^4 (x_{n-1} + y_{n-1}), \\ 0 &= \frac{1}{\kappa^2} x_{n+1} + \left\{ \frac{p}{2} + n + \frac{1}{2} - s \frac{\omega_0}{4} - \frac{E}{2} \right\} y_n \\ &\quad + \{p+n+1+\kappa^2\} x_n + n \kappa^4 (x_{n-1} + y_{n-1}), \end{aligned} \quad (20)$$

where, by definition, $x_{-1} = y_{-1} = 0$. The parameter x_0 simply fixes the norm of $|\Psi\rangle_{-p-1/2}$ and one can take $x_0 = \kappa^2$. After introducing the parameters

$$\begin{aligned} \delta &\equiv -\frac{s\omega_0 + 1}{4}, \\ E &\equiv (v - \frac{1}{2} - 2\kappa^2), \end{aligned} \quad (21)$$

these equations can easily be seen to be equivalent to those of Reik *et al.*¹²

Reik *et al.* noted that Juddian solutions for H_{PJT} occur whenever the Neumann series (19) terminates at finite order; such a termination occurs at the N th term if and only if both the conditions $v=N$ and $\Sigma_N \equiv x_N + y_N = 0$ are met. In particular, for $v=N=0$ the energy lies on the 0th baseline

$$E_0^{\text{Baseline}} = \frac{1}{2} - 2\kappa^2, \quad (22)$$

and the condition $\Sigma_0 = x_0 + y_0 = 0$ reduces to

$$p - 2\delta = 0, \quad (23)$$

which is independent of the coupling κ , and thus yields an analytic solution, valid for all coupling. Specifically, such a solution occurs for the ground ($j = -1/2, p=0$) state of the linear $E \otimes e$ pseudo-Jahn–Teller Hamiltonian at resonance for which $\omega_0 = \omega$, i.e., $\delta=0$. Here, the reference state $|\Psi\rangle_{j=-1/2}^{\text{ref}}$ has the form $|0\rangle|0\rangle|\downarrow\rangle$, where $|0\rangle|0\rangle$ is the bosonic vacuum for any particular realization of the bosonic modes.

Thus, we find that the ground-state wave function $|\Psi_0^{\text{RPJT}}\rangle$ of the resonant pseudo-Jahn–Teller Hamiltonian H_{RPJT} assumes the closed form

$$|\Psi_0^{\text{RPJT}}\rangle = A_{\text{RPJT}} \{I_0(2\kappa c^\dagger) - I_1(2\kappa c^\dagger)\} |0\rangle |0\rangle |\downarrow\rangle, \quad (24)$$

where A_{RPJT} is a normalization constant, and the corresponding ground-state energy is given by Eq. (22). Expressed in terms of bosonic modes of circular polarization, $|\Psi_0^{\text{RPJT}}\rangle$ assumes the explicit form

$$|\Psi_0^{\text{RPJT}}\rangle = A_{\text{RPJT}} \sum_{k=0}^{\infty} \left\{ \frac{\kappa^{2k}}{\sqrt{k!k!}} |k\rangle |k\rangle |\downarrow\rangle - \frac{\kappa^{2k+1}}{\sqrt{k!(k+1)!}} |k\rangle |k+1\rangle |\uparrow\rangle \right\}, \quad (25)$$

which allows for the determination of A_{RPJT} via

$$A_{\text{RPJT}} = \left\{ \sum_{k=0}^{\infty} \left(\frac{\kappa^{4k}}{k!k!} + \frac{\kappa^{4k+2}}{k!(k+1)!} \right) \right\}^{-1/2} \\ = \{I_0(2\kappa^2) + I_1(2\kappa^2)\}^{-1/2}. \quad (26)$$

For $v=N>0$, the conditions $\sum_N = x_N + y_N = 0$ may be used to find other Juddian solutions for H_{JT} and H_{PJT} . It has been conjectured¹⁵ that an expansion of the wave function in generalized spheroidal functions terminates at all values of the coupling, rather than only at the Juddian points. Despite very strong numerical evidence, this conjecture has not been proved. However, the Juddian solutions may be still used to gauge the accuracy of approximate many-body techniques and in particular to confirm that the converged numerical diagonalization results for the spectra of H_{JT} and H_{PJT} are exact for all practical purposes. Also, it can be shown³⁶ that, for large coupling κ , all eigenvalues of H_{JT} and H_{PJT} approach the baselines $v=N$. In particular, the energies of both the ground- and first excited states of these Hamiltonians approach the value $E_0^{\text{Baseline}} = E_0^{\text{RPJT}} = -1/2 - 2\kappa^2$ in the limit $\kappa \rightarrow \infty$.

IV. THE CCM: APPLICATION AND RESULTS

Central to the application of the CCM is the choice of the model state $|\Phi\rangle$ and cluster correlation operator S , in terms of which the exact ground-state eigenket $|\Psi\rangle$ of the Hamiltonian is parametrized as (see, e.g., Ref. 40)

$$|\Psi\rangle = e^S |\Phi\rangle. \quad (27)$$

The state $|\Psi_0^{\text{RPJT}}\rangle$ presents itself as a natural choice for the CCM model state, since it clearly has the correct even-parity and $j = -1/2$ symmetries required of the ground state. Furthermore, since it is easily shown that

$$c |\Psi_0^{\text{RPJT}}\rangle = -\kappa |\Psi_0^{\text{RPJT}}\rangle, \quad (28)$$

the operator $c + \kappa$ annihilates the model state $|\Phi\rangle = |\Psi_0^{\text{RPJT}}\rangle$. This suggests the following (clearly symmetry-conserving) form for the cluster correlation operator S :

$$S = \sum_{n=1}^{\infty} s_n (c^\dagger + \kappa)^n. \quad (29)$$

We shall refer to this choice of the model state and correlation operator as the RPJT scheme. In the first order, or so-called SUB-1 approximation, the operator S is truncated at first order, so that $S = s_1 (c^\dagger + \kappa)$. With the Hamiltonian H_{PJT} (for arbitrary ω_0 , including the JT case $\omega_0 = 0$) written in the convenient form (10), the nested commutator (Haussdorf) expansion

$$e^{-S} H e^S = H + [H, S] + \frac{1}{2!} [[H, S], S] + \cdots \quad (30)$$

may be used to obtain the similarity transformed Hamiltonian

$$e^{-S} H_{\text{PJT}} e^S = \frac{1}{2} \omega_0 \exp\{-2s_1 c^\dagger\} \sigma^z + 2c^\dagger c - \frac{1}{2} \\ + s_1 (c^\dagger + \kappa) + 2\kappa (c^\dagger + c) + \frac{1}{2} (2J) \sigma^z \\ + \frac{1}{2} \sum_{m=0}^{\infty} \frac{2s_1 \kappa (-2s_1 c^\dagger)^m}{(m+1)!} (2J) \sigma^z. \quad (31)$$

For the ground state, one may replace the operator $2J$ by its eigenvalue -1 . Furthermore, given the relation $c|\Phi\rangle = (-\kappa)|\Phi\rangle$ and its Hermitian conjugate $\langle\Phi|c^\dagger = \langle\Phi|(-\kappa)$, it follows that the SUB-1 CCM ground-state energy has the form

$$E_0^{\text{CCM}} = \langle\Phi| e^{-S} H_{\text{PJT}} e^S |\Phi\rangle \\ = -\frac{1}{2} - 2\kappa^2 + \frac{1}{2} (\omega_0 - 1) \exp\{2s_1 \kappa\} \langle\sigma^z\rangle, \quad (32)$$

where the model-state expectation value $\langle\sigma^z\rangle$ is given by

$$\langle\sigma^z\rangle = \langle\Phi| \sigma^z |\Phi\rangle = -\frac{[I_0(2\kappa^2) - I_1(2\kappa^2)]}{[I_0(2\kappa^2) + I_1(2\kappa^2)]}. \quad (33)$$

Using the commutation relations (12), one obtains the overlap equation

$$0 = \langle\Phi| (c + \kappa) e^{-S} H_{\text{PJT}} e^S |\Phi\rangle \\ = \exp\{2s_1 \kappa\} (\omega_0 - 1) (\kappa - \frac{1}{2}s_1) \langle\sigma^z\rangle + \frac{1}{2}s_1 [1 - \langle\sigma^z\rangle] \\ + \frac{\omega_0}{4\kappa} \sinh\{2s_1 \kappa\} + \frac{1}{4\kappa} [1 - \cosh\{2s_1 \kappa\}] \\ + \frac{1}{4\kappa} [1 - \exp\{2s_1 \kappa\}] \langle\sigma^z\rangle, \quad (34)$$

which determines the coefficient s_1 , and thereby also the SUB-1 CCM ground-state energy (32) in the RPJT scheme. It is clear from the form (32) that, as expected, the SUB-1 CCM ground-state energy E_0^{CCM} for the RPJT scheme is exact in the case of resonance $\omega_0 = 1$.

For ease of comparison with other results, we introduce the coupling parameter

$$k^2 \equiv 4\kappa^2 = 2\eta^2. \quad (35)$$

In Table I we compare our SUB-1 CCM results for the ground-state energy of the linear $E \otimes e$ Hamiltonian (for which $\omega_0 = 0$) to the effectively exact results obtained via numerical diagonalization, and also to results obtained via a variety of many-body calculations. It is clear that, even in first order, our CCM calculation based on the RPJT scheme yields a considerable improvement, over the full coupling

TABLE I. Comparison of the ground-state energy E_0^{CCM} of the linear $E \otimes e$ JT ($\omega_0 = 0$) Hamiltonian, obtained as a function of the coupling k^2 from a SUB-1 CCM calculation based on the RPJT scheme, with the results of other many-body calculations. In accordance with the other results quoted here, we have added unity (the zero-point energy of the bosonic modes for $\omega = 1$) to our results. The numerical diagonalization results, which are effectively exact, are labeled E_0^D . The results from Ref. 19 are the so-called optimal CCM ground-state energy results presented there. The other columns, which are reproduced from Ref. 19, represent results obtained via an earlier CCM analysis (Ref. 20), and via variational methods and the method of unitary transformations (Refs. 6–9,17).

k^2	$E_0^D + 1$	$E_0^{\text{CCM}} + 1$	Ref. 19	Ref. 20	Refs. 6,7	Ref. 8	Ref. 9	Ref. 17
0.00	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
0.25	0.7738	0.7739	0.7741	0.7742	0.7766	0.7883	0.7877	0.7767
0.50	0.5780	0.5785	0.5799	0.5806	0.5920	0.6155	0.6119	0.5877
0.75	0.3997	0.4009	0.4045	0.4066	0.4308	0.4609	0.4522	0.4173
1.00	0.2330	0.2350	0.2415	0.2453	0.2838	0.3168	0.3017	0.2586
2.00	-0.3689	-0.3637	-0.3441	-0.3343	-0.2454	-0.2166	-0.2577	-0.3157
3.00	-0.9189	-0.9117	-0.8824	-0.8704	-0.7494	-0.7281	-0.7886	-0.8466
5.00	-1.9610	-1.9532	-1.9173	-1.9051	-1.9750	-1.7371	-1.8225	-1.8716
7.00	-2.9761	-2.9693	-2.9345	-2.9231	-2.7500	-2.7409	-2.8418	-2.8833
10.00	-4.4850	-4.4797	-4.4492	-4.4391	-4.2500	-4.4360	-4.3600	-4.3937
15.00	-6.9907	-6.9870	-6.9625	-6.9538	-6.7500	-6.7458	-6.8780	-6.9042
20.00	-9.4932	-9.4904	-9.4700	-9.4623	-9.2500	-9.2468	-9.3894	-9.4111
30.00	-14.4956	-14.4937	-14.4783	-14.4719	-14.2500	-14.2479	-14.4035	-14.4202

spectrum, on the earlier so-called “optimal” CCM results of Ref. 19, which in turn are far superior to results obtained via other many-body techniques. Furthermore, the CCM results of Wong and Lo given in Ref. 19 were obtained in the third level of their successive coupled cluster approximation scheme, and required the numerical solution of 13 nonlinear coupled equations. It is evident that the proper inclusion of the J and Π_{PJT} symmetries in our calculation, which requires the numerical solution of only the single transcendental equation (34), leads to a much simpler and considerably more accurate CCM calculation of the linear $E \otimes e$ JT ground-state energy.

In Table II we present the results of a SUB-1 CCM calculation, based on the RPJT scheme, of the ground-state energy of the linear $E \otimes e$ PJT Hamiltonian in the subresonant cases $\omega_0 = 0$ (this is again the JT case) and $\omega_0 = 0.5$, as a function of the coupling k^2 . Here, we also show the percentage error in the CCM results, as compared to the (converged) results of a numerical diagonalization of H_{PJT} in a basis consisting of 101 even-parity $j = -1/2$ states. Similar results for the supresonant cases $\omega_0 = 1.5$ and $\omega_0 = 2.0$ are tabulated in Table III. It is clear that, already in the SUB-1 approximation, the CCM ground-state energy results for the RPJT scheme are extremely accurate over the full coupling regime and for a wide range of values of the fermionic level splitting ω_0 , with a percentage error, relative to the diagonalization results, of no more than 0.38% (see Fig. 1) for the range of parameters considered here.

In order to determine ground-state expectation values other than the energy in the SUB-1 RPJT scheme, we construct the energy functional

$$\begin{aligned} \bar{H}_{\text{PJT}}[s_1, \tilde{s}_1] = & \langle \Phi | e^{-s} H_{\text{PJT}} e^s | \Phi \rangle \\ & + \tilde{s}_1 \langle \Phi | (c + \kappa) e^{-s} H_{\text{PJT}} e^s | \Phi \rangle. \end{aligned} \quad (36)$$

The normal coupled cluster method (NCCM) bra state coefficient $\tilde{s}_1$ is determined via the equation

$$\frac{\partial \bar{H}_{\text{PJT}}}{\partial s_1} = T_0 + \tilde{s}_1 T_1 = 0, \quad (37)$$

TABLE II. The ground-state energy E_0^{CCM} of the linear $E \otimes e$ PJT Hamiltonian, in the subresonant cases $\omega_0 = 0.0$ and $\omega_0 = 0.5$, obtained as a function of the coupling k^2 from a SUB-1 CCM calculation based on the RPJT scheme, compared to results (labeled E_0^D) obtained via numerical diagonalization. Also shown is the percentage error $|E_0^{\text{CCM}} - E_0^D|/E_0^D \times 100$.

ω_0	k^2	E_0^D	E_0^{CCM}	%Error
0.0	0.00	0.0000	0.0000	0.00
	0.25	-0.2262	-0.2261	0.04
	0.50	-0.4220	-0.4215	0.12
	0.75	-0.6003	-0.5991	0.20
	1.00	-0.7670	-0.7650	0.26
	2.00	-1.3689	-1.3637	0.38
	3.00	-1.9189	-1.9117	0.38
	5.00	-2.9610	-2.9532	0.26
	7.00	-3.9761	-3.9693	0.17
	10.00	-5.4850	-5.4797	0.10
	15.00	-7.9907	-7.9870	0.05
	20.00	-10.4932	-10.4904	0.03
	30.00	-15.4956	-15.4937	0.01
0.5	0.00	-0.2500	-0.2500	0.00
	0.25	-0.4125	-0.4125	0.00
	0.50	-0.5679	-0.5679	0.00
	0.75	-0.7180	-0.7178	0.03
	1.00	-0.8639	-0.8635	0.05
	2.00	-1.4191	-1.4179	0.08
	3.00	-1.9481	-1.9463	0.09
	5.00	-2.9736	-2.9716	0.07
	7.00	-3.9832	-3.9815	0.04
	10.00	-5.4892	-5.4878	0.03
	15.00	-7.9932	-7.9922	0.01
	20.00	-10.4950	-10.4943	0.01
	30.00	-15.4967	-15.4963	0.00

TABLE III. The ground-state energy E_0^{CCM} of the linear $E \otimes e$ PJT Hamiltonian, in the suprapresonant cases $\omega_0 = 1.5$ and $\omega_0 = 2.0$, obtained as a function of the coupling k^2 from a SUB-1 CCM calculation based on the RPJT scheme, compared to results (labeled E_0^D) obtained via numerical diagonalization. Also shown is the percentage error $|E_0^{\text{CCM}} - E_0^D|/E_0^D \times 100$.

ω_0	k^2	E_0^D	E_0^{CCM}	%Error
1.5	0.00	-0.7500	-0.7500	0.00
	0.25	-0.8510	-0.8510	0.00
	0.50	-0.9540	-0.9539	0.01
	0.75	-1.0589	-1.0588	0.01
	1.00	-1.1656	-1.1654	0.02
	2.00	-1.6095	-1.6085	0.06
	3.00	-2.0745	-2.0728	0.08
	5.00	-3.0402	-3.0382	0.07
	7.00	-4.0264	-4.0245	0.05
	10.00	-5.5174	-5.5159	0.03
	15.00	-8.0111	-8.0101	0.01
	20.00	-10.5082	-10.5074	0.01
	30.00	-15.5054	-15.5048	0.00
2.0	0.00	-1.0000	-1.0000	0.00
	0.25	-1.0845	-1.0845	0.00
	0.50	-1.1714	-1.1713	0.01
	0.75	-1.2607	-1.2604	0.02
	1.00	-1.3525	-1.3519	0.04
	2.00	-1.7440	-1.7407	0.19
	3.00	-2.1708	-2.1645	0.29
	5.00	-3.0945	-3.0861	0.27
	7.00	-4.0625	-4.0549	0.19
	10.00	-5.5413	-5.5354	0.11
	15.00	-8.0266	-8.0224	0.05
	20.00	-10.5196	-10.5164	0.03
	30.00	-15.5129	-15.5107	0.01

where

$$T_0 \equiv \frac{\partial \langle \Phi | e^{-s} H_{\text{PJT}} e^s | \Phi \rangle}{\partial s_1} = \kappa(\omega_0 - 1) \exp\{2s_1 \kappa\} \langle \sigma^z \rangle$$

$$T_1 \equiv \frac{\partial \langle \Phi | (c + \kappa) e^{-s} H_{\text{PJT}} e^s | \Phi \rangle}{\partial s_1}$$

$$= 2\kappa \exp\{2s_1 \kappa\} (\omega_0 - 1) (\kappa - \frac{1}{2}s_1) \langle \sigma^z \rangle$$

$$+ \frac{1}{2} \exp\{2s_1 \kappa\} (\omega_0 - 1) \langle \sigma^z \rangle + \frac{1}{2} [1 - \langle \sigma^z \rangle]$$

$$+ \frac{1}{2} \omega_0 \cosh\{2s_1 \kappa\} - \frac{1}{2} \sinh\{2s_1 \kappa\}$$

$$- \frac{1}{2} \exp\{2s_1 \kappa\} \langle \sigma^z \rangle. \quad (38)$$

It is evident that the other minimization condition

$$\frac{\partial \bar{H}_{\text{PJT}}}{\partial \tilde{s}_1} = 0, \quad (39)$$

simply reproduces Eq. (34) for s_1 . The NCCM ground-state expectation value of the operator σ^z in the SUB-1 RPJT scheme is then given by

$$\langle \sigma^z \rangle^{\text{CCM}} = \exp\{2s_1 \kappa\} \langle \sigma^z \rangle (1 - s_1 \tilde{s}_1 + 2\kappa \tilde{s}_1)$$

$$+ \frac{\tilde{s}_1}{2\kappa} \sinh\{2s_1 \kappa\}, \quad (40)$$

with s_1 and $\tilde{s}_1$ determined via (34) and (38), respectively. In Fig. 2, our results for $\langle \sigma^z \rangle^{\text{CCM}}$, for the representative cases $\omega_0 = 0$ and $\omega_0 = 2.0$, are compared to the numerical diagonalization

FIG. 1. The percentage error, when compared to the results of a numerical diagonalization, in the ground-state energy of the linear $E \otimes e$ PJT Hamiltonian obtained from a SUB-1 CCM calculation based on the RPJT scheme, as a function of the coupling k^2 and the two-level splitting ω_0 .

ization results. Our CCM results, though quantitatively inaccurate for intermediate and large coupling, are at least qualitatively acceptable over the full coupling spectrum.

The first excited state energy of H_{PJT} is useful in, e.g., the analysis of the optical absorption properties of the linear $E \otimes e$ PJT model. Since the symmetries of the Hamiltonian H_{PJT} are built into our calculation, it is straightforward to extend the CCM analysis based on the RPJT scheme to the first excited state of H_{PJT} , which is an odd-parity state corresponding to $j = 1/2$. This can be done by repeating the ground-state analysis above, but with a model state of the form

FIG. 2. The ground-state expectation value $\langle \sigma^z \rangle$ for the linear $E \otimes e$ PJT Hamiltonian, in the representative cases $\omega_0 = 0.0$ and $\omega_0 = 2.0$, obtained as a function of the coupling k^2 from a SUB-1 CCM calculation based on the RPJT scheme (dotted lines labeled $\langle \sigma^z \rangle^{\text{CCM}}$), compared to results obtained via a numerical diagonalization (solid lines labeled $\langle \sigma^z \rangle^{\text{CI}}$).

TABLE IV. The first excited-state energy E_1^{CCM} of the linear $E \otimes e$ PJT Hamiltonian, in the cases $\omega_0 = 0.5$ and $\omega_0 = 1.0$, obtained as a function of the coupling k^2 from a SUB-1 CCM calculation based on the RPJT scheme, compared to results (labeled E_1^D) obtained via numerical diagonalization. Also shown is the percentage error $|E_1^{\text{CCM}} - E_1^D|/E_1^D \times 100$.

ω_0	k^2	E_1^D	E_1^{CCM}	%Error
0.5	0.00	0.2500	0.2500	0.000
	0.25	-0.0935	-0.0930	0.531
	0.50	-0.3325	-0.3307	0.528
	0.75	-0.5351	-0.5317	0.636
	1.00	-0.7176	-0.7124	0.726
	2.00	-1.3505	-1.3387	0.874
	3.00	-1.9123	-1.8967	0.815
	5.00	-2.9620	-2.9454	0.559
	7.00	-3.9785	-3.9641	0.361
	10.00	-5.4874	-5.4763	0.201
	15.00	-7.9925	-7.9848	0.961
	20.00	-10.4946	-10.4888	0.055
	30.00	-15.4966	-15.4927	0.025
1.0	0.00	0.5000	0.5000	0.000
	0.25	-0.0560	-0.0558	0.395
	0.50	-0.3173	-0.3156	0.552
	0.75	-0.5307	-0.5267	0.757
	1.00	-0.7197	-0.7130	0.921
	2.00	-1.3633	-1.3466	1.227
	3.00	-1.9277	-1.9047	1.192
	5.00	-2.9764	-2.9511	0.848
	7.00	-3.9904	-3.9682	0.554
	10.00	-5.4963	-5.4792	0.310
	15.00	-7.9986	-7.9868	0.148
	20.00	-10.4993	-10.4903	0.085
	30.00	-15.4997	-15.4936	-0.039

$$|\Phi\rangle = \frac{1}{\sqrt{I_0(2\kappa^2) + I_1(2\kappa^2)}} \times \{I_0(2\kappa^2) - I_1(2\kappa^2)\} |0\rangle |0\rangle |\uparrow\rangle. \quad (41)$$

However, it is easily shown that this is equivalent to the following procedure: the first excited state of H_{PJT} is, due to the invariance properties of the (exact) Longuet-Higgins relations (18), given by the ground state of the new Hamiltonian obtained by making the replacement $\omega_0 \rightarrow -\omega_0$ in H_{PJT} ; for the first excited state in the CCM, one therefore simply makes this replacement in Eq. (32), which determines the CCM energy, and in Eqs. (34) and (38), which determine the CCM coefficients s_1 and $\tilde{s}_1$. The calculation is otherwise identical to that presented above for the ground state. It is important to note, however, that the model state (41) is not the analytic first excited state of the resonant ($\omega_0 = 1$) linear $E \otimes e$ pseudo-Jahn-Teller Hamiltonian, H_{RPJT} . Also, for the pure JT case ($\omega_0 = 0$), the procedure outlined above clearly gives the same energy results as for the ground state, reproducing the known twofold degeneracy of the H_{JT} ground state.

In Table IV we present the results of a SUB-1 CCM calculation, based on the RPJT scheme, of the first excited-state energy of the linear $E \otimes e$ PJT Hamiltonian, in the cases $\omega_0 = 0.5$ and $\omega_0 = 1.0$, as a function of the coupling k^2 . We also show the percentage error in the CCM results, as compared to the (converged) results of a numerical diagonaliza-

FIG. 3. The percentage error, when compared to the results of a numerical diagonalization, in the first excited-state energy of the linear $E \otimes e$ PJT Hamiltonian obtained from a SUB-1 CCM calculation based on the RPJT scheme, as a function of the coupling k^2 and the two-level splitting ω_0 .

tion of H_{PJT} in a basis consisting of 101 odd-parity $j = 1/2$ states. Though not as good as the ground-state results, the CCM results for the first excited-state energy are still very accurate, over the full coupling spectrum, for the range of ω_0 considered here. For $\omega_0 > 1$, the SUB-1 calculation based on the RPJT scheme breaks down, indicating that the model state (41) is not a physically realistic starting state for the first excited state beyond $\omega_0 = 1$.

In Fig. 3 we plot the percentage error in the results of the SUB-1 RPJT scheme calculation of the first excited-state energy of H_{PJT} as compared to results obtained via numerical diagonalization, as a function of k^2 and ω_0 . For the range $0 \leq \omega_0 \leq 1$, the maximum percentage error of 1.2% occurs at intermediate coupling for the resonant case $\omega_0 = 1$.

V. CONCLUSIONS

We have shown that, even to first order, the CCM can yield very accurate results for the ground- and first excited states of the linear $E \otimes e$ JT and PJT Hamiltonians, provided that one chooses an appropriate model state. Incorporating the correct J and Π_{PJT} symmetries clearly leads to both a simpler calculation and more accurate results than have been previously obtained. It is also important to choose a model state which mimics the physical behavior of these states and in particular reproduces both the small and large coupling behavior. (It can in fact be shown that if one uses the zero coupling or noninteracting state as the model state one obtains an artificial termination in the CCM results.³⁵) It would also be interesting to extend these calculations both to higher lying excited states of the JT and PJT Hamiltonians, and to related nonadiabatic Hamiltonians, in particular the $\Gamma_8 \otimes \tau_2$ Hamiltonian,³ bearing the above points in mind.

To conclude, we have presented approximate calculations for the ground- and first excited-state energies of the JT and PJT Hamiltonians that require the solution of only a single transcendental equation. These calculations thus provide not only accurate but also practicable estimates for these quantities.

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