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# CCM CALCULATIONS ON MODEL NON-ADIABATIC HAMILTONIANS

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## 1. INTRODUCTION

Non-adiabatic models of a two-level fermionic system interacting with one or two independent bosonic modes are of interest for several reasons. The first reason is that they serve as simple prototypical many-particle Hamiltonians for many different physical systems. In quantum optics such models describe the resonant or near-resonant interaction of an atom with one or two perpendicularly polarized modes of a quantized electromagnetic field. For a single mode this model is known as the Rabi Hamiltonian, or equivalently as the Jaynes-Cummings model without the rotating wave approximation (RWA) [1-2]. In quantum chemistry such models describe the vibronic coupling between two electronic levels and two degenerate nuclear vibrational modes in a molecule or crystal. In the case where the electronic levels are degenerate this is known as the linear $E \otimes e$ Jahn-Teller model and in the case where they are not as the linear $E \otimes e$ pseudo Jahn-Teller model [3]. Another realization is the two-site polaron problem describing the interaction of an electron restricted to two lattice sites with one or two lattice phononic modes. Although analytic solutions to both the Rabi and pseudo Jahn-Teller Hamiltonians have been found at isolated values of the fermionic-bosonic coupling [4-5], complete analytic solutions are only available for special values of the bosonic frequency and/or the fermionic level splitting. Since this

class of Hamiltonians is so widely applicable, it is important to find simple tractable approximations.

The second reason such models are interesting is their simplicity. Not only do they contain interesting symmetries, but quasi-exact results are readily obtainable from large-scale diagonalization. They are nonetheless real and non-trivial many-body Hamiltonians, and as such serve as ideal testing grounds for many-body techniques. In particular we shall discuss the application of the coupled cluster method (CCM) (see the review [6]) to these Hamiltonians, underlining some of the drawbacks of the method and suggesting an appropriate resolution. We shall also consider a variational technique in the case of the Rabi Hamiltonian.

The generic form of the non-adiabatic Hamiltonians considered is

$$\hat{H} = \frac{1}{2}\omega_0\sigma^z + \omega_1 b_1^\dagger b_1 + \omega_2 b_2^\dagger b_2 + \eta_1(b_1^\dagger + b_1)\sigma^x + \eta_2(b_2^\dagger + b_2)\sigma^y, \qquad (1)$$

where the two-level fermionic system of level splitting $\omega_0$, represented in terms of the Pauli-matrices $\sigma^x, \sigma^y$ and $\sigma^z$, is interacting with coupling strengths $\eta_1$ and $\eta_2$ with two perpendicular boson modes of angular frequencies $\omega_1$ and $\omega_2$. We have taken $\hbar = 1$, and the usual commutation relations $\left[b_1, b_1^\dagger\right] = 1 = \left[b_2, b_2^\dagger\right]$ apply.

For the case of the Rabi Hamiltonian one has only one bosonic mode

$$\hat{H} = \frac{1}{2}\omega_0\sigma^z + \omega b^\dagger b + 2g(b^\dagger + b)\sigma^x. \qquad (2)$$

where one has written $\eta \equiv 2g$. In this case one expects many-body effects to become more important as one increases the electromagnetic field strength and thus the coupling $g$. For the linear $E \otimes e$ pseudo Jahn-Teller Hamiltonian, the two bosonic modes are degenerate,

$$\hat{H} = \frac{1}{2}\omega_0\sigma^z + \omega b_1^\dagger b_1 + \omega b_2^\dagger b_2 + \eta(b_1^\dagger + b_1)\sigma^x - \eta(b_2^\dagger + b_2)\sigma^y, \qquad (3)$$

and the electronic levels are either degenerate ($\omega_0 = 0$) or nearly degenerate ($\omega_0 << \omega$).

There is an important parity symmetry for these Hamiltonians. The operator that gives the total number of excitation quanta is

$$\hat{N} \equiv b_1^\dagger b_1 + b_2^\dagger b_2 + \frac{1}{2}\left[\sigma^z + 1\right], \qquad (4)$$

and one can define the parity operator by

$$\hat{\Pi} \equiv \exp\left[i\pi\hat{N}\right], \qquad (5)$$

which has eigenvalues $\pm 1$. Since this operator commutes with the Hamiltonian all non-degenerate eigenstates are of good parity. In particular the ground state has even parity or an even number of excitation quanta and the first excited state has odd parity or an odd number of excitation quanta. These states become degenerate

(i.e., of mixed parity) only for zero fermionic level splitting $\omega_0 = 0$ or in the limit of infinite coupling.

## 2. THE COUPLED CLUSTER METHOD (CCM)

At the heart of the coupled cluster method lies the exponential ansatz for the exact ground–state wave function,

$$|\Psi\rangle = \exp[S]|\Phi\rangle; \quad S = \sum_{I \neq 0} s_I C_I^\dagger, \tag{6}$$

in terms of a (normalised) model state $|\Phi\rangle$ and a corresponding complete set of commuting multiconfigurational creation operators $\{C_I^\dagger\}$ defined with respect to it. It is often convenient, although not essential, to choose these such that $C_I|\Phi\rangle = 0 = \langle\Phi|C_I^\dagger, \forall I \neq 0$ where we define $C_0^\dagger \equiv 1$. Apart from the requirements that the model state not be orthogonal to the exact ground state and that the creation operators form a complete set, this choice is in principle arbitrary, although the better the choice the more rapid is likely to be the resulting rate of convergence. The Schrödinger equation $H|\Psi\rangle = E_g|\Psi\rangle$ can then be rewritten in terms of the similarity transformed Hamiltonian as $\exp[-S]H \exp[S]|\Phi\rangle = E_g|\Phi\rangle$, so that $E_g = \langle\Phi|\exp[-S]H \exp[S]|\Phi\rangle$. The similarity transformed Hamiltonian can then be expanded using the nested commutator expansion

$$\exp[-S]H \exp[S] = H + [H, S] + \frac{1}{2}[[H, S], S] + \cdots, \tag{7}$$

which generally terminates at finite order and is therefore computationally tractable, in contrast to the unitary transform $\exp[S^\dagger]H \exp[S]$. The CCM bra ground state, $\langle\tilde{\Psi}|$, is not simply the manifest Hermitian conjugate of $|\Psi\rangle$, but can be parameterized in two ways [7]. The first is the normal CCM (NCCM) for which

$$\langle\tilde{\Psi}| = \langle\Phi|\tilde{S} \exp[-S]; \quad \tilde{S} = 1 + \sum_{I \neq 0} \tilde{s}_I C_I. \tag{8}$$

The second is the extended CCM (ECCM) [7] where the bra state is parameterized as

$$\langle\tilde{\Psi}| = \langle\Phi|\exp(\tilde{\Sigma}) \exp[-S]; \quad \tilde{\Sigma} = \sum_{I \neq 0} \tilde{\sigma}_I C_I. \tag{9}$$

We note that $\langle\tilde{\Psi}|\Psi\rangle = \langle\Phi|\Psi\rangle = \langle\Phi|\Phi\rangle = 1$. In both cases one constructs the energy functional for the Hamiltonian,

$$\overline{H} = \langle\tilde{\Psi}|H|\Psi\rangle, \tag{10}$$

and the coefficients are given by minimizing $\overline{H}$. Thus the NCCM coefficients $\{s_I, \tilde{s}_I\}$ are given by

$$\frac{\partial\overline{H}}{\partial s_I} = 0 = \frac{\partial\overline{H}}{\partial\tilde{s}_I}, \tag{11}$$

and the ECCM coefficients $\{s_I, \tilde{\sigma}_I\}$ by

$$\frac{\partial \overline{H}}{\partial s_I} = 0 = \frac{\partial \overline{H}}{\partial \tilde{\sigma}_I}. \tag{12}$$

Note that the fact that $\langle \tilde{\Psi} |$ is not the manifest Hermitian conjugate of $|\Psi\rangle$ means that an approximate CCM result for $E_g$ does not necessarily provide an upper bound for the true ground–state energy, which in turn implies that convergence may be non-uniform. Furthermore we note that, in general one violates Hermiticity for any finite–order truncation in the sum over the cluster correlation operators in Eqs. (6)–(9). This non-Hermiticity can lead to imaginary values for the CCM energy, but until recently; the appearance of an imaginary part; correctly signalled the presence of a phase transition in the system (see e.g. [8]). On the other hand, the CCM results are clearly size–extensive and these parameterizations do preserve the important Hellmann–Feynman theorem at all orders of approximation.

## 3. A SIMPLE APPLICATION OF THE CCM TO THE RABI HAMILTONIAN

In this section we briefly recall the results [9] obtained by applying the CCM method to the Rabi Hamiltonian (2) with the following choice of model state and operators

$$|\phi>= |0\rangle| \downarrow \rangle, \quad \hat{S} = \hat{S}_1 + \hat{S}_2$$

$$\hat{S}_1 = \sum_{n=1}^{N/2} S_n^{(1)} (b^\dagger)^{2n}; \quad \hat{S}_2 = \sum_{n=1}^{N/2} S_n^{(2)} (b^\dagger)^{2n-1} \sigma^+, \tag{13}$$

where the SUB-$N$ calculation contains a maximum of $N$ excitation quanta. At resonance $\omega = \omega_0 = 1$ and for $N/2$ an odd integer, one obtains a real termination point for the NCCM calculation at $g_c^{(N)}$ which increases with $N$ and converges smoothly to $g_c$. In the corresponding ECCM calculations [9] no termination point is observed but the ground state changes character from good (even) parity and non-degenerate to mixed parity and degenerate at coupling values similar to the termination values in the NCCM. Thus one has an apparent symmetry–breaking phase transition.

However the results of large–scale diagonalization show no evidence for a phase transition and no degeneracy at $g_c$. The results of diagonalization are not necessarily arbitrarily accurate as the order of the matrix increases (see e.g. the multi quantum of $k$–photon Rabi Hamiltonian [10]). Nonetheless for the Rabi Hamiltonian, there exist isolated analytic solutions for the higher–lying states and the large-scale diagonalizations reproduce these energies to within a numerical accuracy of $< 10^{-10}$, strongly suggesting that the large– scale numerical diagonalization is to all practical purposes exact.

Furthermore this termination in the CCM is present even for $\omega_0 = 0$ where the ground and first excited states are known analytically for all couplings and are in fact always degenerate. It therefore appears extremely likely that the phase transition predicted by the CCM is entirely spurious.

The underlying physical reason for the termination of the CCM is the marked change in character in the ground state with increasing coupling. For weak coupling the fermion is predominantly in the lower state. In a rather narrow transitional coupling region this changes to the case of equal probability in the upper and lower states This transition is similar to the localisation-delocalisation transition in the polaron problem and is not in fact a phase transition.

## 4. PROBLEMS WITH THE CCM IN THE RABI HAMILTONIAN

The mathematical reason for the termination of the above CCM method is the lack of uniform convergence for the CCM ansatz. This is most clearly seen by considering the even (and odd) parity solutions for the case of zero level splitting. These are given by

$$|\psi_\pm\rangle = \frac{1}{\sqrt{2}} \left( |\psi_{01}\rangle \pm |\psi_{02}\rangle \right) \tag{14}$$

where

$$|\psi_{01}\rangle = \exp\left(-\frac{2g^2}{\omega^2}\right) \exp\left(\frac{2g}{\omega}b^\dagger\right) |0\rangle |\downarrow\rangle_x \tag{15}$$

$$|\psi_{02}\rangle = \exp\left(-\frac{2g^2}{\omega^2}\right) \exp\left(-\frac{2g}{\omega}b^\dagger\right) |0\rangle |\uparrow\rangle_x, \tag{16}$$

and the states $|\uparrow\rangle_x$ and $|\downarrow\rangle_x$ are eigenstates of $\sigma^x$ with eigenvalues $\pm 1$ respectively. For the resonant Rabi Hamiltonian ($\omega_0 = \omega$) these are only exact for $g = 0$ and in the limit $g \to \infty$. They have the variational estimates for the energy,

$$E_\pm = -\frac{4g^2}{\omega} \mp \frac{1}{2}\omega_0 \exp\left(-\frac{8g^2}{\omega^2}\right). \tag{17}$$

If one tries to write these states in $\exp(S)$ form,

$$|\psi_+\rangle = \exp\left(\sum_{n=1}^{\infty} s_n^{(1)}(b^\dagger)^{2n} + s_n^{(2)}(b^\dagger)^{2n-1}\sigma^+\right) |0\rangle |\downarrow\rangle, \tag{18}$$

in terms of the spin raising operator, $\sigma^+ \equiv \sigma^x + i\sigma^y$, and considers the sequences $s_n^{(1)}$ and $s_n^{(2)}$, one can show analytically that

$$R^{(i)}(g) \equiv \frac{s_{n+1}^{(i)}(g)}{s_n^{(i)}(g)} = \frac{a_{n+1}^{(i)}}{a_n^{(i)}} \left(\frac{4g^2}{\omega}\right), \tag{19}$$

where $a_n^{(i)}$ is independent of $g$. Furthermore one can show numerically that $\lim_{n\to\infty} \frac{a_{n+1}^{(2)}}{a_n^{(2)}} = 0.406$ from which it follows that $R^{(2)}(g) > 1$ for $g > 0.785$. Thus, for $g > 0.785$, the sequence $s^{(2)}(g)$ diverges and the existence of any finite–order CCM expansion is prohibited.

## Table 1

The ground– and first excited–state energies of the scaled resonant ($\omega = \omega_0 = 1$) Rabi Hamiltonian as a function of the coupling $g$ as determined by a SUB-10 NCCM calculation, compared to the results obtained via a CI diagonalization in a basis of 101 states. The model state expectation values given by Eq. (17) are also shown.

| $g$ | $E_0^{CI}$ | $E_+$ | $E_0^{NCCM}$ | $E_1^{CI}$ | $E_-$ | $E_1^{NCCM}$ |
|-----|-----------|---------|------------|-----------|---------|------------|
| 0.0 | -0.50000 | -0.50000 | -0.50000 | 0.50000 | 0.50000 | 0.50000 |
| 0.2 | -0.58333 | -0.52307 | -0.58333 | 0.02337 | 0.20307 | -0.58333 |
| 0.4 | -0.87855 | -0.77902 | -0.87882 | -0.61609 | -0.50098 | -0.87882 |
| 0.6 | -1.52396 | -1.46806 | -1.52343 | -1.46444 | -1.41193 | -1.52343 |
| 0.8 | -2.59070 | -2.56298 | -2.57057 | -2.58432 | -2.55701 | -2.57057 |
| 1.0 | -4.01693 | -4.00016 | -4.00028 | -4.01590 | -3.99983 | -4.00028 |

In fact $|\psi_+\rangle$ can also be written in a different CCM form,

$$|\psi_+\rangle = \exp\left(-\frac{2g^2}{\omega}\right) \exp\left(-\frac{2g}{\omega} b^\dagger \sigma^x\right) |0\rangle| \downarrow\rangle. \qquad (20)$$

Therefore let us consider the first order ansatz $|\psi\rangle = \exp\left(s_1 b^\dagger \sigma^x\right) |0\rangle| \downarrow\rangle$. If one treats $s_1$ as a variational parameter one obtains $s_1 = -2g/\omega$ as $g \to \infty$ as expected. If however one solves for $s_1$ from the CCM one obtains $s_1 = -2g/(\omega + \omega_0)$. Thus, the CCM is incorrect to leading order precisely because of the lack of Hermiticity of the method, and in fact remains poor to all orders. The lack of Hermiticity to all finite orders is therefore also a problem within the CCM.

Possible resolutions include applying a unitary transform to the Hamiltonian as was done for the multimode Rabi model [11] and then applying the NCCM to the transformed Hamiltonian. The results of this procedure are only modestly accurate and one has destroyed the parity symmetry.

Better results can be obtained using coupling–dependent reference states which mimic the change in the exact states. For the ground state we have used $|\phi\rangle = |\psi_+\rangle$ and for the first excited state $|\phi\rangle = |\psi_-\rangle$ together with the following correlation operator for the SUB-$N$ calculation

$$\hat{S} = \sum_{n=1}^{N} s_n(c^\dagger)^n, \qquad c^\dagger \equiv b^\dagger \sigma^x + \frac{2g}{\omega}. \qquad (21)$$

Results are given for the ground and the first excited state SUB-10 calculations at resonance $\omega = \omega_0 = 1$ in Table 1, where we note the considerable improvemnent over the model state expectation values.

## 5. VARIATIONAL CALCULATIONS FOR THE RABI HAMILTONIAN

In this section we present the results of a simple variational calculation for the ground- and first excited–state energies of the Rabi Hamiltonian [12]. First one notes that the $\omega_0 = 0$ or $g \to \infty$ solutions can be written as

$$|x_{1,2}, y_{1,2}\rangle = \frac{1}{\sqrt{1 + y_{1,2}^2}} |x_{1,2}\rangle \exp\left(y_{1,2}\sigma^+/2\right) |\downarrow\rangle \tag{22}$$

where $|x\rangle = e^{-\frac{x^2}{2}} e^{xb^\dagger} |0\rangle$ denotes a coherent state $b|x\rangle = x|x\rangle$ and $x_{1,2} = \pm\frac{2g}{\omega}, y_{1,2} = \mp 1$. One can use $|x, y\rangle$ as a 2-parameter variational ansatz, but the result has a discontinuous derivative at $g = \sqrt{\omega\omega_0/4}$.

This ansatz however neglects the parity symmetry. Using the relationship $\hat{\Pi}|x, y\rangle = |-x, -y\rangle$ it is straightforward to construct states of good even and odd parity respectively $|x, y\rangle_P = |x, y\rangle \pm |-x, -y\rangle$. One notes that the states $|\psi_+\rangle$ and $|\psi_-\rangle$, which become exact in the limit of infinite coupling (and are in fact exact at $g = 0$), are of this form with $x = \frac{2g}{\omega}$ and $y = -1$. Although it is possible to solve for $x$ and $y$ variationally as above and then project out states of good even (odd) parity, it is clearly preferable to use $|x, y\rangle_P$ as our variational ansatz and then solve for these values variationally. This corresponds to projection before variation (PBV) and leads to a dramatic improvement in the results

One can rewrite these ansatzen in the form

$$\{|x\rangle \pm |-x\rangle\}|\downarrow\rangle + y\{|x\rangle \mp |-x\rangle\}|\uparrow\rangle = |x\rangle_\pm|\downarrow\rangle + y|x\rangle_\mp|\uparrow\rangle, \tag{23}$$

where the combinations $|x\rangle_\pm \equiv |x\rangle \pm |-x\rangle$ are of good even (odd) parity. One can thus also propose a 3–parameter variational ansatz

$$|x_1\rangle_\pm|\downarrow\rangle + y|x_2\rangle_\mp|\uparrow\rangle, \tag{24}$$

which yields excellent results for the ground state energy as shown in Figure 1 where the maximal error can be seen to be approximately 1 %. It also yields very good results for the first excited–state energy and the ground–state wavefunction [13].

## 6. CCM FOR THE PSEUDO JAHN-TELLER HAMILTONIAN

The pseudo Jahn-Teller Hamiltonian (3) has two important symmetries. The first is the parity as before. Secondly, the $z$-component of the total angular momentum

$$\hat{J} = i(b_1^\dagger b_2 - b_2^\dagger b_1) + \frac{1}{2}\sigma^z \tag{25}$$

is a constant of the motion with eigenvalues $j = \pm\frac{1}{2}, \pm\frac{3}{2} \cdots$.

It proves very useful to introduce the quasi-boson operator,

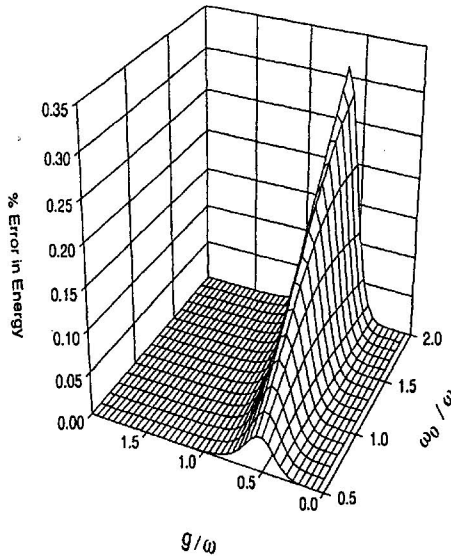$$c^\dagger = b_1^\dagger \sigma^x - b_2^\dagger \sigma^y, \tag{26}$$

**Figure 1.** The percentage error in the three parameter variational approximation to the ground state energy, $E_0$, as a function of the level splitting $\omega_0/\omega$ and the coupling $g/\omega$.

which commutes both with $\hat{J}$ and the parity operator $\hat{\Pi}$ (5). The exact ground state can then be expanded as a power series in the operator $c^\dagger$ acting on the non-interacting ground state, and the first excited state can be shown to be obtained from the ground state by the formal replacement $\omega_0 \rightarrow -\omega_0$.

As is the case of the Rabi Hamiltonian the reference state for the CCM calculation should display the same change in character as the exact state, and in particular, should reproduce the $g = 0$ and $g \rightarrow \infty$ behaviour. An appropriate reference state [13] is the exact ground state [5] of the resonant $\omega_0 = \omega$ pseudo Jahn-Teller Hamiltonian, given by

$$|\psi_0\rangle^{RPJT} = \frac{1}{\sqrt{I_0\left(2\frac{\gamma^2}{\omega^2}\right) + I_1\left(2\frac{\gamma^2}{\omega^2}\right)}} \left\{ I_0\left(2\frac{\gamma}{\omega}c^\dagger\right) - I_1\left(2\frac{\gamma}{\omega}c^\dagger\right) \right\} |0\rangle|0\rangle|\downarrow\rangle, \quad (27)$$

where $I_0$ and $I_1$ are modified Bessel functions of the first kind, and $\gamma \equiv \eta/\sqrt{2}$. This state has energy equal to the baseline energy,

$$E_0^{RPJT} = -\frac{1}{2}\omega - \frac{2\gamma^2}{\omega}. \quad (28)$$

We have used this state together with the correlation operator,

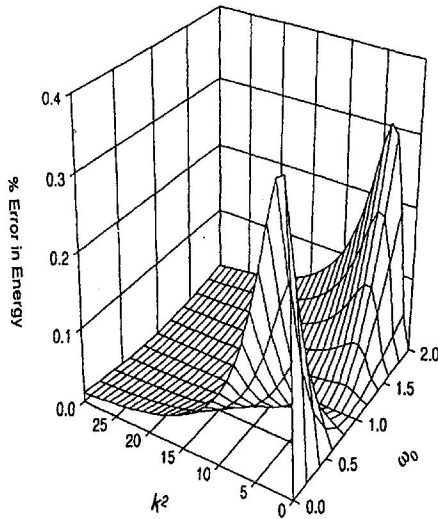$$\hat{S} = s_1\left(c^\dagger + \frac{\gamma}{\omega}\right), \quad (29)$$

**Figure 2.** The percentage error in the ground state energy ($\omega = 1$) of the linear $E \otimes e$ pseudo Jahn–Teller Hamiltonian as obtained from first-order NCCM calculations, as a function of the coupling $k^2 = 2\eta^2$ and of the level splitting $\omega_0$. Note there is zero error at $\omega_0 = \omega = 1$.

to obtain a single transcendental equation for $s_1$, which one can substitute to obtain the CCM approximation to the ground state energy [13]. The results are excellent as is clear from Figure 2 where the maximal error is less than 0.4 %. In the Jahn-Teller case $\omega_0 = 0$ they are better than those obtained via a unitary transformed CCM and a number of variational methods (see [14] and references therein)

One can obtain the solution for the first excited state simply by replacing $\omega_0$ by $-\omega_0$ in all the equations. The results obtained are not quite as good as those for the ground state, but remain remarkably accurate with a maximal error of only 1.2 %.

## 7. CONCLUSIONS AND OUTLOOK

Our results clearly show the central role that symmetry is known to play in many-body calculations. In particular including the parity symmetry leads to excellent variational results for the Rabi Hamiltonian for both the ground– and first–excited state energies. In addition, by incorporating the parity and angular momentum symmetries for the linear $E \otimes e$ pseudo Jahn-Teller Hamiltonian, one obtains results notably better than those previously obtained both via the CCM and other variational calculations [14].

We note that the application of the CCM to these systems is non-trivial since the ground state undergoes a marked change in character with increasing coupling

strength. If the CCM reference state does not reproduce this change, one encounters problems both with an effective incompleteness of the CCM ansatz and with non-Hermiticity. Indeed if one applies the CCM to the non-interacting ground state one even predicts [9], on the basis of the regular termination of the CCM results, a spurious phase transition. In fact this termination simply reflects the absence of a convergent CCM expansion at the relevant coupling.

Our calculations imply that the choice of the CCM model state is not as arbitrary as previously surmised. Ideally one needs to check whether a convergent CCM expansion exists in cases where the ground–state character changes markedly. In practice one needs to choose a reference state that reflects this change in character. If one does this, one can obtain good CCM results both for the Rabi and linear $E \otimes e$ Jahn-Teller Hamiltonians. For the Jahn-Teller case one obtains remarkable results from the solution of a single transcendental equation.

For the future, it would be interesting to study the time dependence of these systems and to study such related models as the multi–mode Rabi Hamiltonian and the $\Gamma_8 \otimes \tau_2$ Jahn–Teller Hamiltonian.

## ACKNOWLEDGMENTS

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