

SIMPLE APPROXIMATIONS FOR THE PSEUDO-JAHN-TELLER HAMILTONIAN USING THE COUPLED CLUSTER METHOD

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The normal coupled cluster method has been used to obtain simple accurate approximations to the ground and first excited state energies of the linear $e \otimes E$ pseudo-Jahn-Teller Hamiltonian.

1 Introduction

We consider a particularly simple, yet non-trivial, many-particle Hamiltonian, namely the linear $e \otimes E$ pseudo-Jahn-Teller (JT) Hamiltonian. This Hamiltonian, which describes the coupling between two degenerate bosonic modes and a two-level fermionic system, is given by

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

Here ω denotes the angular frequency of the bosonic modes; b_1^\dagger and b_2^\dagger denote bosonic creation operators $[b_1, b_1^\dagger] = [b_2, b_2^\dagger] = 1$; ω_0 denotes the fermionic level splitting, σ^x, σ^y and σ^z are the Pauli matrices, and η is the coupling strength. Clearly such a generic boson-fermion Hamiltonian is widely applicable. In particular it is extensively used in quantum chemistry, where it describes the vibronic coupling between two vibrational modes of a molecule/crystal and two (nearly) degenerate electronic levels ($\omega_0 \ll \omega$).

This Hamiltonian is also often written in terms of the circularly polarized modes,

$$a_1 \equiv \frac{1}{\sqrt{2}}(b_1 + ib_2) \quad a_2 \equiv \frac{1}{\sqrt{2}}(b_1 - ib_2), \quad (2)$$

of positive and negative helicity respectively as,

$$\hat{H} = \frac{1}{2}\omega_0\sigma^z + \omega a_1^\dagger a_1 + \omega a_2^\dagger a_2 + \gamma(a_1 + a_2^\dagger)\sigma^+ + \gamma(a_1^\dagger + a_2)\sigma^-, \quad \gamma \equiv \eta/\sqrt{2}. \quad (3)$$

Although this Hamiltonian is remarkably simple, no exact solution has yet been found.^{1a} Analytical values for these energies are however available for isolated values of the coupling η and/or the level splitting ω_0 . These are the so-called Juddian

^aExcellent, yet not exact, results can be obtained using an expansion in terms of generalized spheroidal wave functions

solutions,¹ which have been used here to test the accuracy of the numerical results obtained from a large-scale diagonalization.

One also notes that this Hamiltonian has two symmetries, which should be respected by any approximation. The first is the parity symmetry which says that the eigenstates have either an even or an odd number of “excitation” quanta. The corresponding number operator is given by

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

and the parity operator is defined in terms of it as

$$\hat{\Pi} \equiv \exp [i\pi\hat{N}]. \quad (5)$$

The ground state has even and the first excited state odd parity. The second symmetry is angular momentum. The total angular momentum,

$$\hat{J} \equiv \hat{L}_z + \hat{S}_z = i(b_1^\dagger b_2 - b_1 b_2^\dagger) + \frac{1}{2}\sigma^z, \quad (6)$$

is a constant of the motion with eigenvalues $j = \pm\frac{1}{2}, \pm\frac{3}{2}, \dots$. The ground state has $j = -\frac{1}{2}$ and the first excited state has $j = \frac{1}{2}$.

As a first step, only the ground-state and first excited-state energies for this Hamiltonian have been considered, and simple yet accurate approximations have been found using the normal coupled cluster method.²

2 The coupled cluster method

The coupled cluster method (CCM) is a very popular and successful *ab initio* many-body method. It has been widely applied in fields as diverse as quantum chemistry, nuclear physics, the electron gas, lattice gauge and continuum field theories, and spin and electron lattice models.

The basic idea behind the method is the $\exp(\hat{S})$ parameterization of the ground-state ket,

$$|\psi\rangle = e^{\hat{S}}|\phi\rangle, \quad (7)$$

where \hat{S} is the correlation operator, and $|\phi\rangle$ is the model or reference state, for which $\langle\phi|\psi\rangle \neq 0$. The correlation operator is then expanded as

$$\hat{S} = \sum_I s_I C_I^\dagger, \quad (8)$$

where the set $\{C_I^\dagger\}$ form a complete commuting set of creation operators wrt $|\phi\rangle$, chosen for convenience such that $C_I|\phi\rangle = 0 = \langle\phi|C_I^\dagger$. The Schrödinger equation,

$$\begin{aligned} \hat{H}|\psi\rangle &= E_0|\psi\rangle \\ \Rightarrow e^{-\hat{S}}\hat{H}e^{\hat{S}}|\phi\rangle &= E_0|\phi\rangle, \end{aligned} \quad (9)$$

is then rewritten in terms of the similarity (not unitary) transformed Hamiltonian

$$e^{-\hat{S}}\hat{H}e^{\hat{S}} = \hat{H} + [\hat{H}, \hat{S}] + \frac{1}{2!} [[\hat{H}, \hat{S}], \hat{S}] + \dots \quad (10)$$

In the normal coupled cluster method (NCCM) one projects the Schrödinger equation (9) onto $|\phi\rangle$ and $C_I^\dagger|\phi\rangle$ to give equations for the energy E_0 and the coefficients $\{S_I\}$ respectively,

$$\langle\phi|e^{-\hat{S}}\hat{H}e^{\hat{S}}|\phi\rangle = E_0, \quad (11)$$

$$\langle\phi|C_I e^{-\hat{S}}\hat{H}e^{\hat{S}}|\phi\rangle = 0, \quad \forall I. \quad (12)$$

These equations are of course exact. In practice however one must truncate the infinite sum over I to a finite sum of order N to obtain the so-called SUB- N approximation.

The advantages of the method include its size extensivity (cluster property), the tractability of the similarity transform and the fact that the Feynman–Hellmann theorem is satisfied to all orders. There are however some disadvantages. To any finite order the method is manifestly non-Hermitian and the CCM energy may become complex. One has no lower bound property for the CCM energy and non-uniform convergence may occur. Lastly, although the correlation operator \hat{S} always exists, a convergent expansion of the form (8) in terms of the complete set of creation operators may not exist.²

3 Results from the CCM for the pseudo-Jahn–Teller Hamiltonian

Introducing the quasi-boson operator

$$c^\dagger \equiv b_1^\dagger \sigma^x - b_2^\dagger \sigma^y = \frac{1}{2} (a_2^\dagger \sigma^+ + a_1^\dagger \sigma^-), \quad (13)$$

which commutes with \hat{J} and $\hat{\Pi}$, one can show that the ground (first-excited) state can be expanded as a power series in c^\dagger acting on the state $|0\rangle|0\rangle|\downarrow\rangle$ ($|0\rangle|0\rangle|\uparrow\rangle$), where $|0\rangle|0\rangle$ is the bosonic vacuum, and that the equations for the first excited state are obtained from those for the ground state by the formal replacement $\omega_0 \rightarrow -\omega_0$.

In practice the reference state for the CCM must give the zero coupling $\eta = 0$ and infinite coupling $\eta \rightarrow \infty$ limits of the exact eigenstate. This avoids problems with the existence of a meaningful finite order $\exp(\hat{S})$ expansion. In this case the exact ground state of the resonant ($\omega_0 = \omega$) pseudo-Jahn-Teller Hamiltonian¹ has been used as the CCM reference state, namely,

$$|\phi\rangle = \left[I_0 \left(2 \frac{\gamma^2}{\omega^2} \right) + I_1 \left(2 \frac{\gamma^2}{\omega^2} \right) \right]^{-\frac{1}{2}} \left[I_0 \left(2 \frac{\gamma}{\omega} c^\dagger \right) - I_1 \left(2 \frac{\gamma}{\omega} c^\dagger \right) \right] |0\rangle|0\rangle|\downarrow\rangle, \quad (14)$$

where I_0 and I_1 are modified Bessel functions of the first kind. Only a single correlation operator,

$$\hat{S} = s_1 \left(c^\dagger + \frac{\gamma}{\omega} \right), \quad (15)$$

has been used. One thus obtains only a single transcendental equation for s_1 from (12) and the energy from (11). The equations for the first excited state are obtained by replacing ω_0 by $-\omega_0$.

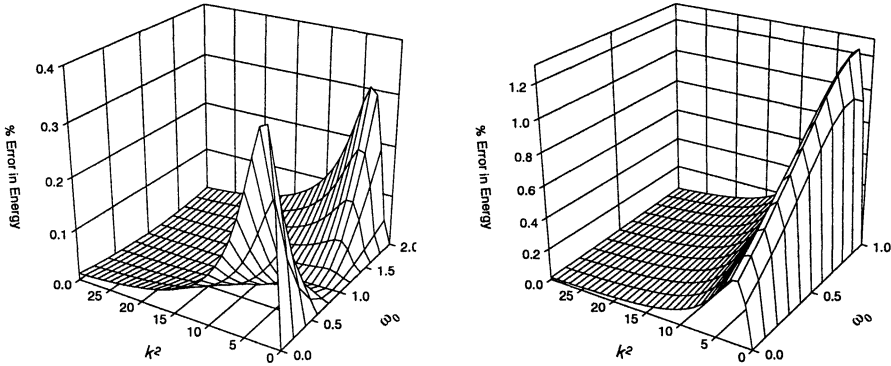


Figure 1. The percentage error in the ground-state and first excited-state energies of the linear $e \otimes E$ pseudo-JT Hamiltonian obtained from first order NCCM calculations as a function of the coupling $k^2 = 2\eta^2$ and the level splitting ω_0 .

4 Conclusions and outlook

As is evident in Fig. 1, the results are excellent. For the JT case ($\omega_0 = 0$), the results are better than results from the CCM when applied to a unitary transform of the Hamiltonian, variational methods and other unitary-transformed methods.³ In particular for the ground-state energy the maximal error (when compared to the essentially exact numerical results) is only 0.4 %. For the first excited-state energy the maximal error is only 1.2 %.

Future work could involve the study of the time and temperature dependence of this Hamiltonian, and the study of related models such as the multi-mode Rabi Hamiltonian, the polaron problem and the $\Gamma_8 \otimes \tau_2$ Hamiltonian.

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