Ground state of a two-level system with phonon coupling

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The ground state of a two-level system coupled to a dispersionless phonon bath is studied using both a connected moments expansion and a truncated Lanczos tridiagonal scheme. We consider the spin-boson Hamiltonian, $\hat{H}=-\delta_o\sigma_x+\Sigma_{\mathbf{k}}\hbar\omega_{\mathbf{k}}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+\Sigma_{\mathbf{k}}g_{\mathbf{k}}(a_{\mathbf{k}}^{\dagger}+a_{\mathbf{k}})\sigma_z$, where δ_0 is the bare tunneling matrix element and $g_{\mathbf{k}}$ represents the coupling to the $\mathbf{k}$ phonon modes. Such systems have found relevance in applications to molecular polaron formation, exciton motion, and attenuation of sound in glasses. Our results are then compared to those of variational methods as well as an exact numerical diagonalization.

The problem of simple quantum-mechanical systems with two degrees of freedom has been the focus of a great deal of attention recently.[1] Such ''two-state systems'' have found application to molecular polaron formation, exciton motion, chaos in quantum systems, spin-phonon relaxation,[2] attenuation of sound in glasses,[3] the motion of defects in certain crystalline solids and also in condensed-matter physics wherein the dissipative effect of a bath on quantum tunneling on a two-state system is of interest. In this work we wish to study the ground-state of a quantum-mechanical two-level system coupled to a dispersionless phonon bath.[4–12] Recently, Wong and Lo have applied a coupled-cluster method (CCM) to this system with great success.[13] For a particle with small tunneling probability, a dissipative two-level system may serve as a first-order approximation. The spin-boson Hamiltonian can be written in second quantized form as

$$\hat{H}=-\delta_o\sigma_x+\sum_{\mathbf{k}}\hbar\omega_{\mathbf{k}}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+\sum_{\mathbf{k}}g_{\mathbf{k}}(a_{\mathbf{k}}^{\dagger}+a_{\mathbf{k}})\sigma_z. \quad (1)$$

Here $a^{\dagger}(a)$ is the boson creation (annihilation) operator and the σ's are the Pauli spin matrices. The bare tunneling matrix element is given by δ_0, while $g_{\mathbf{k}}$ represents coupling to the $\mathbf{k}$ phonon modes. When the bare tunneling matrix element is set to zero, Eq. (1) represents a set of harmonic oscillators whose displacement is dependent on which of the two levels is occupied by the tunneling system. When the system is uncoupled ($g_{\mathbf{k}}=0$) the spin states combine both symmetrically and antisymmetrically with energies $E=\pm\delta_0$. Although there exists a competition between the localization inherent in the interaction with the phonons and the delocalization inherent in the tunneling, it is clear that this system represents a true many-body problem in that a finite number of particles (in this case electrons) is coupled to an essentially infinite number of degrees of freedom arising from the phonon modes.

Lo and Wong[14] have improved upon recent variational treatments of this problem, by obtaining an exact solution for the case of a dispersionless phonon bath, through a combination of unitary transformations and numerical diagonalization and by applying the coupled cluster method[15–18] (CCM) in a systematic fashion. An advantage of the CCM is that each level of approximation may be controlled in a manner which is dictated by the physics of the problem. The rudiments of the method are as follows. For any quantum-mechanical Hamiltonian operator $\hat{H}$, there exists a true ground-state wave function $|\psi\rangle$ and its corresponding eigenvalue E. If $\hat{H}$ is partitioned in such a way that it contains a noninteracting part $\hat{H}_0$ with ground-state wave function $|\phi\rangle$, then one may relate these two wave functions by

$$|\psi\rangle=e^{\lambda}|\phi\rangle. \quad (2)$$

The philosophy of the CCM is, in essence, to compute the quantity λ as a sum $\Sigma_n\lambda_n$, where the operators λ_n describe the excitation of a cluster of n particles (excitations above $|\phi\rangle$). Expansion of the exponential in Eq. (2) yields a sequence of terms which represents successive collections of particle-hole excitations. The energy eigenvalue equation

$$\hat{H}|\psi\rangle=\hat{H}e^{\lambda}|\phi\rangle=E_0|\psi\rangle=E_0e^{\lambda}|\phi\rangle \quad (3)$$

may be multiplied on the left-hand side by $e^{-\lambda}$ to yield a transformed Hamiltonian operator $\tilde{H}$ according to

$$\tilde{H}|\phi\rangle=e^{-\lambda}\hat{H}e^{\lambda}|\phi\rangle=e^{-\lambda}E_0e^{\lambda}|\phi\rangle=E_0|\phi\rangle, \quad (4)$$

which has the virtue that it is of finite order in the amplitude λ_n.[14] A truncation scheme for Eq. (4) yields, for the unknown amplitudes λ_n, a set of coupled nonlinear equations which are of finite order.

Following the prescription of equation Eq. (4) and choosing $\lambda=-\Sigma_{\mathbf{k}}g_{\mathbf{k}}(a_{\mathbf{k}}^{\dagger}-a_{\mathbf{k}})$, Lo and Wong[14] arrive at the following transformed Hamiltonian:

TABLE I. Ground-state energy calculated by different methods for $S=0.02$. E_{CCA} represents the result of the coupled-cluster approximation (Ref. 13), E_{EXACT} is the exact result (Ref. 14).

		$S=0.02$			
δ_0/S	$\mathrm{E}_{\mathrm{CCA}}/S$	$\mathrm{E}_{\mathrm{EXACT}}/S$	$E_{\mathrm{Lanczos}(3\times 3)}/S$	$E_{\mathrm{CMX}(3)}/S$	$E_{\mathrm{AMX}(3)}/S$
0.01	−1.009605	−1.009608	−1.009414	−1.009600	−1.009590
0.04	−1.038429	−1.038434	−1.038240	−1.038403	−1.038362
0.07	−1.067257	−1.067263	−1.067069	−1.067208	−1.067138
0.1	−1.096087	−1.096094	−1.095901	−1.096016	−1.095917
0.4	−1.384535	−1.384553	−1.384366	−1.384252	−1.383871
0.7	−1.673244	−1.673272	−1.673089	−1.672763	−1.672124
1	−1.962204	−1.962242	−1.962064	−1.961538	−1.960663
4	−4.864013	−4.864106	−4.863967	−4.862069	−4.859701
7	−7.783804	−7.783913	−7.783802	−7.781250	−7.778347
10	−10.717092	−10.717200	−10.717111	−10.714286	−10.711294

$$\tilde{H}=-\delta_o\sigma_x+\sum_{\mathbf{k}} a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+(\sigma_z-1)\sum_{\mathbf{k}} q_{\mathbf{k}}(a_{\mathbf{k}}^{\dagger}+a_{\mathbf{k}}) +S(1-2\sigma_z). \tag{5}$$

Here $S=\Sigma_{\mathbf{k}}g_{\mathbf{k}}^2$ and units are chosen such that $\hbar\omega_{\mathbf{k}}=\hbar\omega_0=1$ (for all $\mathbf{k}$). We shall use the transformed Hamiltonian as given by Eq. (5) for our Lanczos calculations.[19–23] The method is as follows: Choosing an initial trial state $|\psi_0\rangle$, an orthogonal set of states $|\psi_n\rangle$ is generated according to the scheme

$$\hat{H}|\psi_n\rangle=\epsilon_{n,n-1}|\psi_{n-1}\rangle+\epsilon_{n,n}|\psi_n\rangle+\epsilon_{n,n+1}|\psi_{n+1}\rangle, \tag{6}$$

where a tridiagonal energy matrix $\tilde{E}$, with matrix elements $\epsilon_{n,m}=\langle\psi_n|\hat{H}|\psi_m\rangle$, is also generated. Here $\epsilon_{n,m}$ is nonzero only for $n=m$ or $n=m\pm1$. An estimate of the ground-state energy is obtained by the direct diagonalization of any submatrix of $\tilde{E}$. It may be shown that state $|\psi_n\rangle$ is given recursively by[23]

$$|\psi_n\rangle=\frac{(\hat{H}-\epsilon_{n-1,n-1})|\psi_{n-1}\rangle-\epsilon_{n-1,n-2}|\psi_{n-2}\rangle}{\epsilon_{n,n-2}}, \tag{7}$$

where each of the states $|\psi_n\rangle$ is related to the initial trial ket $|\psi_0\rangle$ through a polynomial of the Hamiltonian operator

$$|\psi_n\rangle=\hat{p}_n(\hat{H})|\psi_0\rangle \tag{8}$$

and

$$\epsilon_{n,m}=\langle\psi_0|\hat{p}_n(\hat{H})\hat{H}\hat{p}_m(\hat{H})|\psi_0\rangle. \tag{9}$$

With the notation $\langle\hat{H}^n\rangle\equiv\langle\psi_0|\hat{H}^n|\psi_0\rangle$ the diagonal matrix elements $\epsilon_{n,n}$ are related to powers of the Hamiltonian $\langle\hat{H}^n\rangle$ and, to leading order, vary as $\langle\hat{H}\rangle$ for the 1×1 truncation, $\langle\hat{H}^3\rangle$ for the 2×2 truncation, $\langle\hat{H}^5\rangle$ for the 3×3 and so forth.

Another method of calculation which we shall compare results with is that of the connected moments expansion (CMX).[1] The derivation of the CMX expression for the ground-state energy has been given elsewhere.[24–27] The general expression to any order may be written as[27]

$$E_0^{(\mathrm{CMX})}=-\frac{S_{2,1}^2}{S_{3,1}}\left\{1+\frac{S_{2,2}^2}{S_{2,1}^2S_{3,2}}\left[1+\frac{S_{2,3}^2}{S_{2,2}^2S_{3,3}} \times\left(1+\cdots\left(1+\frac{S_{2,m}^2}{S_{2,m-1}^2S_{3,m}}\right)\cdots\right)\right]\right\}, \tag{10}$$

where $S_{k,1}=I_k$, $k=2,3,\ldots,$ and $S_{k,i+1}=S_{k,i}S_{k+2,i}-S_{k+1,i}^2$. This may be written explicitly to third order as

TABLE II. Ground-state energy calculated for $S=2.0$.

		$S=2.0$			
δ_0/S	$\mathrm{E}_{\mathrm{CCA}}/S$	$\mathrm{E}_{\mathrm{EXACT}}/S$	$E_{\mathrm{Lanczos}(3\times 3)}/S$	$E_{\mathrm{CMX}(3)}/S$	$E_{\mathrm{AMX}(3)}/S$
0.01	−1.000029	−1.000212	−0.745727	−0.971538	−0.749238
0.04	−1.000470	−1.001204	−0.749580	−0.902069	−0.565450
0.07	−1.001438	−1.002728	−0.754338	−0.851250	−0.527121
0.1	−1.002935	−1.004789	−0.759994	−0.814286	−0.519989
0.4	−1.047042	−1.055737	−0.863116	−0.784615	−0.684991
0.7	−1.144520	−1.164368	−1.036099	−0.963158	−0.920463
1	−1.295572	−1.330803	−1.255278	−1.200000	−1.178257
4	−4.059590	−4.067174	−4.065555	−4.058824	−4.058081
7	−7.035658	−7.037131	−7.036839	−7.034483	−7.034327
10	−10.025166	−10.025673	−10.025575	−10.024390	−10.024334

TABLE III. Ground-state energy calculated for $S=200$.

			$S=200$		
δ_0/S	E_{CCA}/S	E_{EXACT}/S	$E_{Lanczos(3\times 3)}/S$	$E_{CMX(3)}/S$	$E_{AMX(3)}/S$
0.01	−1.000025	−1.000025	−0.117091	−0.210000	−0.031778
0.04	−1.000401	−1.000401	−0.122915	−0.098824	−0.061906
0.07	−1.001227	−1.001227	−0.135064	−0.104483	−0.093077
0.1	−1.002503	−1.002503	−0.152081	−0.124390	−0.119670
0.4	−1.040051	−1.040051	−0.413028	−0.406211	−0.406117
0.7	−1.122654	−1.122659	−0.706274	−0.703559	−0.703541
1	−1.250266	−1.250336	−1.003880	−1.002494	−1.002488
4	−3.991809	−4.000732	−4.000798	−4.000625	−4.000625
7	−6.998948	−7.000387	−7.000384	−7.000357	−7.000357
10	−9.999807	−10.000264	−10.000262	−10.000250	−10.000250

$$E_0^{(\mathrm{CMX})}=I_1-\frac{I_2^2}{I_3}-\frac{1}{I_3}\frac{(I_2I_4-I_3^2)^2}{(I_5I_3-I_4^2)}-\cdots. \tag{11}$$

The coefficients of expansion I_k are just the connected moments of the Hamiltonian:

$$I_k=\langle\psi_0|\hat{H}^k|\psi_0\rangle-\sum_{i=0}^{k-2}\begin{bmatrix}k-1\\ i\end{bmatrix}I_{i+1}\langle\psi_0|\hat{H}^{k-i-1}|\psi_0\rangle. \tag{12}$$

Recently[28] a related moments expansion was introduced, the alternate moments expansion (AMX). To third order, we have

$$E_0^{(\mathrm{AMX})}=I_1-\frac{I_2I_3}{I_4}-\frac{1}{I_4}\frac{(I_2I_5-I_3I_4)(I_3I_6-I_4I_5)}{(I_4I_7-I_5I_6)}-\cdots. \tag{13}$$

We note that the CMX scheme is computationally more tractable than the AMX. This is evident by comparing equations (11) and (13), where it is seen that, to second order, CMX requires the computation of (to leading order) the third connected moment I_3, whereas the AMX expression requires the evaluation of I_4 which involves $\langle\hat{H}^4\rangle$. It is clear that since both the Lanczos tridiagonal scheme and the CMX and AMX expansions all involve moments of the Hamiltonian, $\langle\hat{H}^n\rangle$, they are related. This relationship has been given elsewhere.[23,29]

In this work we take the ground-state wave function to be

$$|\psi_0\rangle=\frac{1}{\sqrt{2}}(|\uparrow\rangle+|\downarrow\rangle)\,|\mathrm{vac}\rangle, \tag{14}$$

where $|\uparrow\rangle$ and $|\downarrow\rangle$ denote the spin-up and spin-down states respectively, and $|\mathrm{vac}\rangle$ denotes the vacuum state of all the phonon modes. In Tables I, II, and III, we present our results. Here we have followed Lo and Wang[13,14] by evaluating the ground-state energy for different values of the bare tunneling matrix element: $S=0.02$, 2.0, and 200. Also, in accordance with Lo and Wong, we have taken the phonon energy $\hbar\omega_0$ to equal unity. Comparisons of the ground-state energy using the Lanczos (3×3), CMX(3), and AMX(3) truncations are made with the exact[14] as well as the coupled-cluster results[13] of Lo and Wong. In the limit of δ_0 ''small'' wherein the system consists essentially of a set oscillators, our simple two-level system is dominated by interactions with the phonon bath and the energy may be approximated as $E_0\approx -S$. In the opposite extreme with δ_0 ''large,'' that is, in the regime where the bare tunneling matrix element dominates, we have $E_0\approx -\delta_0$. This also agrees with the results of Refs. 13,14. In the intermediate regime our results are also in remarkable agreement with the exact ones, even though we are utilizing the truncated-bases method to model the properties of an essentially infinite (phonon-bath) system.

In Figs. 1–3 we have plotted the magnitude of the ground-state energy scaled by S in a log-log representation as a function of δ_0/S with $S=0.02$, 2.0, and 200, respectively. For $S=0.02$ our results using the Lanczos (3×3) truncation as well as the CMX(3) and AMX(3) series are in excellent agreement with the exact results. As the value of S is increased (strong-coupling limit) we find that our results using these truncated-bases methods, though qualitatively in agreement with the exact results, diverge for small values of the ratio δ_0/S.

In terms of the physics of the approximation schemes it should be noted that in the CCM the transformed wave func-

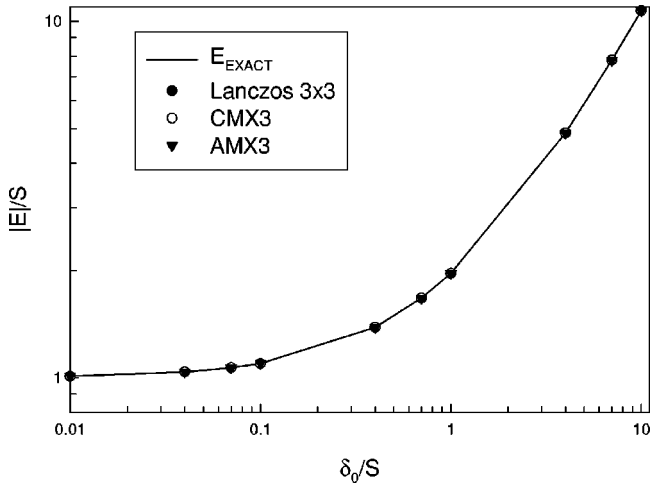

FIG. 1. Ground-state energy of the two-level system with $S=0.02$, plotted in a log-log representation.

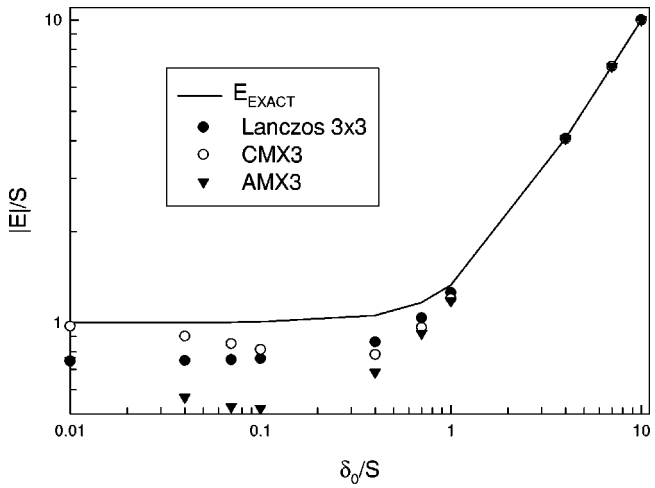

FIG. 2. Ground-state energy of the two-level system with $S=2.0$, plotted in a log-log representation.

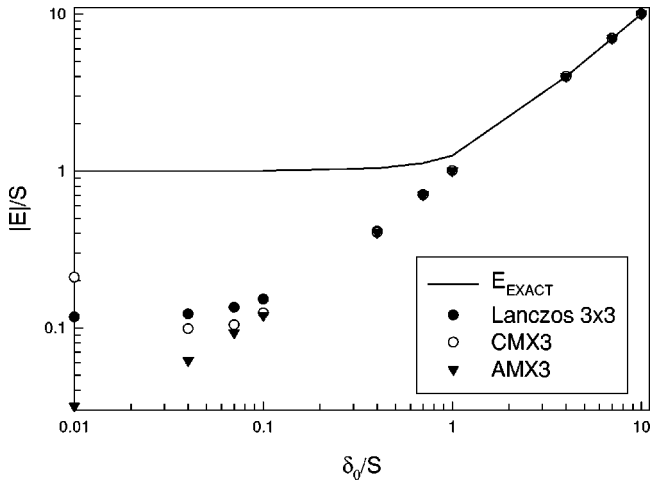

FIG. 3. Ground-state energy of the two-level system with $S=200$, plotted in a log-log representation.

tion $|\tilde{\phi}\rangle$ which yields a value for the ground-state energy E_0 does not necessarily provide an upper bound for the true value of the energy. On the other hand, both the CMX and AMX schemes rely on an ''educated'' guess for the trivial ground-state wave function which, hopefully, maximizes the overlap with the true ground state and hence is dictated by the physics of the given Hamiltonian. In such moment schemes, an essentially infinite system is approximated by a finite matrix truncation. This is valid so long as the system in question is dominated by the low-energy part of the spectrum. For the present spin-boson Hamiltonian this is indeed the case, when S is ''small'' and our results are in excellent agreement with more elaborate and calculationally more complex methods.

We see that the agreement with exact results[14] for both the 3×3 Lanczos truncation and for the third-order AMX expansion are excellent. As a numerical method of evaluation, we believe that the Lanczos scheme is calculationally much simpler than the coupled-cluster method which requires solving a number of coupled, and in general nonlinear equations. By the same token, the AMX expansion is also a fairly straightforward method that is both systematic and simple to program.

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