Ground state of a dissipative two-level system: Coupled-cluster approximation

W. H. Wong and C. F. Lo
Department of Physics, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong

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The ground state of a two-level system coupled to a dispersionless phonon bath is studied by the coupled-cluster method. The estimates of both the ground-state energy and the tunneling reduction factor are found to be in good agreement with the exact values. It is also found that within the coupled-cluster approximation there is no indication of the discontinuous localization-delocalization transition. This is consistent with the exact result. [S0163-1829(96)08042-3]

I. INTRODUCTION

The study of the influence of a phonon bath on a quantum-tunneling system is of fundamental interest, both in physics and chemistry.[1] For a particle with small tunneling probability, the system may be approximated as a dissipative two-state system. In terms of pseudospin formalism, the Hamiltonian of a two-state system coupled linearly to a phonon bath can be written as

$$H=-\Delta_0\sigma_x+\sum_{\mathbf{k}}\hbar\omega_{\mathbf{k}}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+\sum_{\mathbf{k}}g_{\mathbf{k}}(a_{\mathbf{k}}^{\dagger}+a_{\mathbf{k}})\sigma_z, \qquad (1)$$

where $a_{\mathbf{k}}$ and $a_{\mathbf{k}}^{\dagger}$ are boson annihilation and creation operators, respectively, and σ_x and σ_z are usual Pauli matrices. In this Hamiltonian Δ_0 represents the bare tunneling matrix element and $g_{\mathbf{k}}$ the coupling constant to the phonon mode $\mathbf{k}$. When $\Delta_0=0$, the system consists of a set of oscillators, displaced in one direction when the tunneling system is in one of the two levels and displaced in the other direction when the tunneling system is in the other of the two levels. Thus, there is a twofold degenerate localized ground state with energy $E=-\Sigma_{\mathbf{k}}g_{\mathbf{k}}^2(\hbar\omega_{\mathbf{k}})^{-1}$. On the other hand, when $g_{\mathbf{k}}=0$, the eigenstates of the system are the symmetric and antisymmetric combinations of the spin states with energies $E=\pm\Delta_0$. Thus, this two-state system exhibits a competition between the localization inherent in the interaction with the phonons and the delocalization inherent in the tunneling. In the intermediate regime, the effect of the phonons is to modify the tunneling matrix element and damp the oscillations.

Despite the relatively large amount of work in the literature, no exact solution to the problem is yet available in general, except for the dispersionless case ($\omega_{\mathbf{k}}=\omega_0$ for all $\mathbf{k}$).[2] There do exist, however, analytic treatments of the model based upon the variational principle.[3–12] The variational approach has two limitations. First, although the variational method always yields an upper bound of the ground-state energy, it is not trivial to improve the variational results systematically and construction of better variational trial wave functions requires good physical insight. Second, the variational ansatz may not simulate the true ground state well, even though its estimate of the ground-state energy is fairly close to the exact value. For instance, in the dispersionless case the variational calculations predict the existence of the discontinuous localization-delocalization transition and are contrary to the exact result.[9,11] It is, therefore, desirable to find a method which provides a systematic scheme to improve the approximation of the ground-state wave function. In this paper we shall explore the applicability of the coupled-cluster method (CCM) to the ground state of the dissipative two-state system. Instead of dealing with the general case of a dispersive phonon bath, we shall concentrate on the simpler case of dispersionless phonons. The CCM has proved to be a very useful technique, and has been applied to a wide range of physical systems in nuclear physics, quantum chemistry, relativistic quantum field theory, etc.[13] One of its main advantages is its systematic ability to be taken to arbitrary accuracy. The CCM can be used to calculate ground-state and excited-state energies, and also such other physical quantities as correlation functions and density matrices. Recently, the widespread success of the CCM applications has also led to the method being applied to quantum-mechanical systems defined on an extended regular spatial lattice, e.g., quantum spin systems and Hubbard model on a square lattice.[14–21]

The outline of the rest of this paper is as follows. In the next section we describe the basic elements of the CCM and apply it to a two-state system coupled to a dispersionless phonon bath. Numerical results are discussed in Sec. III. Finally, the conclusion is presented in Sec. IV.

II. THEORY

The basic idea of the CCM can be outlined as follows. The ground state of a many-body Hamiltonian H can be expressed as

$$|\psi\rangle=\exp(W)|\psi_0\rangle \qquad (2)$$

with $|\psi_0\rangle$ being an appropriate "starting wave function" which is not orthogonal to the exact ground state. The Schrödinger equation

$$H|\psi\rangle=E_0|\psi\rangle \qquad (3)$$

can be written as

$$\mathcal{H}|\psi_0\rangle\equiv\exp(-W)H\exp(W)|\psi_0\rangle=E_0|\psi_0\rangle, \qquad (4)$$

where

$$\exp(-W)H\exp(W)=H+[H,W]+\frac{1}{2!}[[H,W],W]+\cdots. \qquad (5)$$

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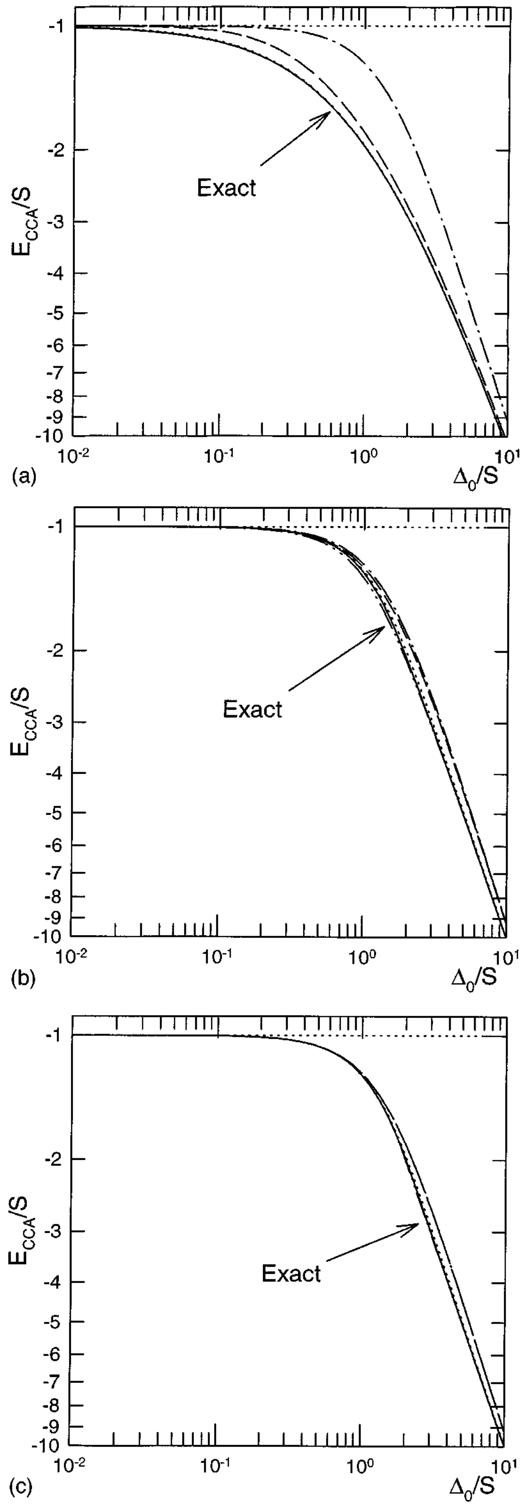

FIG. 1. Ground-state energy E_{CCA} versus Δ_0, for S=(a) 0.02, (b) 2, and (c) 200. The straight dotted line denotes the zeroth-level CCA of energy. For other curves, the dash-dotted, dashed, dotted, and solid lines represent the first-, second-, third-, and fourth-level result of the CCA, respectively. The exact result is denoted by the dash-double-dotted line.

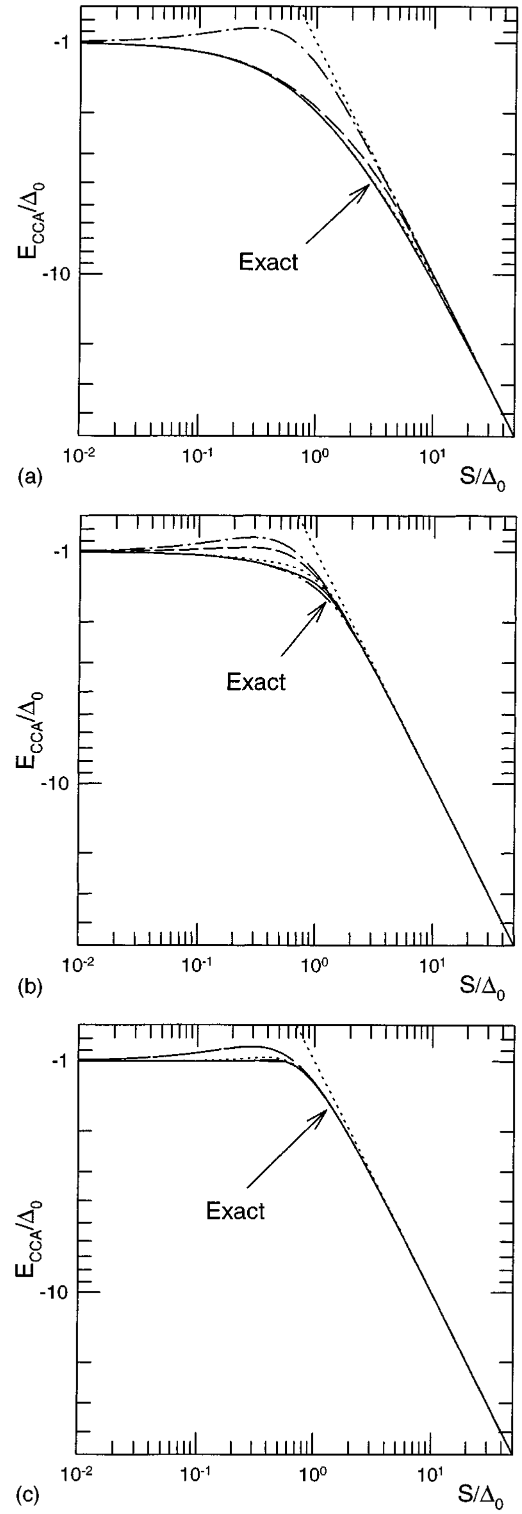

FIG. 2. Ground-state energy E_{CCA} versus S, for Δ_0=(a) 0.01, (b) 1, and (c) 100. The straight dotted line denotes the zeroth-level CCA of energy. For other curves, the dash-dotted, dashed, dotted, and solid lines represent the first-, second-, third-, and fourth-level result of the CCA, respectively. The exact result is denoted by the dash-double-dotted line.

Since $|\psi_0\rangle$ is normalized, we may write

$$\langle \psi_0 | \mathcal{H} | \psi_0 \rangle = \langle \psi_0 | \exp(-W) H \exp(W) | \psi_0 \rangle = E_0, \quad (6)$$

and by projecting Eq. (4) onto the states $|\psi_n\rangle$ which are orthogonal to $|\psi_0\rangle$ we obtain

$$\langle \psi_n | \mathcal{H} | \psi_0 \rangle = \langle \psi_n | \exp(-W) H \exp(W) | \psi_0 \rangle = 0. \quad (7)$$

This orthogonality condition yields a series of nonlinear coupled algebraic equations, each of which contains a finite number of terms. The correlation operator W is determined by solving these equations. Once W is known, the ground-state energy and wave function can be obtained readily. Hence, the problem of finding the ground-state energy and wave function of the many-body system is reduced to computing the operator W. Nevertheless, this is a very formidable task, and we have to resort to some approximation scheme to solve the coupled equations. In the following we shall apply a successive coupled-cluster approximation (CCA) scheme to investigate the ground state of a two-state system coupled to a dispersionless phonon bath. This approximation scheme was proposed by Roger and Hetherington and has been successfully applied to the antiferromagnetic Heisenberg models and the Hubbard model on a square lattice.[14–16,20] Recently, we have also applied the CCM to the linear $E-e$ Jahn-Teller system in which an electronic doublet interacting with a doubly degenerate vibration.[22]

We begin our treatment by first applying a unitary displacement transformation to the Hamiltonian H in Eq. (1): $\widetilde{H}\equiv\exp(T^\dagger)H\exp(T)$, where $T=-\Sigma_{\mathbf{k}}g_{\mathbf{k}}(a^\dagger_{\mathbf{k}}-a_{\mathbf{k}})$. After the transformation, we obtain ($\hbar\omega_{\mathbf{k}}=\hbar\omega_0=1$ for all $\mathbf{k}$)

$$\widetilde{H}=-\Delta_0\sigma_x+\sum_{\mathbf{k}} a^\dagger_{\mathbf{k}}a_{\mathbf{k}}+(\sigma_z-1)\sum_{\mathbf{k}} g_{\mathbf{k}}(a^\dagger_{\mathbf{k}}+a_{\mathbf{k}})+S(1-2\sigma_z), \tag{8}$$

where $S=\Sigma_{\mathbf{k}}g^2_{\mathbf{k}}$. To initiate our CCA, we then choose our "starting state" $|\psi_0\rangle$ to be the state $|\text{vac}\rangle|\uparrow\rangle$, where $|\text{vac}\rangle$ denotes the vacuum state of all the phonon modes, and $|\uparrow\rangle$ denotes the spin-up state. This "starting state" has the advantage that if we apply the $\widetilde{H}$ to this state, the off-diagonal term $(\sigma_z-1)\Sigma_{\mathbf{k}}g_{\mathbf{k}}(a^\dagger_{\mathbf{k}}+a_{\mathbf{k}})$ will vanish automatically. With this $|\psi_0\rangle$, we simply choose the correlation operator W in Eq. (2) to be zero as the zeroth-level approximation. In this zeroth level of CCA we have

$$\exp(-W)\widetilde{H}\exp(W)|\psi_0\rangle=-\left(S+\frac{\Delta_0}{2}\sigma_-\right)|\psi_0\rangle, \tag{9}$$

and the zeroth-level estimate of the ground-state energy $E^{(0)}_{\text{CCA}}$ is equal to $-S$. In order to get rid of the extra term in Eq. (9), we then include in W the operator σ_-, which flips an "up-spin" to a "down-spin", for the first level of CCA:

$$W=\alpha\sigma_-, \tag{10}$$

where the parameter α is to be determined. Using this correlation operator W, we obtain

$$\exp(-W)\widetilde{H}\exp(W)|\psi_0\rangle=E|\psi_0\rangle+F_0\sigma_-|\psi_0\rangle+F_1\sigma_-\sum_{\mathbf{k}} g_{\mathbf{k}}a^\dagger_{\mathbf{k}}|\psi_0\rangle, \tag{11}$$

where $E=-S-2\alpha\Delta_0$, $F_0=4\alpha S-\Delta_0(1/2-2\alpha^2)$ and $F_1=-2\alpha$. The parameter α is determined by setting F_0 equal to zero, from which we get $\alpha=-S/\Delta_0+\sqrt{(S/\Delta_0)^2+1/4}$. This, in turn, gives the first-level estimate of the ground-state energy $E^{(1)}_{\text{CCA}}$: $E^{(1)}_{\text{CCA}}=E=S-2S\sqrt{1+(\Delta_0/2S)^2}$.

Comparing the expressions of $E^{(0)}_{\text{CCA}}$ and $E^{(1)}_{\text{CCA}}$, one immediately realizes that $E^{(0)}_{\text{CCA}}$ takes care of the spin-phonon interaction only while $E^{(1)}_{\text{CCA}}$ also involves the tunneling effect, as Δ_0 appears in the expression of $E^{(1)}_{\text{CCA}}$. This is the effect of the σ_- term in W which makes a spin flip from the spin-up state to the spin-down state. If we examine α more carefully, it can be shown that as $|S/\Delta_0|\gg 1$ (large coupling), α tends to zero. This is consistent with our observation from Eq. (9) that the remaining term is negligible in this limit so that W is no longer important. On the other hand, if $|S/\Delta_0|\ll 1$ (small coupling), α tends to 1/2. In this limit, the Hamiltonian $\widetilde{H}$ is essentially given by $\widetilde{H}\approx-\Delta_0\sigma_x$. Hence, if $\alpha\approx 1/2$, $\exp(-W)\widetilde{H}\exp(W)|\psi_0\rangle\approx\exp(-\sigma_-/2)\widetilde{H}\exp(\sigma_-/2)|\psi_0\rangle=-\Delta_0|\psi_0\rangle$ and our problem is solved.

In the second level of approximation we include in W the terms necessary to cancel the remaining term of Eq. (11):

$$W=\alpha\sigma_-(1+\beta_1A_+), \tag{12}$$

where $A_+=\Sigma_{\mathbf{k}}g_{\mathbf{k}}a^\dagger_{\mathbf{k}}$. The operator A_+ corresponds to single excitations in the phonon modes. With this new correlation factor, we have

$$\exp(-W)\widetilde{H}\exp(W)|\psi_0\rangle=E|\psi_0\rangle+\sum_{n=0}^{2}F_n\sigma_-A^n_+|\psi_0\rangle+G_1A_+|\psi_0\rangle, \tag{13}$$

where

$$\begin{aligned}F_0&=-2\alpha\beta_1S-\frac{\Delta_0}{2}(1-4\alpha^2)+4\alpha S,\\ F_1&=4\alpha^2\Delta_0\beta_1+\alpha\beta_1+4\alpha S\beta_1-2\alpha,\\ F_2&=2\alpha^2\Delta_0\beta_1^2-2\alpha\beta_1,\\ G_1&=2\alpha\Delta_0\beta_1.\end{aligned} \tag{14}$$

By setting F_0 and F_1 equal to zero, a set of two coupled algebraic equations is obtained, from which we may determine the parameters β_1 and α. The corresponding second-level estimate of the ground-state energy is $E^{(2)}_{\text{CCA}}=E=-S-2\alpha\Delta_0$. In the third level of CCA, we pick the correlation operator:

$$W=\alpha\sigma_-(1+\beta_1A_++\beta_2A^2_+)+\alpha\gamma_1A_+, \tag{15}$$

and obtain

$$\exp(-W)\widetilde{H}\exp(W)|\psi_0\rangle=E|\psi_0\rangle+\sum_{n=0}^{4}F_n\sigma_-A^n_+|\psi_0\rangle+\sum_{n=1}^{2}G_nA^n_+|\psi_0\rangle, \tag{16}$$

where

$$\begin{aligned}F_0&=4\alpha S-\frac{\Delta_0}{2}(1-4\alpha^2)-2\alpha S(\beta_1+\alpha\gamma_1),\\ F_1&=4\alpha^2\beta_1\Delta_0+\alpha\beta_1+4\alpha\beta_1S-2\alpha(1+\alpha\beta_1\gamma_1S+2S\beta_2),\\ F_2&=4\alpha^2\beta_2\Delta_0+2\alpha^2\beta_1^2\Delta_0+2\alpha\beta_2+4\alpha\beta_2S\\ &\quad-2\alpha(\beta_1+\alpha\gamma_1\beta_2S),\\ F_3&=4\alpha^2\beta_1\beta_2\Delta_0-2\alpha\beta_2,\\ F_4&=2\alpha^2\beta_2^2\Delta_0,\\ G_1&=\alpha\gamma_1-2\alpha\Delta_0\beta_1,\\ G_2&=-2\alpha\beta_2\Delta_0.\end{aligned} \tag{17}$$

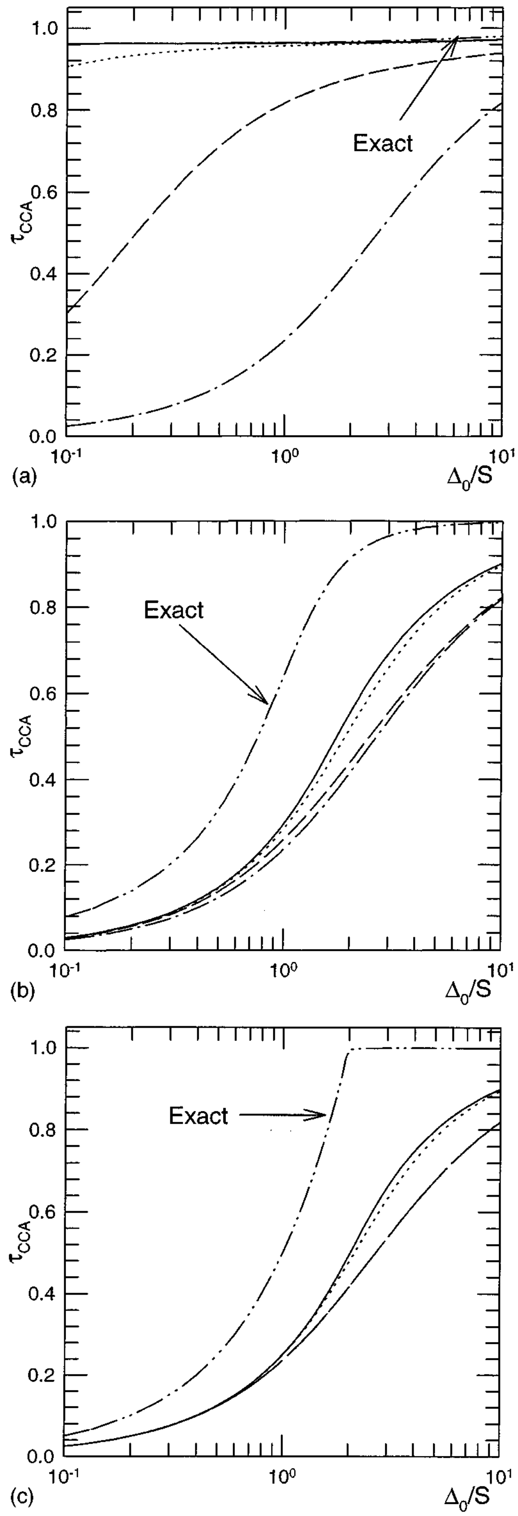

FIG. 3. Tunneling reduction factor τ_{CCA} versus Δ_0, for $S=$(a) 0.02, (b) 2, and (c) 200. The dash-dotted, dashed, dotted, and solid lines represent the first-, second-, third-, and fourth-level result of the CCA, respectively. The exact result is denoted by the dash-double-dotted line.

The parameters α, β_1, β_2, and γ_1 can be determined by equating F_0, F_1, F_2, and G_1 to zero, and the third-level estimate of the ground-state energy is given by $E_{\mathrm{CCA}}^{(3)}=E=-S-2\alpha\Delta_0$.

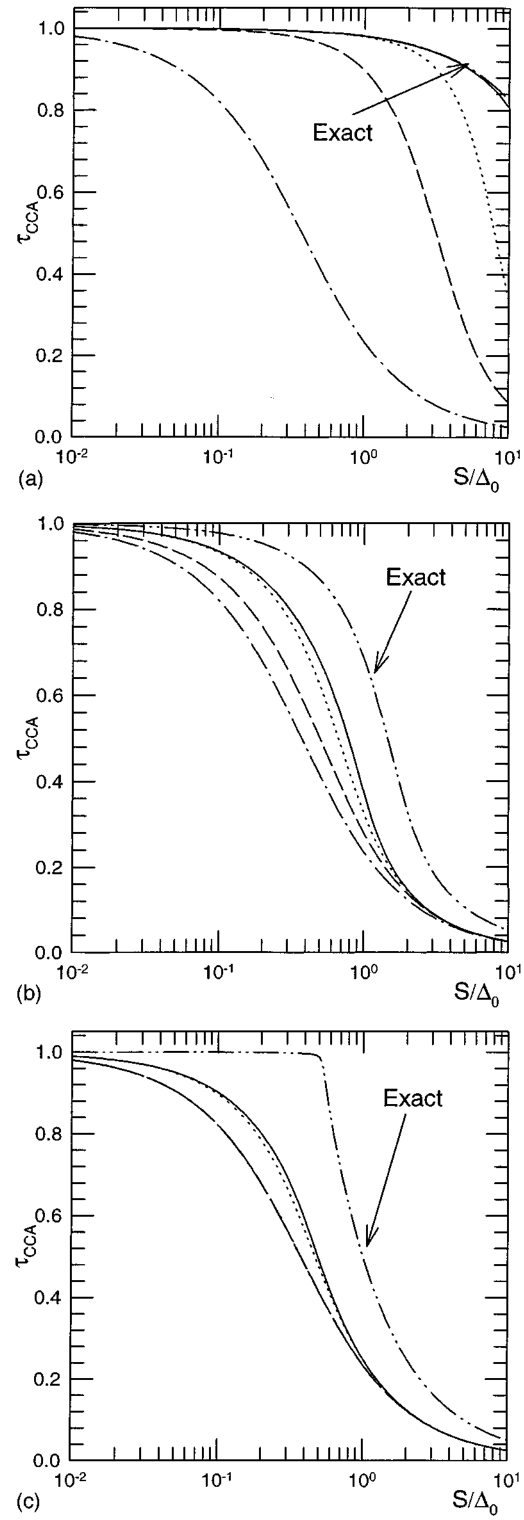

FIG. 4. Tunneling reduction factor τ_{CCA} versus S, for $\Delta_0=$(a) 0.01, (b) 1, and (c) 100. The dash-dotted, dashed, dotted, and solid lines represent the first-, second-, third-, and fourth-level result of the CCA, respectively. The exact result is denoted by the dash-double-dotted line.

Finally, following the same idea as shown above, the correlation operator W for the fourth level of CCA can be chosen as

$$W=\alpha\sigma_-\left(1+\sum_{n=1}^{4}\beta_n A_+^n\right)+\alpha\sum_{n=1}^{2}\gamma_n A_+^n. \tag{18}$$

TABLE I. Ground-state energy calculated by different methods for $S=0.02$, 2, and 200. E_{CSQ} represents the result of the variational correlated squeezed-state approach (Ref. 11).

Δ_0/S	$E^{(4)}_{\mathrm{CCA}}/S$	E_{exact}/S	E_{CSQ}/S
		$S=0.02$	
0.01	−1.009 605	−1.009 608	−1.009 608
0.04	−1.038 429	−1.038 434	−1.038 434
0.07	−1.067 257	−1.067 263	−1.067 263
0.1	−1.096 087	−1.096 094	−1.096 094
0.4	−1.384 535	−1.384 553	−1.384 553
0.7	−1.673 244	−1.673 272	−1.673 272
1	−1.962 204	−1.962 242	−1.962 241
4	−4.864 013	−4.864 106	−4.864 103
7	−7.783 804	−7.783 913	−7.783 907
10	−10.717 092	−10.717 200	−10.717 194
		$S=2$	
0.01	−1.000 029	−1.000 212	−1.000 185
0.04	−1.000 470	−1.001 204	−1.000 760
0.07	−1.001 438	−1.002 728	−1.001 369
0.1	−1.002 935	−1.004 789	−1.002 018
0.4	−1.047 042	−1.055 737	−1.015 492
0.7	−1.144 520	−1.164 368	−1.122 562
1	−1.295 572	−1.330 803	−1.309 130
4	−4.059 590	−4.067 174	−4.067 156
7	−7.035 658	−7.037 131	−7.037 130
10	−10.025 166	−10.025 673	−10.002 567
		$S=200$	
0.01	−1.000 025	−1.000 025	−1.000 000
0.04	−1.000 401	−1.000 401	−1.000 000
0.07	−1.001 227	−1.001 227	−1.000 000
0.1	−1.002 503	−1.002 503	−1.000 000
0.4	−1.040 051	−1.040 051	−1.000 000
0.7	−1.122 654	−1.122 659	−1.000 000
1	−1.250 266	−1.250 336	−1.119 031
4	−3.991 809	−4.000 732	−4.000 732
7	−6.998 948	−7.000 387	−7.000 387
10	−9.999 807	−10.000 264	−10.000 264

TABLE II. Ground-state energy calculated by different methods for $\Delta_0=0.01$, 1, and 100. E_{CSQ} represents the result of the variational correlated squeezed-state approach (Ref. 11).

S/Δ_0	$E^{(4)}_{\mathrm{CCA}}/\Delta_0$	$E_{\mathrm{exact}}/\Delta_0$	$E_{\mathrm{CSQ}}/\Delta_0$
		$\Delta_0=0.01$	
0.01	−1.009 804	−1.009 804	−1.009 804
0.04	−1.039 216	−1.039 216	−1.039 216
0.07	−1.068 628	−1.068 628	−1.068 628
0.1	−1.098 041	−1.098 041	−1.098 041
0.4	−1.392 187	−1.392 187	−1.392 187
0.7	−1.686 365	−1.686 366	−1.686 366
1	−1.980 574	−1.980 579	−1.980 579
4	−4.924 060	−4.924 512	−4.924 510
7	−7.867 917	−7.871 596	−7.871 587
10	−10.806 535	−10.821 663	−10.821 639
		$\Delta_0=1$	
0.01	−1.003 341	−1.003 341	−1.003 341
0.04	−1.013 449	−1.013 453	−1.013 453
0.07	−1.023 683	−1.023 704	−1.023 703
0.1	−1.034 033	−1.034 098	−1.034 094
0.4	−1.141 923	−1.146 829	−1.146 511
0.7	−1.251 728	−1.279 103	−1.276 632
1	−1.375 042	−1.436 545	−1.426 780
4	−4.067 031	−4.067 461	−4.000 345
7	−7.037 094	−7.037 096	−7.000 001
10	−10.025 659	−10.025 659	−10.000 000
		$\Delta_0=100$	
0.01	−1.000 050	−1.000 050	−1.000 050
0.04	−1.000 202	−1.000 203	−1.000 203
0.07	−1.000 350	−1.000 361	−1.000 361
0.1	−1.000 478	−1.000 525	−1.000 525
0.4	−0.991 066	−1.002 726	−1.002 725
0.7	−1.057 693	−1.058 663	−1.027 490
1	−1.250 598	−1.250 674	−1.121 511
4	−4.062 539	−4.062 539	−4.000 000
7	−7.035 727	−7.035 727	−7.000 000
10	−10.025 006	−10.025 006	−10.000 000

The resultant expression for $\exp(-W)\widetilde{H}\exp(W)|\psi_0\rangle$ is very lengthy and will not be presented here. By requiring the appropriate coefficients to vanish, a set of seven nonlinear coupled algebraic equations is obtained, from which the parameters in W can be determined. This, in turn, gives the fourth-level estimate of the ground-state energy $E^{(4)}_{\mathrm{CCA}}=-S-2\alpha\Delta_0$. Furthermore, within the CCA, the tunneling reduction factor $\tau^{(n)}_{\mathrm{CCA}}$ can be identified as

$$\tau^{(n)}_{\mathrm{CCA}}=2\alpha, \tag{19}$$

where n corresponds to the nth level of the CCA. In Sec. III, we shall show the numerical results for both the approximate ground-state energy and the tunneling reduction factor of the CCA.

III. NUMERICAL RESULTS AND DISCUSSION

In Figs. 1–4 we show the CCA results for different levels of approximation. In Figs. 1 and 3 we consider S fixed to the values 0.02, 2, and 200, and let the bare tunneling factor Δ_0 vary. In Figs. 2 and 4 we let S vary while fixing Δ_0 to the values 0.01, 1, and 100. We expect that if Δ_0 is small, the two-state system is mainly controlled by the interaction with phonons and thus $E\approx-S$. On the other hand, if Δ_0 is large, the energy is $E\approx-\Delta_0$. Except for the zeroth level, the results of each level of CCA agree with our expectation in these two extreme cases. For nearly all cases, our results of the ground-state energy indicate apparent convergence, and are in good agreement with the exact results.[2] However, in the intermediate region $\Delta_0\approx S\approx\hbar\omega_0=1$, the convergence is still not perfect, and discrepancy between the CCA results and the exact results is noticeable. Comparing the values of the reduction factor of the third and fourth levels, we observe that there is no significant difference for nearly all cases, except for the cases of $S=0.02$ and $\Delta_0=0.01$. In these two cases, although convergence in energy is apparent, the value of $\tau^{(4)}_{\mathrm{CCA}}$ still differs from that of $\tau^{(3)}_{\mathrm{CCA}}$ by a considerable amount. Nevertheless, we believe that higher levels of CCA will be able to

TABLE III. Tunneling reduction factor calculated by different methods for $S=0.02$, 2, and 200. τ_{CSQ} represents the result of the variational correlated squeezed-state approach (Ref. 11).

Δ_0/S	$\tau^{(4)}_{CCA}$	τ_{exact}	τ_{CSQ}
		$S=0.02$	
0.01	0.960 455	0.960 820	0.960 820
0.04	0.960 732	0.960 910	0.960 910
0.07	0.960 810	0.961 000	0.961 000
0.1	0.960 869	0.961 089	0.961 089
0.4	0.961 337	0.961 968	0.961 968
0.7	0.961 776	0.962 819	0.962 818
1	0.962 204	0.963 641	0.936 641
4	0.966 003	0.970 575	0.970 574
7	0.969 115	0.975 719	0.975 719
10	0.971 709	0.979 635	0.979 635
		$S=2$	
0.01	0.002 935	0.024 195	0.018 644
0.04	0.011 739	0.041 910	0.019 171
0.07	0.020 543	0.059 738	0.020 944
0.1	0.029 349	0.077 684	0.022 363
0.4	0.117 606	0.264 149	0.126 406
0.7	0.206 457	0.460 675	0.523 667
1	0.295 572	0.643 119	0.701 814
4	0.764 898	0.981 842	0.981 868
7	0.862 237	0.994 473	0.994 473
10	0.902 517	0.997 360	0.997 361
		$S=200$	
0.01	0.002 503	0.005 006	0.000 000
0.04	0.010 013	0.020 025	0.000 000
0.07	0.017 522	0.035 044	0.000 000
0.1	0.025 031	0.050 063	0.000 000
0.4	0.100 126	0.200 256	0.000 000
0.7	0.175 221	0.350 468	0.000 000
1	0.250 266	0.500 724	0.714 052
4	0.747 952	0.999 780	0.999 780
7	0.856 993	0.999 940	0.999 940
10	0.899 981	0.999 972	0.999 972

TABLE IV. Tunneling reduction factor calculated by different methods for $\Delta_0=0.01$, 1, and 100. τ_{CSQ} represents the result of the variational correlated squeezed-state approach (Ref. 11).

S/Δ_0	$\tau^{(4)}_{CCA}$	τ_{exact}	τ_{CSQ}
		$\Delta_0=0.01$	
0.01	0.999 804	0.999 808	0.999 808
0.04	0.999 216	0.999 231	0.999 231
0.07	0.998 628	0.998 655	0.998 655
0.1	0.998 041	0.998 079	0.998 079
0.4	0.992 187	0.992 339	0.992 339
0.7	0.986 365	0.986 630	0.986 630
1	0.980 574	0.980 953	0.980 952
4	0.924 060	0.925 882	0.925 879
7	0.867 917	0.873 798	0.873 782
10	0.806 535	0.824 552	0.824 508
		$\Delta_0=1$	
0.01	0.993 341	0.997 770	0.997 770
0.04	0.973 449	0.990 991	0.990 992
0.07	0.953 683	0.984 073	0.984 076
0.1	0.934 033	0.977 013	0.977 021
0.4	0.741 923	0.897 727	0.898 459
0.7	0.551 728	0.800 423	0.805 526
1	0.375 042	0.685 294	0.701 401
4	0.067 031	0.134 732	0.354 852
7	0.037 094	0.074 195	0.000 008
10	0.025 659	0.051 320	0.000 000
		$\Delta_0=100$	
0.01	0.990 050	0.999 950	0.999 950
0.04	0.960 202	0.999 794	0.999 794
0.07	0.930 350	0.999 627	0.999 627
0.1	0.900 478	0.999 447	0.999 447
0.4	0.591 066	0.995 737	0.995 739
0.7	0.357 693	0.718 011	0.876 268
1	0.250 598	0.501 455	0.714 044
4	0.062 539	0.125 079	0.000 000
7	0.035 727	0.071 454	0.000 000
10	0.025 006	0.050 013	0.000 000

take care of these discrepancies and ensure convergence of the results.

One important point worth noticing is that there is no evidence of the discontinuous localization-delocalization transition in our calculations; in other words, as Δ_0 or S varies, there is no abrupt jump in the value of the reduction factor. This is consistent with the exact calculations. However, this observation is far different from those results obtained by the conventional coherent-state or squeezed-state variational approaches which, contrary to the exact results, predict the existence of the discontinuous localization-delocalization transition.[8,9,11] With a correlated squeezed (CSQ) phonon state as an improved variational ansatz, the sudden change in the value of the reduction factor is removed in some cases, but it still persists in the large Δ_0 and large S regimes.[11] This indicates that these variational trial wave functions are incapable of accurately representing the exact ground state of the system. On the other hand, the good agreement of the CCA results with the exact ones seems to suggest that, unlike the variational approaches, the CCM is able to serve as a practical tool which can properly deal with the ground-state properties of the dissipative two-level systems.

In order to have a clearer comparison between the results of different methods, we have also tabulated the results of the ground-state energy in Tables I and II as well as the tunneling reduction factor in Tables III and IV. It is clear that $E^{(4)}_{CCA}$ and E_{exact} show excellent agreement. Even in the intermediate region where $\Delta_0 \approx S \approx \hbar\omega_0 = 1$, their differences are only a few percent. For other cases, the agreement is far better than this. In some cases, for example, $\Delta_0=100$ and $S/\Delta_0=4$, 7, or 10, the agreement is up to seven significant figures. Our results of the tunneling reduction factor also show good accuracy compared with the exact results. On the other hand, the CSQ works well in the region where Δ_0 or S are small enough. However, in the region where S and Δ_0 are both large, the CSQ no longer works properly. Due to its incapability of simulating the exact ground state, it predicts an abrupt jump in the tunneling reduction factor which is absent in the exact results. It seems to suggest that the CCM is able to work well in the whole parameter space, and that, even in the region where the CSQ breaks down, the CCA results agree with the exact ones with high precision.

IV. CONCLUSION

In this paper we have investigated the ground-state properties of a two-state system coupled to a dispersionless phonon bath by the coupled-cluster method. With this method, we can systematically improve not only the estimate of the ground-state energy but also the ground-state wave function. Up to the fourth level of our coupled-cluster approximation scheme, our results show good agreement with the exact results. We have found that the system shows no sign of the discontinuous localization-delocalization transition. In other words, there is no abrupt change in the value of the tunneling reduction factor as the coupling strength or the bare tunneling matrix element varies. This result contradicts those of previous studies by the variational approach but agrees with the exact result. Hence, our results seem to suggest that the coupled-cluster method is able to provide a useful tool for studying the ground-state properties of the dissipative two-state system. We are in the process of applying the coupled-cluster method to the general case of a dispersive phonon bath, and the results will be published elsewhere.

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