Eur. Phys. J. B **6**, 213–223 (1998)

THE EUROPEAN PHYSICAL JOURNAL B

Optimal coupled-cluster approximation for the ground-state properties of a spin-boson model

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Received: 11 March 1998 / Accepted: 23 June 1998

Abstract. In the present work we have developed an optimal coupled-cluster approximation, which can take care of both the accuracies of the ground-state energy and the wavefunction estimates, for the ground state of a two-state system coupled to a dispersionless boson bath. This new approach is also able to give a tight upper bound to the ground-state energy of the system. Up to the fourth level of this approximation our results show excellent agreement with the numerical exact diagonalization results. In particular, our results suggest no discontinuous localization-delocalization transition of the two-state system. This is consistent with the exact result.

PACS. 73.40.Gk Tunneling – 73.20.Jc Delocalization processes – 74.50.+r Proximity effects, weaklinks, tunneling phenomena, and Josephson effets

1 Introduction

In terms of pseudospin formalism, the Hamiltonian of a two-state system coupled linearly to a boson bath can be written as:

$$H_{SB} = -\Delta_0 \sigma_x + \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \sum_{\mathbf{k}} g_{\mathbf{k}} \left(a^\dagger_{\mathbf{k}} + a_{\mathbf{k}} \right) \sigma_z \ , \tag{1}$$

where $a_{\mathbf{k}}$ and $a^\dagger_{\mathbf{k}}$ are bosonic annihilation and creation operators, respectively, and σ_x and σ_z are usual Pauli matrices. In condensed matter physics this system has attracted much interest for the past decade because it provides a simplified description of various complicated problems such as the tunneling between two potential wells, ferroelectrics, and valence fluctuations [1] In the context of a dissipative tunneling system, Δ_0 in the Hamiltonian 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 $E = -\sum_{\mathbf{k}} g^2_{\mathbf{k}} (\hbar\omega_{\mathbf{k}})^{-1}$. 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 $E = \pm\Delta_0$. This two-state system therefore 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 (analytical or numerical) general solution to the problem is yet available, 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 [3–9]. An advantage of the variational method is that it always guarantees the ground-state energy being an upper-bound of the exact one. In other words, if the trial wavefunction is close enough to the exact ground state, the exact ground-state energy should be somewhere near and below the approximate one. However, the variational approach has two limitations. Firstly, it is not trivial to perform systematic improvements to the approximate results and construction of better trial wavefunctions requires good physical insight. The second one, which is worth our attention, is that a wavefunction determined by the variational approach may not simulate the true ground state well, even though the energy estimate is fairly accurate. This limitation is especially apparent in the dissipative tunneling system. In the dispersionless case the variational calculations predict the existence of a discontinuous localization-delocalization transition of the tunneling system [7,8] whereas the existence of such a discontinuous transition has been disproved by the exact result [2]. Accordingly, it is desirable to find a method which can provide a systematic scheme to improve the approximation of both the ground-state energy and the wavefunction.

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In our previous work [10] we applied the successive coupled-cluster approximation scheme [11–16] up to the fourth level to evaluate the ground-state energy and the tunneling reduction factor of a two-level system coupled to a dispersionless phonon bath. Our results were in good agreement with the exact (numerical) results. In this paper, to further improve this, we shall propose a modification to the approximation scheme and develop an optimal coupled-cluster approximation for the spin-boson model. Such an optimal coupled-cluster approximation has been recently applied to the linear E-e Jahn-Teller system [17]. The results are found to be better than those obtained by the conventional successive coupled-cluster approximation. Furthermore, this new approach is able to give a very tight upper bound to the ground-state energy of the system. The outline of this paper is as follows. In the next section we describe the basic elements of the coupled-cluster method and apply it to the two-state system coupled to a dispersionless boson bath within the "optimal" coupled-cluster approximation scheme. Numerical results are discussed in Section 3. Finally, the conclusion is presented.

2 Coupled-cluster method

The basic idea of the coupled-cluster method can be outlined as follows [18]. The ground state of a many-body Hamiltonian H can be expressed as

$$|\Psi\rangle = \exp(W)|\Phi_0\rangle \tag{2}$$

with $|\Phi_0\rangle$ being an appropriate "starting wavefunction" which is not orthogonal to the exact ground state. The Schrödinger equation

$$H|\Psi\rangle = E_0|\Psi\rangle \tag{3}$$

can be written as

$$\mathcal{H}|\Phi_0\rangle \equiv \exp(-W)H\exp(W)|\Phi_0\rangle = E_0|\Phi_0\rangle \tag{4}$$

where

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

Since $|\Phi_0\rangle$ is normalized, we may write

$$\langle\Phi_0|\mathcal{H}|\Phi_0\rangle = \langle\Phi_0|\exp(-W)H\exp(W)|\Phi_0\rangle = E_0, \tag{6}$$

and by projecting equation (4) onto the states $|\Phi_n\rangle$ which are orthogonal to $|\Phi_0\rangle$ we obtain

$$\langle\Phi_n|\mathcal{H}|\Phi_0\rangle = \langle\Phi_n|\exp(-W)H\exp(W)|\Phi_0\rangle = 0. \tag{7}$$

This orthogonality condition yields a series of nonlinear coupled 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 wavefunction can be obtained readily. Hence, the problem of finding the ground-state energy and wavefunction of the many-body system is reduced to computing the operator W. Nevertheless, this is a formidable task, and we have to resort to some approximation scheme to solve the coupled equations.

In our previous work [10] we started by applying a unitary displacement transformation to the Hamiltonian H_{SB} in equation (1) (with $\omega_{\mathbf{k}} \equiv \omega_0$ for all $\mathbf{k}$): $\tilde{H} = \exp(T^\dagger)H_{SB}\exp(T)$, where $T = -\sum_{\mathbf{k}} g_{\mathbf{k}}(a^\dagger_{\mathbf{k}} - a_{\mathbf{k}})/(\hbar\omega_0)$. With the "starting state" chosen to be $|\Phi_0\rangle = |\text{vac}\rangle|\uparrow\rangle$ where $|\text{vac}\rangle$ represented the vacuum boson state and $|\uparrow\rangle$ the "spin-up" state, we found that the correlation operator W might in general be written as

$$W = \mathcal{O}_1 + \mathcal{O}_2 \tag{8}$$

where

$$\mathcal{O}_1 = \alpha\left(1 + \sum_{n=1}^{\infty}\beta_n A_+^n\right)\sigma_- \quad , \quad \mathcal{O}_2 = \alpha\sum_{n=1}^{\infty}\gamma_n A_+^n \ , \tag{9}$$

with $A_+ = \sum_{\mathbf{k}} g_{\mathbf{k}} a^\dagger_{\mathbf{k}}$, $\sigma_- = \sigma_x - i\sigma_y$, as well as β_n's and γ_n's being the parameters to be determined by the coupled-cluster approximation. With W having been determined by the coupled-cluster approximation, we could write down an upper-bound of the ground-state energy:

$$E_{UB} = \frac{\langle\Phi_0|e^{W^\dagger}\tilde{H}e^{W}|\Phi_0\rangle}{\langle\Phi_0|e^{W^\dagger}e^{W}|\Phi_0\rangle} \ . \tag{10}$$

It is not difficult to show that because of the presence of $\mathcal{O}_2$, the calculation of this quantity is very complicated. By using the fact that $\sigma_-^2 = 0$, the calculation may be simplified if $\mathcal{O}_2$ is ignored. This is because in this case $\exp(W) = 1 + \mathcal{O}_1$, which contains two terms only. This simplication will serve as a key to the optimal coupled-cluster approximation to be introduced in the following.

First of all we perform a variable displacement transformation to the Hamiltonian H_{SB}:

$$\begin{aligned}\tilde{H}(\lambda) &\equiv \exp(T^\dagger)H_{SB}\exp(T)\\ &= -\Delta_0\sigma_x + \sum_{\mathbf{k}} a^\dagger_{\mathbf{k}}a_{\mathbf{k}} + \sum_{\mathbf{k}} g^2_{\mathbf{k}}\lambda(\lambda - 2\sigma_z)\\ &\quad +(\sigma_z - \lambda)\sum_{\mathbf{k}} g_{\mathbf{k}}(a^\dagger_{\mathbf{k}} + a_{\mathbf{k}})\end{aligned} \tag{11}$$

where $T = -\lambda\sum_{\mathbf{k}} g_{\mathbf{k}}(a^\dagger_{\mathbf{k}} - a_{\mathbf{k}})$ and the parameter λ is to be determined by the variational principle. For convenience, we have set the energy unit to be $\hbar\omega_0$. As the zeroth-level approximation, we simply choose the correlation operator W to be zero. Projecting $\tilde{H}(\lambda)$ onto our "starting wavefunction" $|\Phi_0\rangle = |\text{vac}\rangle|\uparrow\rangle$, we obtain

$$\begin{aligned}\tilde{H}(\lambda)|\Phi_0\rangle &= \epsilon_0\lambda(2-\lambda)|\Phi_0\rangle - \frac{\Delta_0}{2}\sigma_-|\Phi_0\rangle\\ &\quad -(\lambda - 1)A_+|\Phi_0\rangle\end{aligned} \tag{12}$$

where $\epsilon_0 = -\sum_{\mathbf{k}} g^2_{\mathbf{k}}$. The zeroth-level coupled-cluster

approximation of the ground-state energy is $E^{(0)}_{CCA} = \epsilon_0\lambda(2-\lambda)$. To find an upper-bound of the ground-state energy, we calculate the expectation value given by equation (10) [with $\tilde{H}$ replaced by $\tilde{H}(\lambda)$]:

$$E^{(0)}_{UB}(\lambda) = \frac{\langle\Phi_0|e^{W^\dagger}\tilde{H}(\lambda)e^{W}|\Phi_0\rangle}{\langle\Phi_0|e^{W^\dagger}e^{W}|\Phi_0\rangle} = \langle\Phi_0|\tilde{H}(\lambda)|\Phi_0\rangle$$
$$= E^{(0)}_{CCA} = \epsilon_0\lambda(2-\lambda)\ . \qquad (13)$$

Minimizing $E^{(0)}_{UB}$ with respect to λ, we find that the optimal value of λ is 1. The improved zeroth-level coupled-cluster approximation of the ground-state energy is therefore given by $E^{(0)}_{VCCA} = E^{(0)}_{UB}(\lambda=1) = \epsilon_0$.

There are two remaining terms in equation (12). In order to cancel these terms, both of them are to be included in the correlation operator W of the first-level succesive coupled-cluster approximation scheme. However, for the sake of algebraic simplicity in the calculation of the energy upper-bound and the tunneling reduction factor, we only include the operator with σ_-. Therefore, in the first level we choose $W = \alpha\sigma_-$, which represents the flip of an "up-spin" to a "down-spin". By using this choice, it can be found that

$$\exp(-W)\tilde{H}\exp(W)|\Phi_0\rangle = E^{(1)}_{CCA}|\Phi_0\rangle + F_0 W|\Phi_0\rangle$$
$$- 2\alpha A_+\sigma_-|\Phi_0\rangle + (1-\lambda)A_+|\Phi_0\rangle$$

where $E^{(1)}_{CCA} = \epsilon_0\lambda(2-\lambda) - 2\alpha\Delta_0$ and $\alpha F_0 = -\Delta_0(1-4\alpha^2)/2 - 4\alpha\epsilon_0\lambda$. By setting F_0 to be zero, a quadratic equation of the parameter α is obtained, which can be easily solved to give two roots. The admissible solution is given by $\alpha = \lambda\epsilon_0/\Delta_0 + \sqrt{(\lambda\epsilon_0/\Delta_0)^2 + 1/4}$. With the remaining terms being neglected, the first-level coupled-cluster approximation of the ground-state energy is given by $E^{(1)}_{CCA}$. Using equation (10) [with $\tilde{H}$ replaced by $\tilde{H}(\lambda)$], one can obtain an upper-bound of the ground-state energy, which is expressed as

$$E^{(1)}_{UB} = E^{(1)}_{CCA} = -\epsilon_0\lambda^2 - 2\Delta_0\sqrt{\left(\frac{\lambda\epsilon_0}{\Delta_0}\right)^2 + \frac{1}{4}}\ . \qquad (14)$$

Minimizing $E^{(1)}_{UB}$ with respect to λ, we obtain an optimal value, λ^*, of the variational parameter λ. Detailed calculation is not shown here. After some steps, the improved first-level coupled-cluster approximation of the ground-state energy is given by $E^{(1)}_{VCCA} = E^{(1)}_{UB}(\lambda=\lambda^*) = \epsilon_0\{1 + [\Delta_0/(2\epsilon_0)]^2\}$ for $\Delta_0 \le 2S$ and $-\Delta_0$ for $\Delta_0 > 2S$, where $S = \sum_{\mathbf{k}} g^2_{\mathbf{k}} = -\epsilon_0$. Besides, we also evaluate the tunneling reduction factor defined as

$$\tau_{VCCA} \equiv \left.\frac{\langle\Phi_0|e^{W^\dagger}e^{T^\dagger}\sigma_x e^{T}e^{W}|\Phi_0\rangle}{\langle\Phi_0|e^{W^\dagger}e^{W}|\Phi_0\rangle}\right|_{\lambda=\lambda^*}\ . \qquad (15)$$

For the first level, the tunneling reduction factor is simply given by

$$\tau^{(1)}_{VCCA} = \left.\frac{4\alpha}{1+4\alpha^2}\right|_{\lambda=\lambda^*}\ . \qquad (16)$$

In order to improve the approximation we shall include in W the terms necessary to cancel the remaining terms with $\sigma_- A_+$: $W = \alpha(1+\beta_1 A_+)\sigma_-$. The second term of W represents the simultaneous spin-flip and collective excitation of the boson modes. By setting the coefficients of $\sigma_-|\Phi_0\rangle$ and $A_+\sigma_-|\Phi_0\rangle$ to be zero, a set of two equations is obtained,

$$-\Delta_0(1-4\alpha^2) - 8\alpha\epsilon_0\lambda + 2\alpha\epsilon_0(1+\lambda)\beta_1 = 0$$
$$(4\alpha\Delta_0 + 1 - 4\epsilon_0\lambda)\beta_1 - 2 = 0\ , \qquad (17)$$

which by solving we can obtain the parameters, α and β_1, as functions of λ. The second-level coupled-cluster approximation of the ground-state energy is given by $E^{(2)}_{CCA} = \epsilon_0\lambda(2-\lambda) - 2\alpha\Delta_0$. By using equation (10) [with $\tilde{H}$ replaced by $\tilde{H}(\lambda)$], it can be shown that an energy upper-bound is given by

$$E^{(2)}_{UB} = E^{(2)}_{CCA} + \frac{8\alpha^3\Delta_0\beta_1^2\epsilon_0 - 4(1-\lambda)\alpha^2\beta_1\epsilon_0}{1+4\alpha^2(1-\beta_1^2\epsilon_0)}\ . \qquad (18)$$

$E^{(2)}_{UB}$ is minimized with respect to λ and thus an optimal value of λ, λ^*, is obtained. The improved second-level coupled-cluster approximation of the ground-state energy is $E^{(2)}_{VCCA} = E^{(2)}_{UB}(\lambda=\lambda^*)$. It is obvious that provided the parameter β_1 is not zero, there is considerable improvement beyond the first-level results (see Figs. 1 and 2 as well as Tabs. 1 to 4). By using equation (15), we have calculated the second-level coupled-cluster approximation of the tunneling reduction factor:

$$\tau^{(2)}_{VCCA} = \left.\frac{4\alpha}{1+4\alpha^2(1-\beta_1^2\epsilon_0)}\right|_{\lambda=\lambda^*}\ . \qquad (19)$$

In the third and the fourth levels we repeat the previous procedure and choose the correlation operator W for the third level as follows:

$$W = \alpha(1+\beta_1 A_+ + \beta_2 A_+^2)\sigma_-\ , \qquad (20)$$

while for the fourth level,

$$W = \alpha(1+\beta_1 A_+ + \beta_2 A_+^2 + \beta_3 A_+^3 + \beta_4 A_+^4)\sigma_-\ . \qquad (21)$$

After some straightforward, though tedious, calculations similar to those in the second-level approximation, a set of three (five) nonlinear coupled algebraic equations of the parameters, α and β_n's, is obtained, for the third (fourth) level. One needs to resort to numerical methods to solve these equations. Then, these parameters, α and β_n's, which are functions of λ, will in turn give the third-level (fourth-level) coupled-cluster approximation of the ground-state energy $E^{(3)}_{CCA} = \epsilon_0\lambda(2-\lambda) - 2\alpha\Delta_0$ [$E^{(4)}_{CCA} = \epsilon_0\lambda(2-\lambda) - 2\alpha\Delta_0$]. Using equation (10) again [with $\tilde{H}$ replaced by $\tilde{H}(\lambda)$], one obtains an upper-bound of the ground-state energy, $E^{(3)}_{UB}$ ($E^{(4)}_{UB}$), for the third (fourth) level. The expressions will not be presented here. Minimizing $E^{(3)}_{UB}$ ($E^{(4)}_{UB}$) with respect to λ, we obtain an optimal value of λ, λ^*. The improved third-level (fourth-level) coupled-cluster approximation of the ground-state

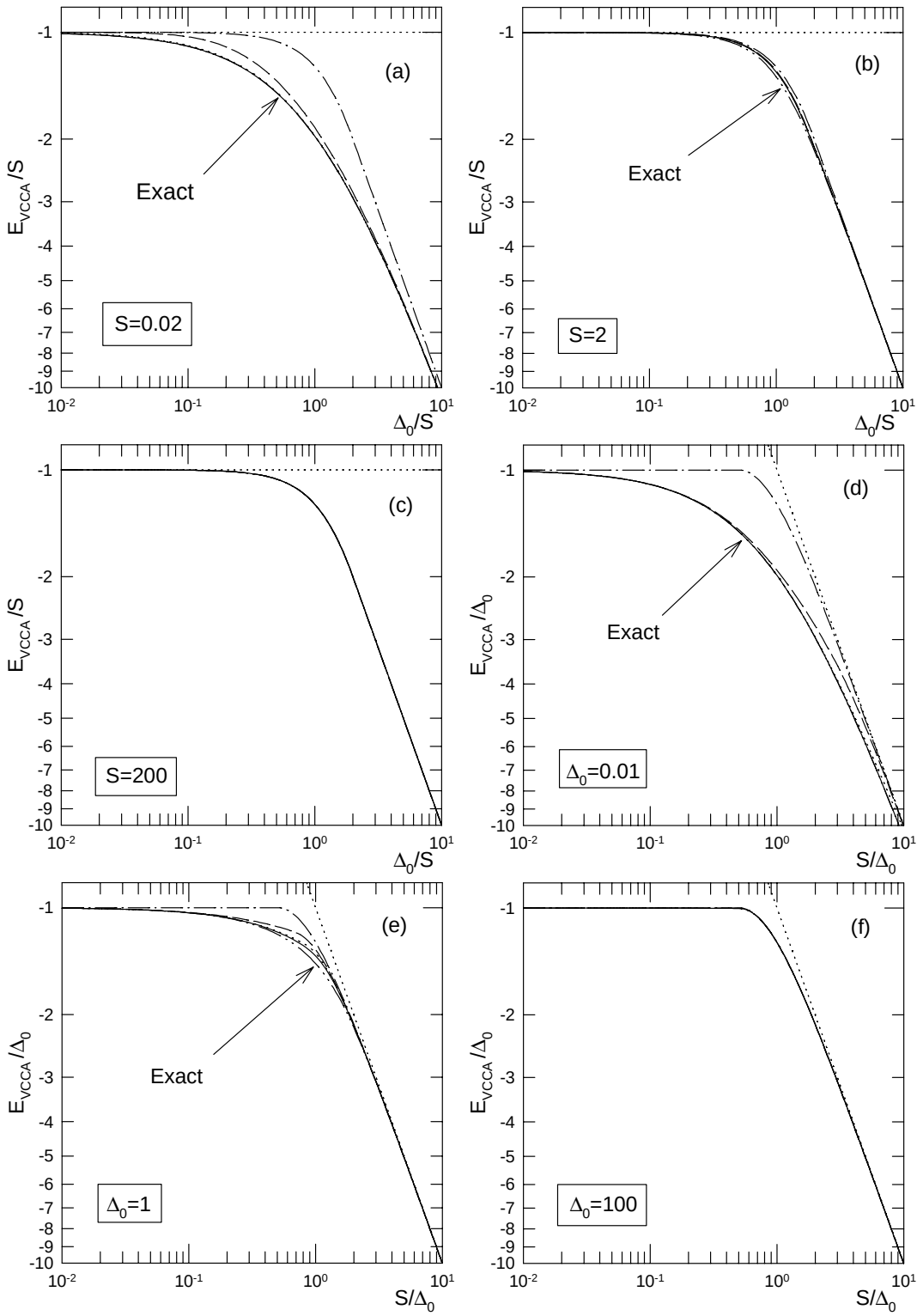

Fig. 1. Ground-state energy E_{VCCA} *versus* (a)-(c): Δ_0, for S = (a) 0.02; (b) 2; (c) 200; and (d)-(f): S, for Δ_0 = (d) 0.01; (e) 1; (f) 100. The straight dotted line denotes the zeroth-level result. For other curves, the dash-dotted, dashed, dotted, and solid lines represent the first-, second-, third-, and fourth-level results, respectively. The exact result is denoted by the dash-double-dotted line. In most regions the fourth-level result and the exact one are very close.

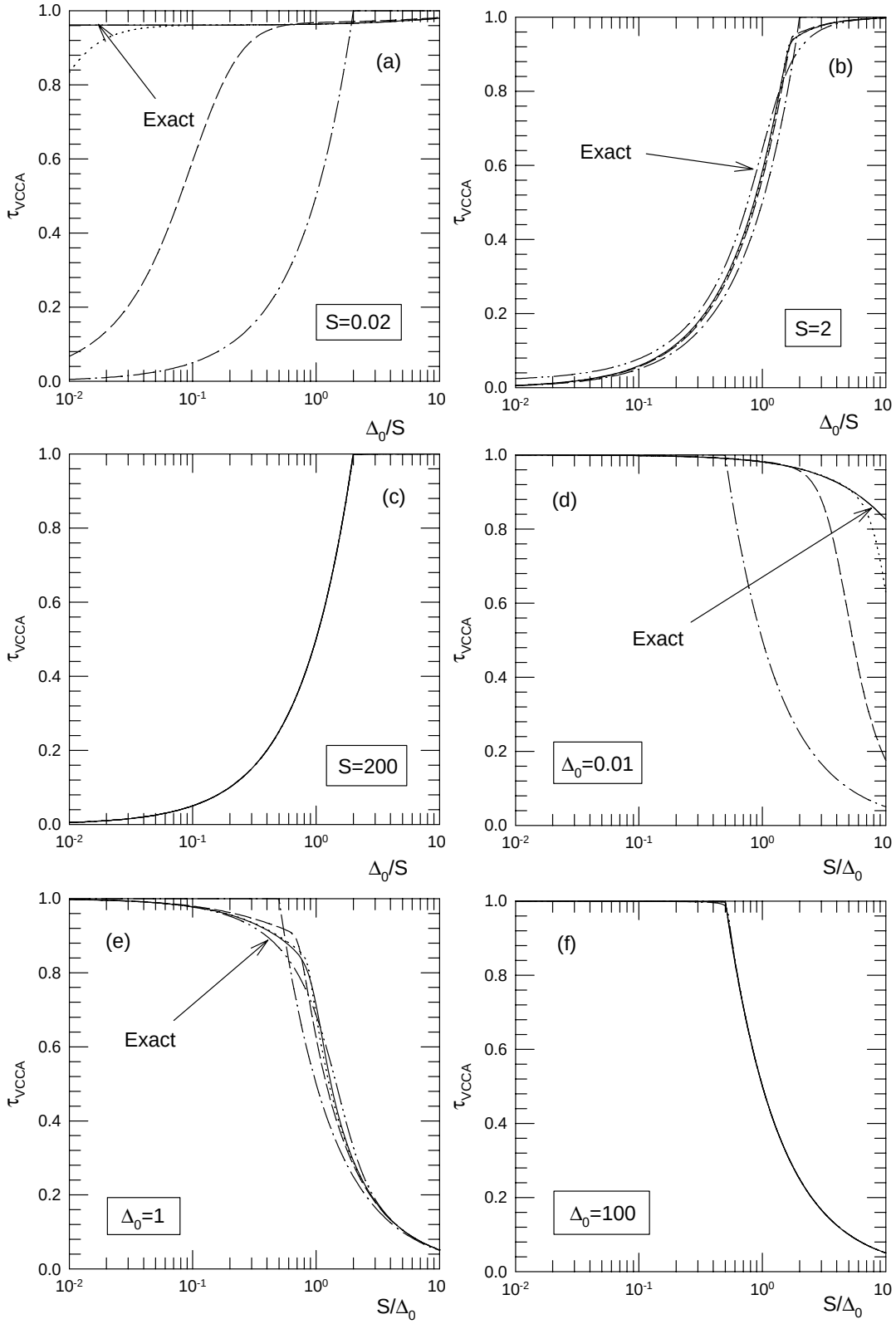

Fig. 2. Tunneling reduction factor τ_{VCCA} *versus* (a)-(c): Δ_0, for S = (a) 0.02; (b) 2; (c) 200; and (d)-(f): S, for Δ_0 = (d) 0.01; (e) 1; (f) 100. The dash-dotted, dashed, dotted, and solid lines represent the first-, second-, third-, and fourth-level results, respectively. The exact result is denoted by the dash-double-dotted line. In most regions the fourth-level result and the exact one are very close.

Table 1. Ground-state energy calculated by different methods for $S =$ (a) 0.02, (b) 2, and (c) 200. $E^{(4)}_{pre}$ represents the fourth-level result of our previous work (Ref. [10]). E_{CSQ} represents the result of the variational correlated squeezed-state approach (Ref. [8]).

Table 1a: ($S = 0.02$)

Δ_0/S	$E^{(4)}_{pre}/S$	$E^{(4)}_{VCCA}/S$	$E^{(4)}_{OP}/S$	E_{exact}/S	E_{CSQ}/S
0.01	− 1.009605	− 1.009605	− 1.009605	− 1.009608	− 1.009608
0.04	− 1.038429	− 1.038431	− 1.038429	− 1.038434	− 1.038434
0.07	− 1.067257	− 1.067259	− 1.067257	− 1.067263	− 1.067263
0.1	− 1.096087	− 1.096091	− 1.096087	− 1.096094	− 1.096094
0.4	− 1.384535	− 1.384545	− 1.384535	− 1.384553	− 1.384553
0.7	− 1.673244	− 1.673254	− 1.673245	− 1.673272	− 1.673272
1	− 1.962204	− 1.962210	− 1.962206	− 1.962242	− 1.962241
4	− 4.864013	− 4.863801	− 4.864032	− 4.864106	− 4.864103
7	− 7.783804	− 7.783292	− 7.783837	− 7.783913	− 7.783907
10	− 10.717092	− 10.716322	− 10.717135	− 10.717200	− 10.717194

Table 1b: ($S = 2$)

Δ_0/S	$E^{(4)}_{pre}/S$	$E^{(4)}_{VCCA}/S$	$E^{(4)}_{OP}/S$	E_{exact}/S	E_{CSQ}/S
0.01	− 1.000029	− 1.000029	− 1.000029	− 1.000212	− 1.000185
0.04	− 1.000470	− 1.000470	− 1.000470	− 1.001204	− 1.000760
0.07	− 1.001438	− 1.001438	− 1.001438	− 1.002728	− 1.001369
0.1	− 1.002935	− 1.002935	− 1.002935	− 1.004789	− 1.002018
0.4	− 1.047042	− 1.046945	− 1.047067	− 1.055737	− 1.015492
0.7	− 1.144520	− 1.143637	− 1.144925	− 1.164368	− 1.122562
1	− 1.295572	− 1.292487	− 1.298691	− 1.330803	− 1.309130
4	− 4.059590	− 4.059176	− 4.067179	− 4.067174	− 4.067156
7	− 7.035658	− 7.034560	− 7.037131	− 7.037131	− 7.037130
10	− 10.025166	− 10.024418	− 10.025673	− 10.025673	− 10.002567

Table 1c: ($S = 200$)

Δ_0/S	$E^{(4)}_{pre}/S$	$E^{(4)}_{VCCA}/S$	$E^{(4)}_{OP}/S$	E_{exact}/S	E_{CSQ}/S
0.01	− 1.000025	− 1.000025	− 1.000025	− 1.000025	− 1.000000
0.04	− 1.000401	− 1.000401	− 1.000401	− 1.000401	− 1.000000
0.07	− 1.001227	− 1.001227	− 1.001227	− 1.001227	− 1.000000
0.1	− 1.002503	− 1.002503	− 1.002503	− 1.002503	− 1.000000
0.4	− 1.040051	− 1.040050	− 1.040051	− 1.040051	− 1.000000
0.7	− 1.122654	− 1.122654	− 1.122659	− 1.122659	− 1.000000
1	− 1.250266	− 1.250313	− 1.250336	− 1.250336	− 1.119031
4	− 3.991809	− 4.000625	− 4.000732	− 4.000732	− 4.000732
7	− 6.998948	− 7.000357	− 7.000387	− 7.000387	− 7.000387
10	− 9.999807	− 10.000250	− 10.000264	− 10.000264	− 10.000264

Table 2. Ground-state energy calculated by different methods for Δ_0 = (a) 0.01, (b) 1, and (c) 100. $E^{(4)}_{pre}$ represents the fourth-level result of our previous work (Ref. [10]). E_{CSQ} represents the result of the variational correlated squeezed-state approach (Ref. [8]).

Table 2a: ($\Delta_0 = 0.01$)

S/Δ_0	$E^{(4)}_{pre}/\Delta_0$	$E^{(4)}_{VCCA}/\Delta_0$	$E^{(4)}_{OP}/\Delta_0$	E_{exact}/Δ_0	E_{CSQ}/Δ_0
0.01	− 1.009804	− 1.009804	− 1.009804	− 1.009804	− 1.009804
0.04	− 1.039216	− 1.039216	− 1.039216	− 1.039216	− 1.039216
0.07	− 1.068628	− 1.068628	− 1.068628	− 1.068628	− 1.068628
0.1	− 1.098041	− 1.098041	− 1.098041	− 1.098041	− 1.098041
0.4	− 1.392187	− 1.392186	− 1.392187	− 1.392187	− 1.392187
0.7	− 1.686365	− 1.686365	− 1.686365	− 1.686366	− 1.686366
1	− 1.980574	− 1.980575	− 1.980575	− 1.980579	− 1.980579
4	− 4.924060	− 4.924286	− 4.924075	− 4.924512	− 4.924510
7	− 7.867917	− 7.869159	− 7.868055	− 7.871596	− 7.871587
10	− 10.806535	− 10.809939	− 10.807118	− 10.821663	− 10.821639

Table 2b: ($\Delta_0 = 1$)

S/Δ_0	$E^{(4)}_{pre}/\Delta_0$	$E^{(4)}_{VCCA}/\Delta_0$	$E^{(4)}_{OP}/\Delta_0$	E_{exact}/Δ_0	E_{CSQ}/Δ_0
0.01	− 1.003341	− 1.003336	− 1.003341	− 1.003341	− 1.003341
0.04	− 1.013449	− 1.013372	− 1.013453	− 1.013453	− 1.013453
0.07	− 1.023683	− 1.023449	− 1.023700	− 1.023704	− 1.023703
0.1	− 1.034033	− 1.033564	− 1.034086	− 1.034098	− 1.034094
0.4	− 1.141923	− 1.136321	− 1.145885	− 1.146829	− 1.146511
0.7	− 1.251728	− 1.241796	− 1.271813	− 1.279103	− 1.276632
1	− 1.375042	− 1.367342	− 1.396707	− 1.436545	− 1.426780
4	− 4.067031	− 4.067009	− 4.067032	− 4.067461	− 4.000345
7	− 7.037094	− 7.037092	− 7.037094	− 7.037096	− 7.000001
10	− 10.025659	− 10.025659	− 10.025659	− 10.025659	− 10.000000

Table 2c: ($\Delta_0 = 100$)

S/Δ_0	$E^{(4)}_{pre}/\Delta_0$	$E^{(4)}_{VCCA}/\Delta_0$	$E^{(4)}_{OP}/\Delta_0$	E_{exact}/Δ_0	E_{CSQ}/Δ_0
0.01	− 1.000050	− 1.000050	− 1.000050	− 1.000050	− 1.000050
0.04	− 1.000202	− 1.000199	− 1.000203	− 1.000203	− 1.000203
0.07	− 1.000350	− 1.000348	− 1.000361	− 1.000361	− 1.000361
0.1	− 1.000478	− 1.000498	− 1.000525	− 1.000525	− 1.000525
0.4	− 0.991066	− 1.001992	− 1.002729	− 1.002726	− 1.002725
0.7	− 1.057693	− 1.058427	− 1.058659	− 1.058663	− 1.027490
1	− 1.250598	− 1.250628	− 1.250674	− 1.250674	− 1.121511
4	− 4.062539	− 4.062539	− 4.062539	− 4.062539	− 4.000000
7	− 7.035727	− 7.035727	− 7.035727	− 7.035727	− 7.000000
10	− 10.025006	− 10.025006	− 10.025006	− 10.025006	− 10.000000

energy is given by $E^{(3)}_{VCCA} = E^{(3)}_{UB}(\lambda = \lambda^*)$ [$E^{(4)}_{VCCA} = E^{(4)}_{UB}(\lambda = \lambda^*)$]. The tunneling reduction factor for the third level is given by

$$\tau^{(3)}_{VCCA} = \left.\frac{4\alpha}{1+4\alpha^2(1-\beta_1^2\epsilon_0+2\beta_2^2\epsilon_0^2)}\right|_{\lambda=\lambda^*}, \quad (22)$$

while for the fourth level,

$$\tau^{(4)}_{VCCA} = \left.\frac{4\alpha}{1+4\alpha^2(1-\beta_1^2\epsilon_0+2\beta_2^2\epsilon_0^2-6\beta_3^2\epsilon_0^3+24\beta_4^2\epsilon_0^4)}\right|_{\lambda=\lambda^*}. \quad (23)$$

In Figures 1–2 and Tables 1–4, one can see that our fourth-level results are in good agreement with the exact results. To improve our estimates, we make use of the optimal value of the variational parameter, λ^*, to obtain an "optimal" Hamiltonian to which we then apply the usual coupled-cluster approximation.

Now we apply the usual coupled-cluster approximation to the following "optimal" Hamiltonian $\bar{H}$ which is defined as

$$\begin{aligned}\bar{H} &\equiv e^{T^\dagger(\lambda^*)} H_{SB} e^{T(\lambda^*)} \\ &= -\Delta_0\sigma_x + \sum_{\mathbf{k}} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \sum_{\mathbf{k}} g^2_{\mathbf{k}}\lambda^*(\lambda^* - 2\sigma_z) \\ &\quad +(\sigma_z - \lambda^*)\sum_{\mathbf{k}} g_{\mathbf{k}}(a^\dagger_{\mathbf{k}} + a_{\mathbf{k}}) \,. \end{aligned} \quad (24)$$

This is identical to equation (11) but with the variational parameter λ replaced by the fixed value λ^*. It is expected that our results will be good for two reasons. Firstly, since λ^* is determined by the variational principle, the optimal Hamiltonian somehow provides us a good starting point in terms of energy. Secondly, since in the usual coupled-cluster approximation the restriction on W is relaxed, one may include those terms without σ_-, and thus the wavefunction should be more accurate.

In the fourth level the correlation operator W is given by

$$\begin{aligned} W &= \alpha(1 + \beta_1 A_+ + \beta_2 A_+^2 + \beta_3 A_+^3 + \beta_4 A_+^4)\sigma_- \\ &\quad +\alpha(\gamma_1 A_+ + \gamma_2 A_+^2). \end{aligned} \quad (25)$$

After some straightforward calculations, a set of seven nonlinear coupled algebraic equations of the parameters, α, β_n's, and γ_n's, is obtained. Numerical methods are needed in solving these equations. Then, these parameters will in turn give the ground-state energy $E^{(4)}_{OP} = \epsilon_0\lambda^*(2-\lambda^*) - 2\alpha\Delta_0 - \epsilon_0(1-\lambda^*)\alpha\gamma_1$. We have also calculated the tunneling reduction factor which is given by

$$\tau^{(4)}_{OP} = \frac{\langle\Phi_0|e^{W^\dagger}e^{T^\dagger(\lambda^*)}\sigma_x e^{T(\lambda^*)}e^W|\Phi_0\rangle}{\langle\Phi_0|e^{W^\dagger}e^W|\Phi_0\rangle}\,. \quad (26)$$

The final expression of the tunneling reduction factor is lengthy and will not be presented here. The numerical results are presented in Tables 1 to 4.

3 Discussion

In Figure 1 we show the upper bound of the ground-state energy for different levels of the coupled-cluster approximation. In (a)-(c) we consider S fixed to values 0.02, 2, and 200, and let the bare tunneling parameter Δ_0 vary. In (d)-(f), we let S vary while fixing Δ_0 to values 0.01, 1, and 100. We expect that if Δ_0 is small, then the two-state system is mainly controlled by the interaction with bosons and thus $E \approx -S$. On the other hand, if Δ_0 is large, then the energy is $E \approx -\Delta_0$. Except for the zeroth level, the results of all levels agree with our expectation in these two limiting cases. For nearly the whole parameter space, our estimates of energy show apparent convergence, and our results show good agreement with the exact results. However, in the intermediate region where $\Delta_0 \approx S \approx \hbar\omega_0$ convergence is still not trivial and discrepancy between the fourth-level result and the exact one is noticeable.

In Figure 2 we show the coupled-cluster approximation of the tunneling reduction factor. The results are arranged in the same way as that of Figure 1. The fourth-level results have already shown good agreement with the exact results. One important point worthy of noticing is that there is no evidence of any discontinuous localization-delocalization transition. This is consistent with the exact result. This observation is far different from those results obtained by the conventional coherent-state or squeezed-state approaches which predict the existence of a discontinuity in the reduction factor in certain cases [7]. With a correlated squeezed-state as an improved trial wavefunction [8], although in some cases the discontinuity is removed, it still persists in the large-coupling and large-Δ_0 regimes. It shows that these conventional trial wavefunctions are incapable of representing the ground state of the system. The agreement of our result with the exact result in this aspect suggests that our approach is a practical tool which can properly deal with the ground-state properties of spin-boson systems. It not only takes care of the accuracy of the ground-state energy estimate, but also that of the wavefunction estimate.

Our results of the optimal coupled-cluster approximation in Section 2, $E^{(4)}_{OP}$ and $\tau^{(4)}_{OP}$, are qualitatively the same as those discussed above. In order to have a clearer comparison between our results of the optimal coupled-cluster approximation and those of the other methods, we have tabulated the results of the ground-state energy in Tables 1 and 2, and also the tunneling reduction factor in Tables 3 and 4. In each table the rightmost column is the result of the variational correlated-squeezed state approach (CSQ) [8]. The results of our previous work [10] by using the conventional successive coupled-cluster approximation are shown in Tables 1 to 4 as well.

$E^{(4)}_{OP}$ and the exact ground-state energy E_{exact} show excellent agreement. Even in the intermediate region where $\Delta_0 \approx S \approx \hbar\omega_0$, their difference is only a few percents. For other cases, the agreement is far better than this. In some cases, for example, $\Delta_0 = 100$ and $S/\Delta_0 = 1$, 4, or 7, the agreement is up to seven significant figures.

Table 3. Tunneling reduction factor calculated by different methods for S = (a) 0.02, (b) 2, and (c) 200. $\tau_{pre}^{(4)}$ represents the fourth-level result of our previous work (Ref. [10]). τ_{CSQ} represents the result of the variational correlated squeezed-state approach (Ref. [8]).

Table 3a: ($S = 0.02$)

Δ_0/S	$\tau_{pre}^{(4)}$	$\tau_{VCCA}^{(4)}$	$\tau_{OP}^{(4)}$	τ_{exact}	τ_{CSQ}
0.01	0.960455	0.960820	0.960820	0.960820	0.960820
0.04	0.960732	0.960912	0.960910	0.960910	0.960910
0.07	0.960810	0.961004	0.961000	0.961000	0.961000
0.1	0.960869	0.961095	0.961090	0.961089	0.961089
0.4	0.961337	0.961992	0.961969	0.961968	0.961968
0.7	0.961776	0.962858	0.962820	0.962819	0.962818
1	0.962204	0.963694	0.963643	0.963641	0.963641
4	0.966003	0.970713	0.970579	0.970575	0.970574
7	0.969115	0.975883	0.975723	0.975719	0.975719
10	0.971709	0.979800	0.979638	0.979635	0.979635

Table 3b: ($S = 2$)

Δ_0/S	$\tau_{pre}^{(4)}$	$\tau_{VCCA}^{(4)}$	$\tau_{OP}^{(4)}$	τ_{exact}	τ_{CSQ}
0.01	0.002935	0.005869	0.005869	0.024195	0.018644
0.04	0.011739	0.023476	0.023478	0.041910	0.019171
0.07	0.020543	0.041082	0.041089	0.059738	0.020944
0.1	0.029349	0.058685	0.058707	0.077684	0.022363
0.4	0.117606	0.234452	0.235706	0.264149	0.126406
0.7	0.206457	0.409805	0.415357	0.460675	0.523667
1	0.295572	0.584717	0.596597	0.643119	0.701814
4	0.764898	0.986258	0.981822	0.981842	0.981868
7	0.862237	0.995255	0.994472	0.994473	0.994473
10	0.902517	0.997623	0.997360	0.997360	0.997361

Table 3c: ($S = 200$)

Δ_0/S	$\tau_{pre}^{(4)}$	$\tau_{VCCA}^{(4)}$	$\tau_{OP}^{(4)}$	τ_{exact}	τ_{CSQ}
0.01	0.002503	0.005006	0.005006	0.005006	0.000000
0.04	0.010013	0.020025	0.020025	0.020025	0.000000
0.07	0.017522	0.035044	0.035044	0.035044	0.000000
0.1	0.025031	0.050063	0.050063	0.050063	0.000000
0.4	0.100126	0.200251	0.200256	0.200256	0.000000
0.7	0.175221	0.350439	0.350465	0.350468	0.000000
1	0.250266	0.500627	0.500704	0.500724	0.714052
4	0.747952	0.999844	0.999780	0.999780	0.999780
7	0.856993	0.999949	0.999940	0.999940	0.999940
10	0.899981	0.999975	0.999972	0.999972	0.999972

Table 4. Tunneling reduction factor calculated by different methods for Δ_0 = (a) 0.01, (b) 1, and (c) 100. $\tau_{pre}^{(4)}$ represents the fourth-level result of our previous work (Ref. [10]). τ_{CSQ} represents the result of the variational correlated squeezed-state approach (Ref. [8]).

Table 4a: ($\Delta_0 = 0.01$)

S/Δ_0	$\tau_{pre}^{(4)}$	$\tau_{VCCA}^{(4)}$	$\tau_{OP}^{(4)}$	τ_{exact}	τ_{CSQ}
0.01	0.999804	0.999808	0.999808	0.999808	0.999808
0.04	0.999216	0.999231	0.999231	0.999231	0.999231
0.07	0.998628	0.998655	0.998655	0.998655	0.998655
0.1	0.998041	0.998080	0.998079	0.998079	0.998079
0.4	0.992187	0.992340	0.992339	0.992339	0.992339
0.7	0.986365	0.986634	0.986630	0.986630	0.986630
1	0.980574	0.980960	0.980953	0.980953	0.980952
4	0.924060	0.925998	0.925896	0.925882	0.925879
7	0.867917	0.874186	0.873904	0.873798	0.873782
10	0.806535	0.825464	0.824870	0.824552	0.824508

Table 4b: ($\Delta_0 = 1$)

S/Δ_0	$\tau_{pre}^{(4)}$	$\tau_{VCCA}^{(4)}$	$\tau_{OP}^{(4)}$	τ_{exact}	τ_{CSQ}
0.01	0.993341	0.997780	0.997770	0.997770	0.997770
0.04	0.973449	0.991151	0.990992	0.990991	0.990992
0.07	0.953683	0.984567	0.984078	0.984073	0.984076
0.1	0.934033	0.978029	0.977027	0.977013	0.977021
0.4	0.741923	0.915240	0.898773	0.897727	0.898459
0.7	0.551728	0.853480	0.806590	0.800423	0.805526
1	0.375042	0.713071	0.695424	0.685294	0.701401
4	0.067031	0.134009	0.134107	0.134732	0.354852
7	0.037094	0.074184	0.074192	0.074195	0.000008
10	0.025659	0.051318	0.051319	0.051320	0.000000

Table 4c: ($\Delta_0 = 100$)

S/Δ_0	$\tau_{pre}^{(4)}$	$\tau_{VCCA}^{(4)}$	$\tau_{OP}^{(4)}$	τ_{exact}	τ_{CSQ}
0.01	0.990050	0.999950	0.999950	0.999950	0.999950
0.04	0.960202	0.999802	0.999794	0.999794	0.999794
0.07	0.930350	0.999654	0.999627	0.999627	0.999627
0.1	0.900478	0.999505	0.999447	0.999447	0.999447
0.4	0.591066	0.998022	0.995703	0.995737	0.995739
0.7	0.357693	0.716855	0.717462	0.718011	0.876268
1	0.250598	0.501256	0.501413	0.501455	0.714044
4	0.062539	0.125078	0.125079	0.125079	0.000000
7	0.035727	0.071454	0.071454	0.071454	0.000000
10	0.025006	0.050013	0.050013	0.050013	0.000000

However, we should be careful that $E_{OP}^{(4)}$ is not necessarily an upper-bound of the exact value. For instance, in the case of $S = 2$ and $\Delta_0/S = 4$, $E_{OP}^{(4)}$ is even lower than the exact value. The optimal coupled-cluster approximation of the tunneling reduction factor $\tau_{OP}^{(4)}$ also shows very good accuracy compared with the exact result.

One can observe that the CSQ results of the ground-state energy and the tunneling reduction factor are even better than those of the optimal coupled-cluster approximation in the region where Δ_0 or S are small. However, in the region where S and Δ_0 are both large, CSQ no longer works properly. Due to its incapability of accurately simulating the ground state, it predicts a discontinuous localization-delocalization transition which is absent in the exact result. On the contrary, the optimal coupled-cluster approximation works well in the whole parameter space. It is surprising to note that in the region where CSQ results deteriorate, the results of the optimal coupled-cluster approximation agree with the exact results with high precision. Furthermore, in many cases $E_{OP}^{(4)}$ and $\tau_{OP}^{(4)}$ are closer to the exact values than the results of the conventional successive coupled-cluster approximation. This significant improvement (especially in the estimate of the tunneling reduction factor τ) is expected because the correlation operator (and hence the wavefunction) is more accurate in the optimal coupled-cluster approximation than that in the conventional successive coupled-cluster approximation.

4 Conclusion

In this paper we have proposed the optimal coupled-cluster approximation to investigate the ground-state properties of a two-state system which is coupled linearly to a dispersionless boson bath. With this approximation scheme we can systematically improve not only the estimate of the ground-state energy but also the ground-state wavefunction. This new approach is also able to give a very tight upper bound of the ground-state energy of the system. Up to the fourth level of the optimal coupled-cluster approximation, our results of the ground-state energy and the tunneling reduction factor show excellent 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 agrees with the exact result but contradicts the results of the conventional variational approaches. Hence, our results seem to suggest that the optimal coupled-cluster approximation is a practical tool for studying the ground-state properties of spin-boson systems. Furthermore, if an additional variable squeezing or correlated squeezing transformation is also performed to the Hamiltonian H_{SB}, then a better "optimal" Hamiltonian will be obtained, the use of which may allow better ground-state energies and wavefunctions to be obtained. The mathematical treatment in this work is simple and could be easily extended to the studies of other fermion-boson interacting systems.

This work is partially supported by the Earmarked Grant for Research from the Research Grants Council of the Hong Kong Government. The authors would like to thank Dr. K.L. Liu for many helpful discussions.

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