Quality of variational ground states for a two-state system coupled to phonons

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We generalize the variational approach proposed by Chen, Zhang, and Wu [Phys. Rev. B 40, 11326 (1989)] to the ground state of a two-level system coupled to a single boson mode. The resulting displaced-squeezed state is compared to the true ground state (calculated numerically), and to further variational states, by computing energy differences and overlaps. These states are able to describe a bifurcation occurring in the ground state of the quantum system as well as in the equilibrium state of its classical limit, and they are excellent approximations to the true ground state.

In a recent paper, Chen, Zhang, and Wu discussed variational approaches to the ground state of the Hamiltonian

\[ H = -\Delta \sigma_\chi + b^\dagger b + g(\sigma_\chi + \sigma_\sigma) \]  

(1)

describing a two-state system interacting with a single boson mode. The boson operators \( b \) and \( b^\dagger \) describe a harmonic oscillator, the natural frequency of which we use as unit of energy, the Pauli spin matrices \( \sigma_\chi \) and \( \sigma_\sigma \) (eigenvalues \( \pm 1 \)) characterize the two-state system, \( 2\Delta \) and \( g \) are the level splitting and the coupling parameter, respectively. The model (1) enjoys great popularity in various fields of physics, such as molecular and solid-state physics, quantum optics, quantum dissipation, and quantum chaos. Out of the large body of existing literature on (1) and related models we only wish to mention Refs. 2–5. Despite the apparent simplicity of the Hamiltonian, the eigenstates and eigenvalues are not known analytically in general. Apart from the trivial cases \( \Delta = 0 \) or \( g = 0 \), analytic solutions have been obtained so far only for special combinations of the parameters \( \Delta \) and \( g \), see, for example, so that there is an obvious need for good approximate solutions. Variational Ansätze corresponding to a displaced ground state (coherent state) of the oscillator were studied during the decade-long discussion on self-trapping phenomena in polaronic systems. Chen, Zhang, and Wu discussed a state of this type, with a spin-dependent displacement as a variational parameter, and compared it to a state with fixed displacement and an additional variable “squeeze.” We shall use a state with both variable displacement and variable squeeze parameter, namely

\[ |\phi\rangle = \exp[-\sigma, \lambda(b^\dagger b - b b^\dagger)] \exp[-\gamma(b^2 - b^2)]|\text{vac}\rangle \]  

(2)

The first exponential in (2) describes the spin-dependent displacement, the second one the squeeze; \(|\text{vac}\rangle\) denotes the \( g = 0 \) ground state of (1). \(|\phi\rangle\) is a normalized state, as both exponentials are unitary; \( \gamma \) and \( \lambda \) are variational parameters used to minimize \( \langle \phi | H | \phi \rangle \). For \( \gamma = 0 \) (\( \lambda = g \)), \(|\phi\rangle\) corresponds to the state \( \phi_1(\phi_2) \) of Ref. 1. Thus \(|\phi\rangle\) is a slightly more general variational state than those used in Ref. 1. The energy expectation value may be easily calculated using the properties of the two unitary operators occurring in (2):

\[ E(\gamma, \lambda) := \langle \phi | H | \phi \rangle = \sinh^2 2\gamma + \lambda(\lambda - 2g) - \Delta \exp[-2\lambda^2 \exp(-4\gamma)] \]  

(3)

Minimizing \( E(\gamma, \lambda) \) with respect to \( \gamma \) and \( \lambda \) leads to

\[ \gamma = \frac{1}{4} \ln [1 + 8\lambda^2 \Delta \exp(-2\lambda^2 \exp(-4\gamma))] \]  

(4)

\[ \lambda = g / [1 + 2\Delta \exp(-4\gamma) \exp(-2\lambda^2 \exp(-4\gamma))] \]  

These equations generalize Eqs. (7) and (13) of Ref. 1. We note in passing that the solution of (4) is not necessarily unique. In fact, multiple solutions already occur in the special cases discussed in Ref. 1, and the “optimal” solution must be determined by comparing energies. Of course, due to the variational principle, any solution of (4) yields an upper bound to the true ground-state energy when inserted into (3). For later comparison to the numerically computed exact ground state of (1) we need a more explicit representation of the state \(|\phi\rangle\). To obtain it, one may bring the unitary squeezing operator into normal order. It is then easy to compute the scalar product of \(|\phi\rangle\) with a coherent state \(|\sigma\rangle\), which may be used as a generating function for the coefficients in the occupation number representation of \(|\phi\rangle\). In order to get rid of the Pauli matrices one may perform these operations in subspaces corresponding to \( \sigma_\chi = \pm 1 \) and reassemble the full Hilbert space in the end. The result is

\[ |\phi\rangle = (\cosh 2\gamma)^{-1/2} \exp \left[ -\frac{\lambda^2}{2} (1 - \tanh 2\gamma) \right] \sum_{n=0}^{\infty} \frac{(\tanh 2\gamma)^n}{n!} G_n \]  

(5)

Here, the basis states \(|\nu\rangle\) are defined by

\[ b^\dagger b |\nu\rangle = \nu |\nu\rangle, \quad \sigma_\chi |\nu\rangle = (-1)^\nu |\nu\rangle, \quad (\nu = 0, 1, \ldots). \]  

(6)

(Obviously \(|\text{vac}\rangle\) corresponds to \( \nu = 0 \).) The polynomials \( G_n(x) \) are related to Hermite polynomials \( H_n(x) \).
\begin{align}
G_n(x) &= i^n H_n(-ix) ; \\
\text{they may be easily calculated by the recursion} \\
G_{n+1}(x) &= 2x G_n(x) + n G_{n-1}(x) , \\
G_0(x) &= 1, \quad G_1(x) = 2x .
\end{align}

Let us now turn to the exact (numerical) calculation of the ground state. The Hamiltonian commutes with the “parity” operator

\begin{equation}
P \equiv \exp \left[ \frac{i\pi}{2} \sigma_x + 1 + 2b^\dagger b \right] .
\end{equation}

The \( g = 0 \) ground state \( |\text{vac}\> \) has positive parity.

Combining continuity arguments with the nondegeneracy\(^{11}\) of the ground state one may conclude that the exact ground state has positive parity for all values of \( g \). We may thus restrict ourselves to the subspace of positive parity, spanned by the states \( |\psi\> \) (6). The Hamiltonian matrix \( \langle \psi | H | \mu \rangle \) is tridiagonal and may be easily treated by standard numerical methods. We have used the bisection method\(^{12}\) for the eigenvalues and the inverse iteration method\(^{12}\) for the eigenvectors of the Hamiltonian matrix truncated at \( \nu = 79 \).

Let us denote the exact ground-state vector by \( |\phi_0\> \), and the ground-state energy by \( E_0 \), respectively. To assess the quality of the variational state (2) we have computed the modulus-squared overlap with the exact ground state \( \langle \phi | \phi_0 \rangle \), and the energy difference

\begin{equation}
\Delta E \equiv \min E(\gamma, \lambda) - E_0 \geq 0
\end{equation}

for various values of \( g \) and \( \Delta \). As was to be expected, the variational state performs very well if either of the parameters \( g \) and \( \Delta \) is small, and less well if both are of the same order of magnitude and large. For \( g \) and \( \Delta \) both varying between 0 and 2 we obtain

\[ \Delta E \leq 0.302 \]

and

\[ \langle \phi | \phi_0 \rangle^2 \geq 0.818 . \]

The corresponding numbers for the slightly less general ansatz of Ref. 1 are 0.438 and 0.754, respectively. The exact ground-state energy \( E_0 \) varies between 0 and \(-4.27\) in this range of coupling constants. (Remember that we use the harmonic-oscillator frequency as unit of energy.) For \( g \leq 2.8 \) and \( \Delta \leq 5 \), the energy difference increases to 0.859 and the overlap (squared) decreases to 0.568; \( E_0 \) decreases to \(-8.67\).

It is interesting to compare the above results to those obtained by Shore and Sander\(^{2}\) using a different variational ansatz. Motivated by the shape of the numerically calculated exact ground-state wave function \( \phi_0(x) \), these authors suggested a linear combination of two displaced Gaussian wave functions:

\begin{equation}
|\psi\> = \text{exp}[-\sigma^u (b^\dagger - b)] + w \text{exp}[-\sigma^v (b^\dagger - b)] |\text{vac}\> .
\end{equation}

Here \( u, v, \) and \( w \) are real variational parameters. The relative weight \( w \) may be restricted to \( 0 \leq w \leq 1 \). (Note that \( |\psi\> \) is not normalized.) It is instructive to compare the shape of \( |\psi\> \) to that of the variational state \( |\phi\> \) (2) or of the exact ground state \( |\phi_0\> \) in a suitable representation. We have chosen a “parity-projected Husimi representation,” i.e., we consider \( \langle a \alpha | \psi \rangle \), where

\[ |\alpha\> \equiv \exp[-\alpha a^\dagger (b^\dagger - b)] |\text{vac}\> \]

is a “parity-projected coherent state.” \( \alpha \) is an arbitrary complex number. In this representation, the state \( |\phi\> \) (2) corresponds to a two-dimensional Gaussian centered at \( \alpha = \lambda \) with different half-widths along the real and imaginary directions. For \( \gamma = 0 \) the Gaussian becomes isotropic. In contrast, the state \( |\phi\> \) (11) proposed by Shore and Sander yields two isotropic Gaussian hills centered at \( u \) and \( v \), respectively, plus an interference term, if \( |u - v| \) is not too large. The same kind of structure is observed in the exact ground state for large values of \( g \) and \( \Delta \), i.e., in the region where the variational ansatz (2) fails.

We wish to point out that the double maximum structure of the quantum-mechanical “phase-space density”\(^{13}\) \( \langle \phi | \phi_0 \rangle \), of the ground state is not surprising from a classical point of view. The classical limit of the Hamiltonian (1) —i.e., a classical angular momentum vector coupled to a classical oscillator— shows interesting non-linear behavior\(^{14}\) including a transition to chaos. The classical ground-state (phase-space point of minimum energy) shows a bifurcation.\(^{14}\) For large values of \( \gamma \), the oscillator is at rest at \( x = 0 \), whereas for smaller values of \( \gamma \) this position becomes unstable and two new stable equilibrium positions \( \pm x_0 \) show up, with \( x_0 \) proportional to \( g \) for very strong coupling. This is only one of the many interesting parallels between the phase-space descriptions of the classical system and the Husimi (coherent state) representation of the quantum system.\(^{15}\) (Note, however, that the quantum ground state is nondegenerate, in contrast to the “classical ground state.”)

The energy expectation value corresponding to the state \( |\psi\> \) (11) is easily calculated and (numerically) minimized with respect to the parameters \( u, v, \) and \( w \). Again, we have studied the energy difference \( \Delta E \) [analogous to (10)] and the squared overlap with the exact ground state for the two parameter ranges \( 0 \leq \Delta \leq 2, 0 \leq g \leq 2, \) and \( 0 \leq \Delta \leq 5, 0 \leq g \leq 2.8 \). For the smaller range we obtain

\[ \Delta E \leq 10^{-2} , \quad \langle \phi | \phi_0 \rangle \geq 0.995 , \]

and for the larger range

\[ \Delta E \leq 0.0376 , \quad \langle \phi | \phi_0 \rangle \geq 0.973 . \]

It is tempting to follow the correspondence between the classical and quantum systems still a little bit further. We have tried to do so by studying a variational state

\[ |\psi\> = \beta |\text{vac}\> + \gamma |\alpha\> + \gamma' |\alpha'\> , \]

(13)

The \( \beta \) term obviously represents the classical equilibrium position \( x = 0 \) (which is stable for weak coupling), the other terms correspond to the two symmetrically displaced classical equilibria for strong coupling. \( \alpha, \beta, \gamma, \) and \( \gamma' \) are real variational parameters, \( |\psi\> \) is not normalized. Due to the presence of the \( \beta \) term, one may expect im-

proved results especially in the weak- and intermediate-coupling regimes. In fact, it turns out that the state (13) is not generally superior to (11), however, it leads to a further improvement in the expected regime. Combining both states (i.e., choosing the one with lower energy-expectation value), we obtained

$$\Delta E \leq 7 \times 10^{-3} \ (0.0237)$$

and

$$|\langle \psi | \phi_0 \rangle|^2 \geq 0.9981 \ (0.9944)$$

for the two coupling ranges mentioned above. (Values in parentheses correspond to the larger range.)

Thus, the states (11) and (13) yield an improvement of the minimum-energy difference by more than an order of magnitude, as compared to ansatz (2). An inspection of the numerical results reveals that the optimum values of the variational parameters depend rather regularly on the system parameters $g$ and $\Delta$. By an empirical fit to some simple functional dependence one might thus obtain a simple but precise analytical approximation to the ground state and its energy. A state of this type would be simple enough to be useful even in the physically interesting case of more than one oscillator mode interacting with a single two-level system.

To summarize, we have studied the quality of several variational ground states proposed for the model (1) of a two-level system coupled to an oscillator. We have unified and generalized the two different variational states proposed by Chen, Zhang, and Wu. It turns out, however, that different variational states perform much better in the interesting intermediate-coupling region. The reason for the success of these states (which exhibit more than one maximum in "quantum phase space") may be traced back to a bifurcation in the equilibrium position of the corresponding classical system.

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7See, H. B. Shore and L. M. Sander (Ref. 3) and references therein; for a generalization to nonzero temperatures see, for example, R. Mańka, Phys. Status Solidi B 94, K67 (1979).


13Note that the real and imaginary parts of the complex variable $\alpha$ are related to the oscillator position and momentum, respectively.
