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Variational treatment of entanglement in the Dicke model

L Bakemeier, A Alvermann and H Fehske

Institute of Physics, Ernst-Moritz-Arndt-University, 17487 Greifswald, Germany

E-mail: alvermann@physik.uni-greifswald.de

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Abstract

We introduce a variational ansatz for the Dicke model that extends mean-field theory through the inclusion of spin–oscillator correlations. The correlated variational state is obtained from the mean-field product state via a unitary transformation. The ansatz becomes correct in the limit of large oscillator frequency and in the limit of a large spin, for which it captures the leading quantum corrections to the classical limit exactly including the spin–oscillator entanglement entropy. We explain the origin of the unitary transformation before we show that the ansatz improves substantially upon mean-field theory, giving near exact results for the ground state energy and very good results for other observables. We then discuss why the ansatz still encounters problems in the transition regime at moderate spin lengths, where it fails to capture the precursors of the superradiant quantum phase transition faithfully. This observation illustrates the principal limits of semi-classical formulations, even after they are extended with correlations and entanglement.

Keywords: quantum phase transition, semiclassical limit, variational ansatz, quantum correlations

(Some figures may appear in colour only in the online journal)

1. Introduction

A quantum phase transition (QPT) of mean-field type arises in the semi-classical limit of a quantum system whenever a bifurcation of the equilibria of the associated classical Hamiltonian system occurs [1, 2]. A standard example is that of a particle moving in a one-dimensional potential $V(x) \propto x^4 + ax^2$, where the classical limit is realized through $\hbar \to 0$ or the equivalent scaling of the particle mass and potential. A QPT occurs because the number of potential energy minima changes as the control parameter a is adjusted from $a > 0$ to $a < 0$. The QPT corresponds to breaking of the $x \mapsto -x$ reflection symmetry of $V(x)$ in the ground state.

The properties of this example are characteristic for the more general situation, in particular for the superradiant QPT in the Dicke model addressed in the present paper. First, the QPT takes place only in the classical limit but not in the quantum regime. Prior to the classical limit the ground state is always non-degenerate because of tunneling between the two potential wells. Because of this the QPT itself is fully described by the classical bifurcation. Quantum effects enter the description of the QPT as corrections to the classical limit for small but finite $\hbar$. Second, the leading quantum corrections can be computed analytically, but the description of the system at larger $\hbar$, i.e. away from the classical limit, requires solution of the full Schrödinger equation.

In this contribution we ask whether it is possible to go beyond the semi-classical—or mean-field—description and directly include quantum effects in a variational ansatz for the ground state. The ansatz is variational because the values of its parameters will be determined through energy minimization. Variational ansätze have long been used for the Dicke model and related spin–boson models [3–7], often with the exclusive aim of improving the computation of the ground state energy and other simple observables. Little attention has been paid to the relevance of quantum correlations and fluctuations for the construction of a variational ansatz.

Our requirement is not only that the ansatz performs reasonably well before the classical limit is performed, i.e. in those regimes where the mean-field description fails. We also demand that the ansatz becomes exact in the classical limit in the sense that the leading order quantum corrections are captured faithfully. To go beyond mean-field theory thus requires not only the construction of some improved variational ansatz but to describe quantum correlations and quantum fluctuations in the ground state in a controlled way.

We discuss these questions here for the superradiant QPT in the Dicke model [8, 9], for which we establish our notation in section 2. We summarize the mean-field description of the QPT and the theory of quantum corrections in sections 3, 4 before we introduce the correlated variational ansatz in section 5. There, we explain the construction of the ansatz and the origin of the unitary transformation used therein, and show that it does indeed capture the leading quantum corrections to the classical limit of the Dicke model. In section 6 we evaluate the variational ansatz in comparison to quasi-exact numerical data for finite spin length, before we conclude in section 7.

2. The Dicke model

The Dicke model [10]

$$H = \Delta J_z + \kappa J_x \left(a^\dagger + a \right) + \Omega a^\dagger a \tag{1}$$

describes an ensemble of N two-level systems, e.g. atomic levels, interacting with a quantum harmonic oscillator, e.g., the photons in a cavity. The two-level systems are combined into a pseudo spin with length $j = N/2$ and operators $J_{x,y,z}$. The cavity photon field is described as a harmonic oscillator with bosonic ladder operators $a^{(\dagger)}$.

In addition to the three parameters Δ, Ω, κ and the spin length j we will use also the dimensionless coupling constant $\bar{\kappa}$ with

$$\kappa = \sqrt{\frac{\Delta \Omega \bar{\kappa}}{2j}}. \tag{2}$$

The above Hamiltonian has a combined spin–oscillator reflection symmetry. It is implemented by the unitary operator

$$R = \exp\left[\mathrm{i}\pi \left(J_z - j \right) \right] \exp\left[\mathrm{i}\pi a^\dagger a \right] \tag{3}$$

with

$$R J_x R^\dagger = -J_x, \quad R a^{(\dagger)} R^\dagger = -a^{(\dagger)} \tag{4}$$

such that $[R, H] = 0$.

The reflection symmetry can be broken in the classical limit $j \to \infty$ of a large spin [8, 9]. Then, the superradiant QPT from the symmetric ground state with $\langle J_x \rangle = \langle a \rangle = 0$ to a symmetry-broken two-fold degenerate ground state with $\langle J_x \rangle, \langle a \rangle \neq 0$ takes place at the critical coupling $\bar{\kappa} = 1$.

The QPT cannot occur at finite j because the energy of a hypothetical symmetry-broken ground state $|\phi\rangle$ could always be lowered by forming a linear combination with the opposite state $R|\phi\rangle$. Thus, symmetry-breaking is possible only for zero overlap $\langle \phi | R | \phi \rangle = 0$, which requires $j \to \infty$.

Precursors of the QPT at finite j are visible, e.g., in the entanglement entropy or the spin susceptibility [11]. Nearly degenerate symmetry-broken ground states can be obtained in a situation with small $\langle \phi | R | \phi \rangle \ll 1$ in the usual way by adding a small symmetry-breaking perturbation ϵJ_x to H.

3. Mean-field theory of the QPT

The semi-classical—or mean-field—theory of the QPT in the Dicke model is based on the ansatz

$$\left| \psi_{\mathrm{mf}} \right\rangle = |\phi\rangle \otimes |\chi\rangle \tag{5}$$

for the ground state, which is the product of a (yet unkown) spin state $|\phi\rangle$ and oscillator state $|\chi\rangle$.

Because of the product form of the ansatz (5) minimization of the mean-field energy

$$\begin{aligned} E_{\mathrm{mf}} = \left\langle \psi_{\mathrm{mf}} | H | \psi_{\mathrm{mf}} \right\rangle &= \Delta \langle \phi | J_z | \phi \rangle \\ &+ \kappa \langle \phi | J_x | \phi \rangle \langle \chi | a^\dagger + a | \chi \rangle + \Omega \langle \chi | a^\dagger a | \chi \rangle \end{aligned} \tag{6}$$

splits into two individual minimization problems for the spin and oscillator state, which are coupled only through expectation values formed with the respective other state.

Specifically, the spin state $|\phi\rangle$ has to be the ground state of the effective spin Hamiltonian

$$H_{\mathrm{mf}}^{\mathrm{s}} = \Delta J_z + \xi_1 J_x, \tag{7}$$

with the one parameter $\xi_1 = \kappa \langle \chi | a^\dagger + a | \chi \rangle$. Such a state is a spin coherent state $|\theta\rangle$, with rotation angle $\tan\theta = \xi_1/\Delta$ relative to the z-axis (see appendix A for notation).

Conversely, the oscillator state $|\chi\rangle$ has to be the ground state of the effective boson Hamiltonian

$$H_{\mathrm{mf}}^{\mathrm{b}} = \xi_2 \left(a^\dagger + a \right) + \Omega a^\dagger a, \tag{8}$$

where $\xi_2 = \kappa \langle \phi | J_x | \phi \rangle$. The ground state is a boson coherent state $|\alpha\rangle$, with $\alpha = -\xi_2/\Omega$.

Therefore, the mean-field ground state is

$$\left| \psi_{\mathrm{mf}} \right\rangle = |\theta\rangle \otimes |\alpha\rangle, \tag{9}$$

a product state of a spin coherent state $|\theta\rangle$ and an oscillator coherent state $|\alpha\rangle$. It only depends on the two real parameters θ, α. In particular, the absence of spin–oscillator correlations or entanglement in the product state (5) implies that the individual spin and oscillator state is a coherent state.

The mean-field energy then is

$$E_{\mathrm{mf}} = -j\Delta \cos\theta + 2j\kappa\alpha \sin\theta + \Omega\alpha^2, \tag{10}$$

which has to be minimized as a function of θ and α. The optimal α follows immediately as

$$\alpha = -\frac{j\kappa}{\Omega} \sin\theta, \tag{11}$$

such that

$$\begin{aligned} E_{\mathrm{mf}} &= -j\Delta \cos\theta - j^2 \frac{\kappa^2}{\Omega} \sin^2\theta \\ &= -j\Delta \left(\cos\theta + \frac{1}{2} \bar{\kappa} \sin^2\theta \right). \end{aligned} \tag{12}$$

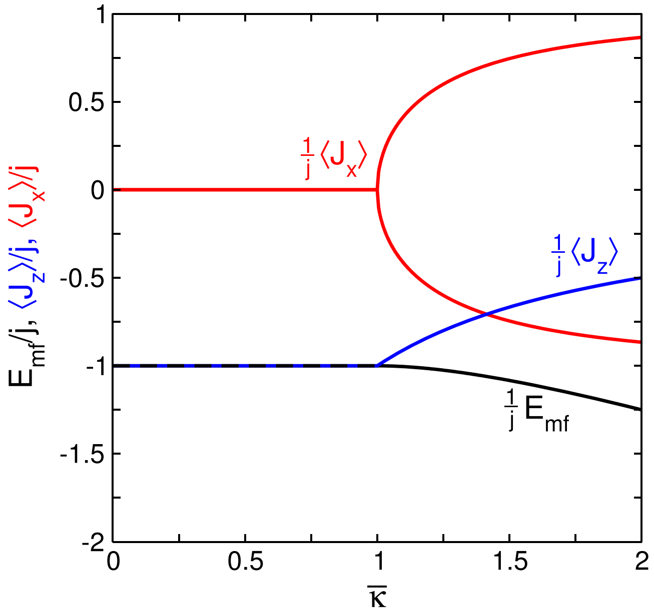

Figure 1. Energy E_{mf} and spin expectation values $\langle J_x \rangle$, $\langle J_z \rangle$ of the Dicke model in mean-field theory. At $\bar{\kappa} = 1$ the superradiant QPT from $\langle J_x \rangle = 0$ to $\langle J_x \rangle \neq 0$ takes place.

The functional form of E_{mf} gives rise to a bifurcation of the minima at the critical value $\kappa = 1$. The optimal θ is

$$\theta = \begin{cases} 0 & \text{if } \bar{\kappa} < 1, \\ \pm\arccos\left(1/\bar{\kappa}\right) & \text{if } \bar{\kappa} > 1. \end{cases} \tag{13}$$

The relevant observables (cf figure 1) are $E_{\mathrm{mf}} = -j\Delta$, $\langle J_z \rangle = -j$, $\langle J_x \rangle = 0$ for $\bar{\kappa} < 1$, and

$$E_{\mathrm{mf}} = -\frac{1}{2} j\Delta\left(\bar{\kappa} + 1/\bar{\kappa}\right), \quad \left\langle J_z \right\rangle = -j/\bar{\kappa},$$
$$\left\langle J_x \right\rangle = \pm j\sqrt{1 - 1/\bar{\kappa}^2} \quad \text{for } \bar{\kappa} > 1. \tag{14}$$

The mean-field theory thus predicts a QPT transition at $\bar{\kappa} = 1$. This prediction is independent of j, which has dropped out of the mean-field equations entirely because of the particularly simple (j-independent) form of H^s_{mf} and H^b_{mf}. As we noted earlier the QPT transition is in fact realized only in the limit $j \to \infty$.

4. Quantum corrections to the classical limit

Mean-field theory becomes valid in the classical limit of large $j \to \infty$. At finite j correlations between the spin and oscillator occur together with non-classical spin and oscillator fluctuations.

The quantum corrections to the classical limit were obtained in [12–15] in leading order of a $1/j$ expansion using the Holstein–Primakoff (H–P) transformation of the spin operators. The H–P transformation gives

$$J_z = -j + b^\dagger b, \tag{15a}$$

$$J_x = \sqrt{\frac{j}{2}}\left(b^\dagger + b\right) + O\left(j^{-1/2}\right), \tag{15b}$$

for the spin operators in the Dicke Hamiltonian H, with new bosonic operators $b^{(\dagger)}$. In the symmetric phase ($\langle J_z \rangle = \langle a \rangle = 0$) we get the expansion

$$H = -j\Delta + H_{\mathrm{qc}} + O(1/j), \tag{16}$$

with the bosonic Hamilton operator

$$H_{\mathrm{qc}} = \Delta b^\dagger b + \frac{1}{2}\sqrt{\Delta\Omega\bar{\kappa}}\left(b^\dagger + b\right)\left(a^\dagger + a\right) + \Omega a^\dagger a \tag{17}$$

for the leading order quantum corrections. In the symmetry-broken phase spin (oscillator) operators have to be rotated (shifted) to the new equilibrium values first, before the H–P transformation can be applied.

The two oscillators in H_{qc} can be decoupled with a unitary transformation of the form

$$U_2 = \exp\left[\mathrm{i}\left(\gamma_1 X_1 P_2 + \gamma_2 P_2 X_1\right)\right]. \tag{18}$$

Then, the ground state of the transformed Hamiltonian $U_2 H_{\mathrm{qc}} U_2^\dagger$ is a simple product state of two squeezed oscillator states. Back transformation with U_2 reintroduces the correlations present in the ground state of H_{qc} but absent in the product ground state of the transformed Hamiltonian.

A useful measure for correlations between the spin and oscillator, and thus for the relevance of quantum corrections to the mean-field state, is the spin–oscillator entanglement entropy

$$S = -\mathrm{tr}\left[\rho_S \ln \rho_S\right]. \tag{19}$$

It is computed, e.g., from the reduced spin density matrix ρ_S after a trace over the bosonic degree of freedom. S is bounded by $S \leqslant \ln(2j + 1)$. The mean-field state gives $S = 0$ independently of j. In the limit $j \to \infty$ the entropy S converges to a value that can be computed from H_{qc} [15].

The entropy S, which is shown in figure 2, diverges at the QPT and thus provides a characterization of the QPT through the amount of quantum corrections to the classical limit [14]. Larger values of S in the vicinity of the QPT show that deviations from the mean-field state (5) occur not only for small j but remain important in the limit $j \to \infty$. The divergence of S at the QPT indicates the breakdown of the classical limit and of mean-field theory.

5. Correlated mean-field theory

By construction, the mean-field ansatz does not account for spin–oscillator correlations. It also does not account for quantum fluctuations of the spin or oscillator at finite j. Indeed, we have seen in section 3 that the assumption of a product state implies that the spin and oscillator are in coherent (i.e., classical) states. Therefore, to improve the mean-field ansatz one has to include spin–oscillator entanglement and correlations.

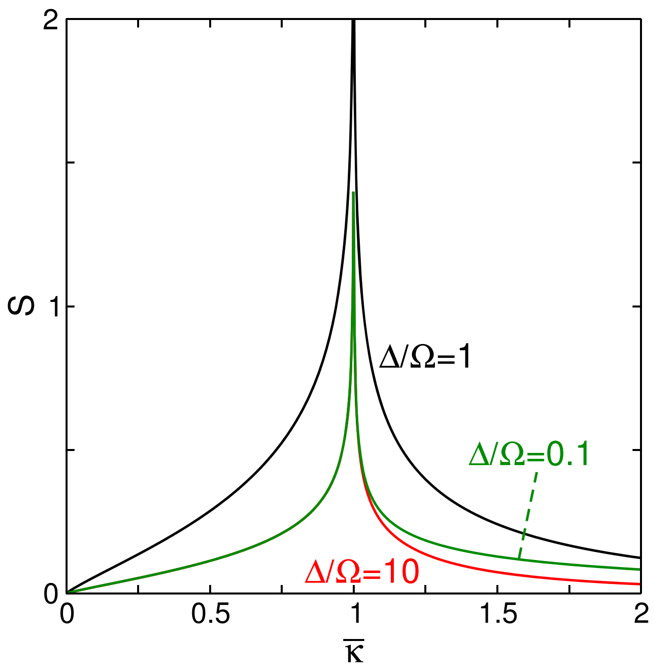

Figure 2. Spin–oscillator entanglement entropy S for $j \to \infty$. For $\bar{\kappa} < 1$ curves with equal ratio Δ/Ω and $(\Delta/\Omega)^{-1}$ coincide. Note that S for $\bar{\kappa} > 1$ is given for the situation where one of the two opposite degenerate ground states is selected through inclusion of a small ϵJ_x term. Therefore, $S \to 0$ for $\bar{\kappa} \to \infty$.

To go beyond mean-field theory we propose the variational ansatz

$$|\psi\rangle = D_x(\eta)|\phi\rangle \otimes |\chi\rangle \tag{20}$$

with the unitary transformation

$$D_x(\eta) = \exp\left[\eta J_x\left(a^\dagger - a\right)\right]. \tag{21}$$

The transformation depends on the variational parameter η ($\eta \in \mathbb{R}$). It can be interpreted as an oscillator shift that depends on the J_x-eigenvalues for $\eta \neq 0$. This J_x-dependence is the crucial difference to the mean-field ansatz, which is recovered for $\eta = 0$. It introduces spin–oscillator correlations and, thereby, allows for non-classical fluctuations. The spin state $|\phi\rangle$ and the oscillator state $|\chi\rangle$ remain to be determined in dependence on η. In particular, they will not be coherent states.

The above ansatz is partly modeled after the famous Lang–Firsov transformation of polaron physics, which describes the phonon-dressing of electronic states [16]. Here, the unitary transformation describes the dressing of the spin with bosons. We will later provide further justification for the above choice of the transformation through consideration of the $j \to \infty$ limit. A similar transformation has been used in [17–19] for the Rabi model ($j = 1/2$) at weak spin–oscillator coupling ($\bar{\kappa} \ll 1$), but the QPT was not addressed.

5.1. Entanglement entropy

The variational state (20) contains spin–oscillator correlations. This is exemplified by the fact that the spin–oscillator entanglement entropy S is non-zero for $\eta \neq 0$.

Working in the J_x eigenbasis $|m^x\rangle$, the reduced spin density matrix is given by

$$\begin{aligned}\rho_{mn} &= \langle m^x|\,\rho_S\,|n^x\rangle \\ &= \langle m^x\,|\phi\rangle\langle\phi\,|n^x\rangle\langle\chi|\,D(\eta(n-m))|\chi\rangle,\end{aligned} \tag{22}$$

where $D(\,\cdot\,)$ is the standard oscillator displacement operator (cf equation (A1)). For $\eta = 0$, $\rho_S = |\phi\rangle\langle\phi|$ is a pure state and $S = 0$. For $\eta \to \infty$, ρ_S evolves into a diagonal matrix with entries $|\langle m^x|\phi\rangle|^2$, and the entropy S becomes maximal for the given $|\phi\rangle$. Note that still $S \leqslant \ln(2j + 1)$.

5.2. Variational equations

Instead of explicit transformation of the product state in equation (20) it is more convenient to consider the transformed Hamiltonian

$$\breve{H} = D_x(-\eta)HD_x(\eta). \tag{23}$$

With the relations from appendix B one finds

$$\begin{aligned}\breve{H} &= \Delta J_z \cosh\left[\eta\left(a^\dagger - a\right)\right] + \mathrm{i}\Delta J_y \sinh\left[\eta\left(a^\dagger - a\right)\right] \\ &\quad + \Omega a^\dagger a + \left(2\eta\kappa + \Omega\eta^2\right)J_x^2 \\ &\quad + (\kappa + \Omega\eta)J_x\left(a^\dagger + a\right).\end{aligned} \tag{24}$$

The original Hamiltonian is real, and therefore we can assume real states $|\phi\rangle, |\chi\rangle$. Then, the term $\mathrm{i}J_y \sinh[\eta(a^\dagger - a)]$ gives no contribution to the variational energy E_V, and thus drops out of the following equations.

Just as in the derivation of the mean-field ansatz we now obtain the spin state $|\phi\rangle$ as the ground state of an effective spin Hamiltonian

$$H_{\rm sp} = \xi_1 J_z + \xi_2 J_x^2 + \xi_3 J_x, \tag{25}$$

with parameters

$$\begin{aligned}&\xi_1 = \Delta\langle\chi|\,\cosh\left[\eta\left(a^\dagger - a\right)\right]|\chi\rangle, \quad \xi_2 = 2\eta\kappa + \Omega\eta^2, \\ &\xi_3 = (\kappa + \Omega\eta)\langle\chi|\,a^\dagger + a\,|\chi\rangle.\end{aligned} \tag{26}$$

The oscillator state $|\chi\rangle$ is the ground state of an effective bosonic Hamiltonian

$$H_{\rm bos} = \xi_4 \cosh\left[\eta\left(a^\dagger - a\right)\right] + \Omega a^\dagger a + \xi_5\left(a^\dagger + a\right), \tag{27}$$

with parameters

$$\begin{aligned}\xi_4 &= \Delta\langle\phi|\,J_z\,|\phi\rangle, \\ \xi_5 &= (\kappa + \Omega\eta)\langle\phi\,|J_x|\,\phi\rangle.\end{aligned} \tag{28}$$

The variational energy is

$$\begin{aligned}E_V &= \langle\psi|\,H\,|\psi\rangle = \left(\langle\phi|\otimes\langle\chi|\right)\breve{H}\left(|\phi\rangle\otimes|\chi\rangle\right) \\ &= \langle\phi|\,H_{\rm sp}\,|\phi\rangle + \Omega\langle\chi|\,a^\dagger a\,|\chi\rangle \\ &= \langle\chi|\,H_{\rm bos}\,|\chi\rangle + \xi_2\langle J_x^2\rangle\end{aligned} \tag{29}$$

obtained either with $H_{\rm sp}$ or $H_{\rm bos}$. Note that one could include $\Omega\langle\chi|\,a^\dagger a\,|\chi\rangle$ as a scalar constant in $H_{\rm sp}$, or $\xi\langle J_x^2\rangle$ as a constant in $H_{\rm bos}$, to get a perfectly symmetric expression.

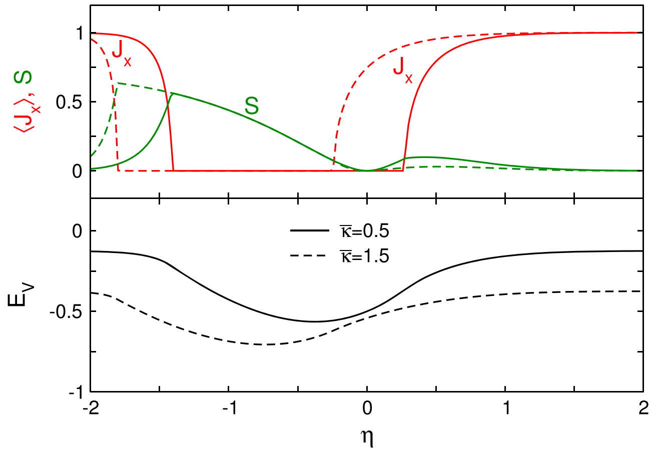

Figure 3. Variational energy E_V, spin expectation value $\langle J_x \rangle$, and spin–oscillator entanglement entropy S as a function of η, for $j = 1/2$ and $\bar{\kappa} = 0.5$ (solid), $\bar{\kappa} = 1.5$ (dashed). In this and all following figures we use the Dicke model at resonance $\Omega = \Delta$, and measure energies in units of Δ or Ω equivalently.

In contrast to the mean-field ansatz the ground states of the effective Hamiltonians $H_{\rm sp}$, $H_{\rm bos}$ are no longer simple coherent states because of the J_x^2 and $\cosh[\cdots]$ term. Instead, we have to determine $|\phi\rangle$, $|\chi\rangle$ freely through a self-consistent computation of the respective ground states. The parameters ξ_i of each effective Hamiltonian depend on expectation values formed with the respective other state, which results in a non-parabolic minimization problem. In practice, we can use a simple iterative strategy and determine the ground states of $H_{\rm sp}$ and $H_{\rm bos}$ alternately, always with the respective updated parameters ξ_1, ξ_2, ξ_3 or ξ_4, ξ_5.

The result of such a computation for short spin $j = 1/2$ is shown in figure 3. The transformation parameter η is determined from the minimum of $E_V(\eta)$, given in the lower panel. Minima occur for $\eta < 0$. We observe the significant lowering of the energy in comparison to the mean-field energy at $\eta = 0$. More interestingly, at the optimal η-value the ansatz gives the correct result $\langle J_x \rangle \approx 0$ also for $\bar{\kappa} = 1.5 > 1$, in contrast to the wrong (and j-independent) prediction $\langle J_x \rangle / j \approx 0.75$ of mean-field theory, which fails completely for the $j = 1/2$ case. We also observe substantial values of S (it is $S \leqslant \ln 2 \approx 0.69$ for $j = 1/2$) at the optimal η: the ansatz succeeds because it includes spin–oscillator entanglement. We continue with the evaluation in section 6.

Notice that for $j = 1/2$ the term $J_x^2 = 1/4$ is constant. Then, and only then, the effective spin Hamiltonian gives a spin coherent state $|\phi\rangle$ also for $\xi_2 \neq 0$. Nevertheless, the oscillator state $|\chi\rangle$ is not a coherent state but shows significant squeezing because still $\xi_4 \neq 0$ in equation (27). Simplifications occur in the two limiting cases discussed next.

5.3. The fast oscillator limit

In the limit of large Ω, the optimal $|\chi\rangle$ is the boson vacuum $|\text{vac}\rangle$. Then, the transformation parameter η occurs only in the term $(2\eta\kappa + \Omega\eta^2)J_x^2$ of $H_{\rm sp}$, and energy minimization gives $\eta = -\kappa/\Omega$. The effective spin Hamiltonian now reads

$$H_{\rm sp}^{\Omega=\infty} = \Delta J_z - \frac{\kappa^2}{\Omega} J_x^2. \tag{30}$$

This is the Lipkin–Meshkov–Glick model of nuclear physics [20]. Because we allow for free variation of $|\phi\rangle$, the variational ansatz here gives the exact ground state $|\phi\rangle \otimes |\text{vac}\rangle$ of $\breve{H}$, and hence the exact ground state $|\psi\rangle$ of H. For $j < \infty$, $|\phi\rangle$ is not a spin coherent state.

We have discussed elsewhere [11] the two possible variations of the limit $\Omega \to \infty$ for $j = 1/2$ and $j > 1/2$, either with constant κ/Ω or constant κ^2/Ω, and their relation to the Lang–Firsov transformation of polaron physics.

5.4. The large spin limit

Second, consider the limit of large $j \to \infty$. In this limit, the transformation $D_x(\eta)$ assumes the form

$$D_x(\eta) \underset{j\to\infty}{=} \exp\left[\eta\sqrt{j/2}\left(b^\dagger + b\right)\left(a^\dagger - a\right)\right] \tag{31}$$

after H–P transformation. For the sake of the argument we assume being in the ordered phase, otherwise a spin rotation has to be applied first, similar to section 4.

If we compare the above transformation to the transformation (18) we see that it gives only half of the transformation. It is not general enough to achieve full decoupling of the two harmonic oscillators in the Hamiltonian $H_{\rm qc}$ (equation (17)). However, the transformation $D_x(\eta)$ can achieve separation of the ground state of $H_{\rm qc}$, which is all that is required for the variational ansatz.

As explained in appendix C the appropriate choice of η gives the Hamiltonian

$$\begin{aligned} &D_x(-\eta) H_{\rm qc} D_x(\eta) \\ &= \omega_1 B^\dagger B + \lambda\left(B^\dagger A + B A^\dagger\right) + \omega_2 A^\dagger A + \text{constant}. \end{aligned} \tag{32}$$

Here, new bosonic operators $A^{(\dagger)}$, $B^{(\dagger)}$ appear as linear combinations of either the $a^{(\dagger)}$ or $b^{(\dagger)}$ operators. The actual computations are rather technical and collected in appendix C.

Although the two oscillators are still coupled in the transformed Hamiltonian (32), its true ground state is a simple product state $|\phi\rangle \otimes |\chi\rangle$. Here, $|\phi\rangle$, $|\chi\rangle$ are the squeezed oscillator states annihilated by B and A, respectively. Because the coupling operator contains only terms with either A or B, it annihilates the product state. In the language of quantum optics the transformation $D_x(\eta)$ achieves elimination of the counter-rotating terms in $H_{\rm qc}$.

Because of this property the variational ansatz (20) can give the correct ground state of H for large j including the leading order quantum corrections. This observation gives the justification for the particular form of $D_x(\eta)$ promised earlier.

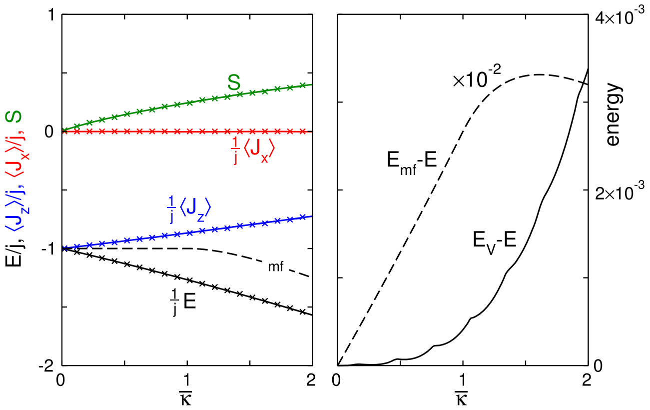

Figure 4. Comparison of results from the variational ansatz to the true ground state from numerics, for $j = 1/2$. Left panel: ground state energy E, spin expectation values $\langle J_z \rangle$, $\langle J_x \rangle$, and spin–oscillator entanglement entropy S as a function of coupling $\bar{\kappa}$. The crosses indicate the corresponding results from the variational ansatz. For orientation we include the mean-field energy (dashed curve). Right panel: deviation $E_V - E$ of the variational energy E_V from the true energy E. For orientation the dashed curve gives the difference $E_{\rm mf} - E$ to the mean-field energy, scaled by 10^{-2} to fit into the panel.

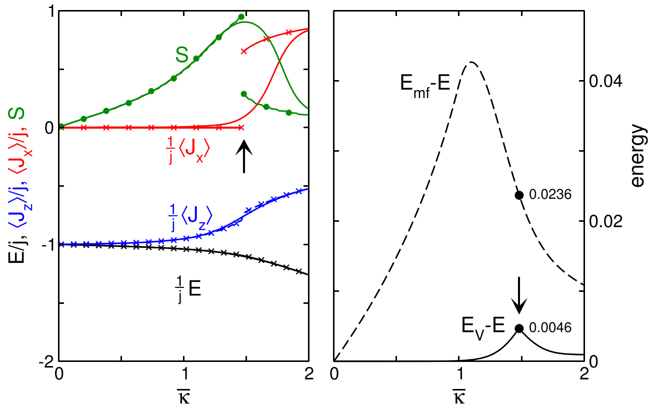

Figure 5. Comparison of results from the variational ansatz to the true ground state from numerics as in the previous figure, now for $j = 5$. Left panel: ground state energy E, spin expectation values $\langle J_z \rangle$, $\langle J_x \rangle$, and spin–oscillator entanglement entropy S as a function of coupling $\bar{\kappa}$. The crosses and circles indicate corresponding curves from the variational ansatz. The arrow indicates the 'jump' at $\bar{\kappa} \approx 1.48$ of the variational results for S and $\langle J_x \rangle$. Right panel: deviation $E_V - E$ of the variational energy E_V from the true energy E. The dashed curve gives the difference $E_{\rm mf} - E$ to the mean-field energy. At $\bar{\kappa} = 1.48$, it is $E_V - E = 0.0046$ in comparison to $E_{\rm mf} - E = 0.0236$.

6. Evaluation of the correlated ansatz

We now continue the evaluation of the variational ansatz for finite j through comparison to quasi-exact data from numerical diagonalization of H.

To prevent ambiguities with the $j \to \infty$ limit above the QPT, we include a small symmetry breaking term ϵJ_x in $H + \epsilon J_x$, with $\epsilon = 10^{-3}$. This perturbation suffices to select one of the two nearly symmetry broken states for $\bar{\kappa} > 1$ and larger j, but does not affect results in the symmetric phase.

The results shown in figure 4 for $j = 1/2$ correspond to the situation of figure 3. Here, we plot the optimal results of the variational ansatz after the minimization over η has been performed. The agreement between the variational and exact results is very good in this case. The variational energy deviates from the true ground state energy by less than 0.4%, which is hundred times smaller than the deviation from the mean-field energy (with $\eta = 0$). This picture shows the overall success of the correlated variational ansatz: it gives near-exact results for the energy, spin–observables, and the spin–oscillator entanglement. In particular, it gives the correct $\langle J_x \rangle \approx 0$ where mean-field theory would predict symmetry breaking with large $\langle J_x \rangle$. The finite value of S shows that inclusion of spin–oscillator correlations through the unitary transformation $D_x(\eta)$ is the crucial step to go beyond mean-field theory.

The ansatz is however not perfect, and we report in figure 5 how it can fail for moderate spin length $j = 5$. There, we observe a jump in S and $\langle J_x \rangle$ at $\bar{\kappa} \approx 1.48$ while the true result is a continuous curve. The jump is accompanied by a small kink in the result for $\langle J_z \rangle$.

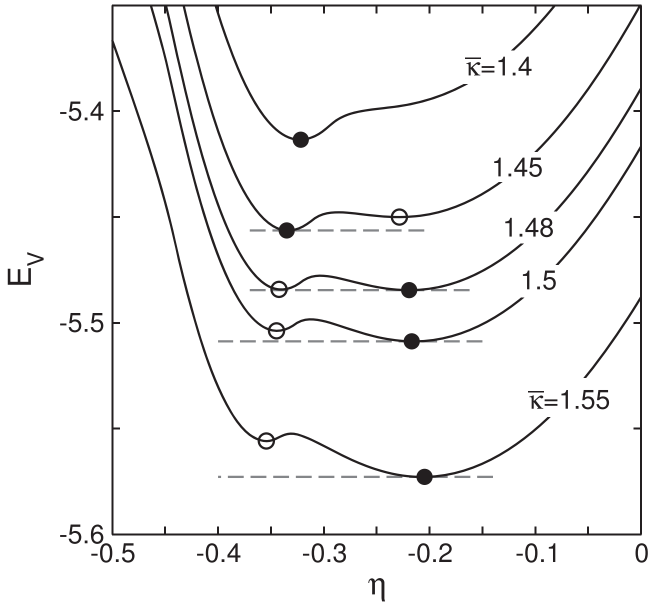

Figure 6. Variational energy E_V as a function of η, for $j = 5$ and $\bar{\kappa} = 1.4, 1.45, 1.48, 1.5, 1.55$ as indicated. A circle marks a local minimum, a filled circle the global minimum of $E_V(\eta)$. Horizontal gray dashed lines give the respective minimal values of E_V.

We note that the variational energy remains very accurate: the deviation from the true ground energy is below 0.5% for all $\bar{\kappa}$, and even precisely at the jump it is still five times more accurate than the mean-field energy.

The origin of the artificial jump is depicted in figure 6, where the variational energy $E_V(\eta)$ is shown in the vicinity of the jump. A single minimum exists for smaller $\bar{\kappa}$, but a second minimum appears as $\bar{\kappa}$ approaches the jump value. Both

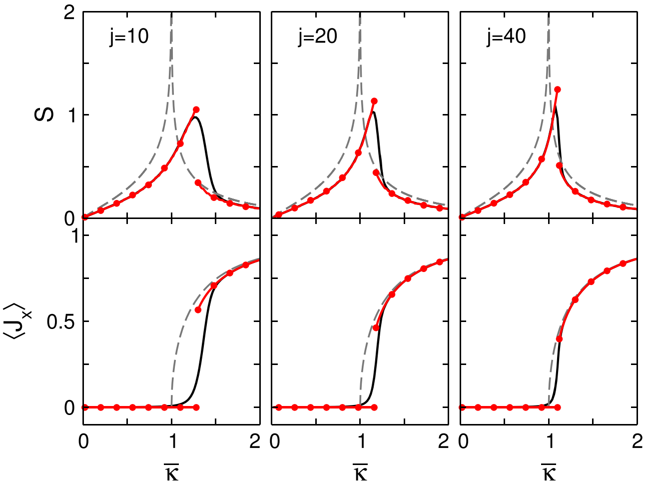

Figure 7. Comparison of spin–oscillator entanglement entropy S (upper row) and spin expectation values $\langle J_x \rangle$ (lower row) from the variational ansatz (red curves with small circles) to the exact results from numerics (black curves). Curves are given for $j = 10, 20, 40$ in the left, middle, right column. The dashed gray curves in all panels give the analytical $j \to \infty$ result for $\langle J_x \rangle$ and S.

minima switch the role of the global minimum at $\bar{\kappa} \approx 1.48$, and a first order phase transition with a jump is predicted where in reality no such transition occurs. At even larger $\bar{\kappa}$ the second minimum would disappear again. This behavior is a typical artefact of a variational ansatz, known, e.g., from polaron physics, the spin–boson model or general Hartree–Fock computations.

One should note that the energy is computed to much higher accuracy than other observable. This is, quite directly, the consequence of the variational approach: we optimize for the energy. In any case, the energy is not a very sensitive quantity and tiny energy changes can correspond to huge changes in other observables. Therefore, comparison of variational energies is not sufficient to argue for the quality of a variational ansatz.

As we have shown in section 5.4 the variational ansatz becomes exact in the large spin limit $j \to \infty$. Therefore, we expect that the artificial jump becomes less significant with increasing j. Figure 7 shows that this expectation holds true. At $j = 40$ the jump is still present, but now it traces the true rapid change of S and $\langle J_x \rangle$ slightly above the QPT.

For even larger j the theoretical argument section 5.4 shows that we can observe convergence of the variational result for S towards the analytical result in the $j \to \infty$ limit. Note that the similar convergence of the $\langle J_x \rangle$ expectation value is not surprising: it only expresses the fact that this observable is obtained from mean-field theory for $j \to \infty$, and does not make a statement about the quality of the variational ansatz.

7. Conclusions

For the example of the Dicke model we introduced and analyzed a correlated variational ansatz that extends mean-field theory with quantum correlations and fluctuations. The extension of mean-field theory is not arbitrary but controlled by the behavior in the $j \to \infty$ limit, where the variational ansatz gives correct results for the quantum corrections to the classical limit.

We show that the ansatz can give very good results not only for the ground state energy, but also for more crucial quantities such as the spin–oscillator entanglement. The agreement achieved there provides a better test for the quality of the variational ansatz than the near-exact results achieved for the ground state energy.

Nevertheless, the ansatz still suffers from a typical error found with variational ansätze in general: an artificial jump, here in S and the $\langle J_x \rangle$ expectation value, that occurs whenever several minima appear in the variational energy and the global mimimum changes discontinuously as the coupling is increased. This erroneous effect diminishes for larger spin, as expected from the construction of the ansatz. As we show analytically, the variational ansatz becomes exact for $j \to \infty$ including the leading quantum corrections.

In the present example, the jump of observables appears in spite of the high accuracy of the variational energy. This illustrates the general concerns one should have about a variational ansatz, for which it is sometimes hard to tell which results are real and which are artifacts. To overcome this problem one has to devise a scheme that allows for systematic improvement. The present ansatz is rigid in the sense that one cannot easily include more parameters in the unitary transformation, or additional variational degrees of freedom. Essentially the only way out of this situations would be to start from a linear combination of a few instead of the single product state in equation (20). In this way, also the reflection symmetry of the Dicke Hamiltonian could be explicitly accounted for in the variational ansatz.

However, it would be overkill to pursue this avenue for the Dicke model, which can be solved quasi-exactly with standard small-scale numerics. More interesting is the development of improved variational schemes for models such as the spin–boson model with a coupling to continuous bosonic degrees [21, 22]. The QPTs in these systems are different in nature from the QPT in the Dicke model, because they do not require a classical limit, and are still hard to tackle even with advanced numerical methods [23–25].

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Appendix A. Spin and oscillator coherent states

We use standard definitions of spin and oscillator coherent states (see [26] for a review).

An oscillator coherent state is defined through

$$|\alpha\rangle = D(\alpha)|\text{vac}\rangle = \exp\left[\alpha a^\dagger - \alpha^* a\right]|\text{vac}\rangle, \quad \text{(A1)}$$

where $|\text{vac}\rangle$ is the boson vacuum. It is

$$\langle\alpha|\, a^{(\dagger)}|\alpha\rangle = \alpha^{(*)}. \quad \text{(A2)}$$

In the main text, α is real.

A spin coherent state is defined through

$$|\theta\rangle = \mathrm{e}^{\mathrm{i}\theta J_y}\, |-j\rangle, \quad \text{(A3)}$$

where $|-j\rangle$ is the J_z eigenstate with minimal eigenvalue $-j$. It is

$$\langle\theta|\, J_z\, |\theta\rangle = -j\cos\theta, \quad \langle\theta|\, J_x\, |\theta\rangle = j\sin\theta. \quad \text{(A4)}$$

Only these spin coherent states, which result from a rotation around the y-axis, are needed in the main text.

Appendix B. Algebraic properties of the unitary transformation $D_x(\eta)$

Direct application of $\mathrm{e}^A B \mathrm{e}^{-A} = \sum_{n=0}^{\infty}(1/n!)[A, B]_n$, with iterated commutators $[A, B]_0 = B$, $[A, B]_{n+1} = [A, [A, B]_n]$, gives the transformation rule

$$D_x(-\eta) a D_x(\eta) = a + \eta J_x, \quad \text{(B1)}$$

from which one gets

$$D_x(-\eta)\left(a^\dagger + a\right)D_x(\eta) = a^\dagger + a + 2\eta J_x, \quad \text{(B2)}$$

and

$$D_x(-\eta)\left(a^\dagger a\right)D_x(\eta) = a^\dagger a + \eta J_x\left(a^\dagger + a\right) + \eta^2 J_x^2. \quad \text{(B3)}$$

These rules depend only on the bosonic commutation relations and can be generalized for an arbitrary operator replacing J_x.

For the spin operator J_z one finds

$$\begin{aligned} D_x(-\eta) J_z D_x(\eta) &= J_z \sum_{n=0}^{\infty} \frac{1}{(2n)!}\eta^{2n}\left(a^\dagger - a\right)^{2n} \\ &\quad + \mathrm{i}J_y \sum_{n=0}^{\infty} \frac{1}{(2n+1)!}\eta^{2n+1}\left(a^\dagger - a\right)^{2n+1} \\ &= J_z \cosh\left[\eta\left(a^\dagger - a\right)\right] \\ &\quad + \mathrm{i}J_y \sinh\left[\eta\left(a^\dagger - a\right)\right]. \end{aligned} \quad \text{(B4)}$$

The simple form of this transformation rule depends on the spin commutation relations. It does not generalize to arbitrary operators.

Appendix C. Partial decoupling of H_{qc}

After the H–P transformation the bosonic operator for the quantums corrections has the form

$$\begin{aligned} H_{\text{qc}} &= \omega_b b^\dagger b + \lambda\left(b^\dagger + b\right)\left(a^\dagger + a\right) + \omega_a a^\dagger a \\ &= \frac{1}{2}\omega_b\left(X_b^2 + P_b^2\right) + 2\lambda X_b X_a \\ &\quad + \frac{1}{2}\omega_a\left(X_a^2 + P_a^2\right) - E_{\text{qc}} \end{aligned} \quad \text{(C1)}$$

(cf equation (17)), with parameters ω_a, ω_b, λ that depend on Δ, Ω, $\bar{\kappa}$.

Here, we introduced position and momentum operators as

$$X_a = \frac{1}{\sqrt{2}}\left(a^\dagger + a\right), \quad P_a = \frac{\mathrm{i}}{\sqrt{2}}\left(a^\dagger - a\right), \quad \text{(C2}a\text{)}$$

$$X_b = \frac{1}{\sqrt{2}}\left(b^\dagger + b\right), \quad P_b = \frac{\mathrm{i}}{\sqrt{2}}\left(b^\dagger - b\right), \quad \text{(C2}b\text{)}$$

and $E_{\text{qc}} = \frac{1}{2}(\omega_a + \omega_b)$. Notice the stability condition $4\lambda^2 < \omega_a\omega_b$ for a H_{qc} bounded from below. The specific form of H_{qc} in equation (C1) holds below the QPT. Above the QPT an additional $(b + b^\dagger)^2$ term appears which can be accounted for by a redefinition of the X_b, P_b operators. The following argument does not change.

Our goal is to show that the ground state of H_{qc} can be written in the form $D_x(\gamma)\left[|\chi_b\rangle \otimes |\chi_a\rangle\right]$, where the unitary transformation is

$$\begin{aligned} D_x(\gamma) &= \exp\left[\mathrm{i}\gamma X_b P_a\right] \\ &= \exp\left[\frac{1}{2}\mathrm{i}\gamma\left(b^\dagger + b\right)\left(a^\dagger - a\right)\right] \end{aligned} \quad \text{(C3)}$$

(cf equation (31)).

The transformed Hamiltonian is

$$\begin{aligned} &D_x(-\gamma) H_{\text{qc}} D_x(\gamma) \\ &\quad = \frac{1}{2}\left(\omega_b + \omega_a\gamma^2 - 4\lambda\gamma\right)X_b^2 + \frac{1}{2}\omega_b P_b^2 \\ &\quad + \frac{1}{2}\omega_a X_a^2 + \frac{1}{2}\left(\omega_a + \omega_b\gamma^2\right)P_a^2 \\ &\quad + \left(2\lambda - \omega_a\gamma\right)X_a X_b + \omega_b\gamma P_a P_b. \end{aligned} \quad \text{(C4)}$$

Notice that all parameters are real.

Now make the ansatz

$$A = a_1 X_a + \mathrm{i}a_2 P_a, \quad B = b_1 X_b + \mathrm{i}b_2 P_b, \quad \text{(C5}a\text{)}$$

$$A^\dagger = a_1 X_a - \mathrm{i}a_2 P_a, \quad B^\dagger = b_1 X_b - \mathrm{i}b_2 P_b, \quad \text{(C5}b\text{)}$$

in the Hamiltonian

$$\begin{aligned}\tilde{H} &= B^\dagger B + \mu\left(B^\dagger A + BA^\dagger\right) + A^\dagger A \\ &= a_1^2 X_a^2 + a_2^2 P_a^2 + b_1^2 X_b^2 + b_2^2 P_b^2 \\ &\quad + 2\mu a_1 b_1 X_a X_b \\ &\quad + 2\mu a_2 b_2 P_a P_b - \tilde{E}. \end{aligned} \tag{C6}$$

Here, $\tilde{E} = a_1 a_2 + b_1 b_2$. The ground state of $\tilde{H}$ is a product state $|\chi_b\rangle \otimes |\chi_a\rangle$, where the two states $|\chi_{a/b}\rangle$ are those squeezed oscillator states that are annihilated by the operator A or B, respectively. Thus, to achieve the above goal, we must try to choose the transformation parameter γ in such a way that the transformed Hamiltonian from equation (C4) assumes the form of $\tilde{H}$. Comparison of the two expressions gives the condition

$$\begin{aligned}\frac{2\lambda - \omega_a\gamma}{\omega_b\gamma} &= \frac{a_1 b_1}{a_2 b_2} \\ &= \frac{\sqrt{\omega_a\left(\omega_b + \omega_a\gamma^2 - 4\lambda\gamma\right)}}{\sqrt{\omega_b\left(\omega_a + \omega_b\gamma^2\right)}},\end{aligned} \tag{C7}$$

or the equivalent equation

$$\begin{aligned}&\left(2\lambda - \omega_a\gamma\right)\sqrt{\omega_b\left(\omega_a + \omega_b\gamma^2\right)} \\ &= \omega_b\gamma\sqrt{\omega_a\left(\omega_b + \omega_a\gamma^2 - 4\lambda\gamma\right)}.\end{aligned} \tag{C8}$$

Under the above stability condition the argument of the square root on the right hand side of the equation is always positive. The left and right hand side of the equation diverge towards opposite values $\pm\infty$ for $\gamma \to \pm\infty$, such that there is always a choice of γ to satisfy the above condition. Therefore, we have achieved our goal. We note that the specific value of γ can be obtained from a quadratic equation that follows from equation (C8). It could be used to fix the parameter η in equation (20) as an alternative to energy minimization, at least for large j.

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