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A beyond mean-field study of the Tavis-Cummings model

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Abstract. A beyond mean-field study of the Tavis-Cummings (TC) model is developed. This is the simplest model for describing the interaction of a radiation field with a system composed by an array of two-level atoms. The first correction to the mean-field ground state energy and the energy gap between the ground and the first excited states are computed. For the ground-state energy our result improves the mean-field calculation, as expected. For the gap, that cannot be calculated at mean-field level, a drop down to zero is obtained at the critical point where the system undergoes a second-order quantum phase transition.

INTRODUCTION

The simplest model describing the interplay between matter (represented by a two-level system) and radiation is the Jaynes-Cummings (JC) model with the Rotating Wave Approximation (RWA) [1]. In order to describe the interaction of a single mode radiation with many quantum dipoles, a generalization of the JC model, called Tavis-Cummings (TC) model, was introduced [2]. All these models including the simplest Rabi model [3] and the more general Dicke model [4] have gained renewed interest in the last years with the development of quantum computing, entanglement, Josephson phase qubits, etc. For all these models, their phase space and ground state quantum phase transitions (QPT) at the mean-field level (large system sizes) have been studied.

Mean-field models have been successfully used for many years to interpret and characterise thermodynamical phase transitions in many different branches of Physics. However, they are not well suited to study regions around the critical point in mesoscopic systems where finite size effects are important. For these cases, theories beyond mean-field are of use. In this work, we start reviewing the mean-field theory based on an intrinsic state for the Tavis-Cummings model [2], of interest in quantum optics and quantum computation. Then, we introduce a beyond mean-field treatment based on three consecutive transformations. First, a Holstein-Primakoff change is proposed to produce an expansion of the energy surface in terms of the system size, $1/N$. The leading term in this expansion generates the mean field results and successive terms provide size corrections. Then, a shift transformation allows for a displacement (deformation) of the solution. Finally, a Bogoliubov transformation is used to diagonalize the first relevant beyond mean-field term. This procedure allows to study finite size effects in observables of interest. As an example, we present here the beyond mean-field calculation of the ground state energy and of the system gap, and compare these results with the exact numerical treatment for finite sizes.

In this contribution, we solve the TC model beyond the mean-field theory so as to catch finite particle number effects. This contribution is dedicated to Professor Francesco Iachello as a recognition of all his career. He has impulsed the algebraic models in many Physics branches. His influence started in mid 70s with the introduction of the Interacting Boson Model of Nuclear Structure, then extended to the Vibron Model of Molecular Physics, and after-

wards brought similar formalisms to Particle Physics, Condensed Matter, etc. In addition, his introduction in 2000 of the ideas of critical point symmetries was a real breakthrough in the research in the field of quantum phase transitions. The present contribution is along this last line and is our way of thanking Professor Iachello for his invaluable help, advise, support, and friendship since 1983, year in which he started directing the PhD work of one of the authors (JMA) on the Interacting Boson-Fermion model. Thanks a lot, Franco!

The model

The Dicke model describes a system given by an array of two-level atoms interacting with a radiation field [4]. Due to these characteristics, this model is very popular in quantum optics and, more recently, in quantum computing. On the one hand, it includes a subsystem given by a radiation field which is typically modeled by a single bosonic mode in terms of creation and annihilation operators b^\dagger and b . These operators are described by the Heisenberg-Weyl algebra HW(1). On the other hand, the atomic field is represented by pseudospin operators $J_\pm = J_x \pm iJ_y$ and $J_0 = J_z$ satisfying the commutation relations of the su(2) algebra. Thus, the Dicke Hamiltonian, using natural units, is written as,

$$H_D(\lambda) = \omega_0 J_z + \omega b^\dagger b + \frac{\lambda}{\sqrt{2J}} [(b + b^\dagger)(J_+ + J_-)]. \quad (1)$$

It depends on a control parameter, λ , that takes into account the strength of the interaction between matter and the radiation field. The frequencies, ω and ω_0 , are linked to the single bosonic mode and to the energy splitting of the two-level system of the matter field, respectively. Finally, $J = N/2$, where N is the total number of atoms in the atomic field.

From the Dicke Hamiltonian, one can obtain the, so called, Tavis-Cummings model by means of the Rotating Wave Approximation (RWA). In this approximation, the counter rotating terms $b^\dagger J_+$ and $b J_-$ are dropped down. Therefore, the Tavis-Cummings Hamiltonian reads [1, 2]:

$$H_{TC}(\lambda) = \omega_0 J_z + \omega b^\dagger b + \frac{\lambda}{\sqrt{2J}} [b J_+ + b^\dagger J_-]. \quad (2)$$

This Hamiltonian, unlike the Dicke Hamiltonian, conserves the quantity $N = N_b + J_z + J$. In other words, the total number of photons (N_b) plus the number of excited atoms ($J_z + J$) are conserved and it is equal to the total number of atoms in the atomic field. The conservation of this quantity implies a finite dimension of the Hilbert space, that can be spanned by a basis of states given by $\{|N_b, M\rangle\}$. These states are simultaneous eigenstates of the operators $b^\dagger b$ and J_z :

$$\begin{aligned} b^\dagger b |N_b, M\rangle &= N_b |N_b, M\rangle, \\ J_z |N_b, M\rangle &= M |N_b, M\rangle. \end{aligned} \quad (3)$$

Thus, the Hamiltonian given by Equation 2 can be exactly diagonalized in the basis (3).

Results

The TC Hamiltonian, Equation 2, can be studied within a mean-field theory by means of bosonic coherent states for the radiation field [5] and spin coherent states for the atomic field [6]. That is, the normalized bosonic coherent state is given by

$$|z\rangle = e^{-zz^*/J/2} e^{z\sqrt{J}b^\dagger} |0\rangle, \quad (4)$$

where z is, in general, a complex variational parameter and $|0\rangle$ is the vacuum state of the radiation field. On the other hand, the normalized spin coherent state is given by

$$|J, y\rangle = \frac{e^{yJ_+}}{(1 + yy^*)^J} |J, -J\rangle, \quad (5)$$

where y is, in general, a complex variational parameter and $|J, -J\rangle$ is the lowest spin projection for the atomic field. Thus, the state of the system in the mean field framework is $|z; J, y\rangle = |z\rangle \otimes |J, y\rangle$.

Now, the ground-state energy of the system is computed minimizing the energy functional $E(z, y, \lambda) = \langle z; J, y | H_{\text{TC}} | z; J, y \rangle$, which depends on the variational parameters z and y , and on the control parameter λ . The z and y parameters are not free, since they are constrained by the conservation of the total number of atoms in the atomic field. This produces the relation $y = \sqrt{\frac{2}{z^2} - 1}$. Consequently, the energy functional can be expressed as a function of only one variational parameter, i.e z , and the strength of the interaction λ , so

$$E(z, \lambda) = 2J \left(\frac{\omega_0}{2} (1 - z^2) + \frac{\omega}{2} z^2 - \frac{\lambda}{\sqrt{2}} z^2 \sqrt{2 - z^2} \right). \quad (6)$$

By minimizing Equation 6 for fixed values of the control parameter λ one obtains the optimal z -parameter value. It is found, that there is a critical value for $\lambda = \lambda_c = |(\omega - \omega_0)/2|$ for which the structure of the system, characterised by the value of z , changes. For $\lambda < \lambda_c$ the value of z that minimizes Equation 6 is $z_{\min} = 0$, whereas for $\lambda > \lambda_c$, the z value is given by

$$z_{\min} = \frac{1}{3} \sqrt{-\frac{(\omega - \omega_0)^2 - 12\lambda^2 + \sqrt{(\omega - \omega_0)^4 + 12(\omega - \omega_0)^2 \lambda^2}}{\lambda^2}}. \quad (7)$$

Consequently, from this analysis, it is found that the system undergoes a second-order QPT at the critical point λ_c [7]. Indeed, the energy and its first derivative with respect the λ parameter are continuous, while the second derivative for the energy becomes non-analytic at the critical point.

This approach is exact in the thermodynamic limit, $J \rightarrow \infty$ [8, 9]. If one wants to describe a finite-size system, then a beyond-mean-field description [10] should be addressed. With this objective, we introduce the Holstein-Primakoff transformation [11] followed by a shift transformation. In this way, it is possible to describe at once the two different quantum phases that appear in the system. Finally, it is necessary to perform a Bogoliubov transformation, so we could bring the Hamiltonian into a diagonal form. All these transformations are canonical, thus, the new operators introduced by them still verify the original commutation relations. Particularly, the Holstein-Primakoff transformation is defined as,

$$\begin{aligned} J_z &= N/2 - d^\dagger d, \\ J_+ &= -\sqrt{N - d^\dagger} d, \\ J_- &= -d^\dagger \sqrt{N - d^\dagger}, \end{aligned} \quad (8)$$

where we have introduced new bosonic operators d (d^\dagger) that fulfill the commutation relation $[d, d^\dagger] = 1$. Furthermore, the bosonic operators describing the radiation field, b (b^\dagger), can be related with these new operators due to the constraint on the conservation of the total number of particles N . This constraint leads to the relation $d^\dagger d = b^\dagger b$. Therefore, the TC Hamiltonian, Equation 2, can be written in terms of just the operators d (d^\dagger).

Now, we perform a shift transformation which depends on a real parameter μ . This is a variational parameter that allows us to describe the symmetry breaking in the system due to the QPT. This transformation reads

$$\begin{aligned} d^\dagger &= c^\dagger + \mu \sqrt{N/2}, \\ d &= c + \mu \sqrt{N/2}. \end{aligned} \quad (9)$$

This is a canonical transformation in which we have introduced a new kind of operators c (c^\dagger) that still fulfill the commutation relation $[c, c^\dagger] = 1$. With this transformation and expanding the square root that appears in the Holstein-Primakoff transformation, the TC Hamiltonian, Equation 2, can be rewritten as a power series in the size of the system, N . Therefore, it can be written as

$$H_{\text{TC}} = H_1 N + H_{1/2} N^{1/2} + H_0 N^0 + \mathcal{O}(N^{-1/2}), \quad (10)$$

where H_i , $i = 1, 1/2, 0$, denotes the dependence of the Hamiltonian on the system size, N (the last term, \mathcal{O} , represents all contributions N^i with i smaller than $-1/2$). Furthermore, we find that the first term H_1 coincides with the energy Equation 6 computed within the mean-field approach. This is something expected since H_1 is the contribution to the system energy that is proportional to N . On the other hand, the next term $H_{1/2}$ is proportional to $\frac{dH_1}{d\mu}$. This means that it is null when μ is set to minimize the first term, H_1 . This means that the first correction to the mean-field approach for the ground state energy is given by H_0 , which is independent of N .

H_0 has form

$$H_0 = A c^\dagger c + B (c^\dagger c^\dagger + cc) + C,$$

where $A = A(\lambda, \mu)$, $B = B(\lambda, \mu)$ and $C = C(\lambda, \mu)$ are real functions that depend on the parameters λ and μ . An additional Bogolibov transformation allows us to bring H_0 into a diagonal form in terms of a new kind of bosonic operators a (a^\dagger). This transformation reads

$$\begin{aligned} c &= u a + v a^\dagger, \\ c^\dagger &= v a + u a^\dagger. \end{aligned} \quad (11)$$

The functions u and v are complex in general, however, they can be taken as real functions in our case. These functions are determined by imposing that the transformation given by Equation 11 is canonical. This means that the new operators a (a^\dagger) must fulfill the commutation relation $[a, a^\dagger] = 1$. In addition, in order to have H_0 as diagonal in the basis defined by the new operators a (a^\dagger), it is necessary to cancel the coefficients accompanying the terms $a^\dagger a^\dagger$ or aa . As a consequence, the two constraints that define the functions u and v in the Bogoliubov transformation read

$$\begin{aligned} u^2 - v^2 &= 1, \\ A u v + B(u^2 + v^2) &= 0. \end{aligned} \quad (12)$$

It is straightforward to check that Equation 12 can be solved using hyperbolic functions. Indeed, a solution is $u = \cosh(\alpha)$ and $v = \sinh(\alpha)$, with $\alpha = -\text{artanh}(2B/A)/2$.

Once performed the Bogoliubov transformation, H_0 can be written as $H_0 = E_0 + \Delta a^\dagger a$. The terms $E_0 = A v^2 + 2B u v + C$ and $\Delta = A(u^2 + v^2) + 4B u v$ are functions that depend on λ as well as on μ , u , and v . However, the μ parameter is fixed since it is set to minimize the mean-field term H_1 , and the functions u and v are also known once we have solved the Equation 12. Consequently, the only dependence of E_0 and Δ is on the λ parameter. To sum up, with the three transformations performed on the TC Hamiltonian, Equation 2, we get

$$H_{\text{TC}} = H_1 N + E_0 + \Delta a^\dagger a. \quad (13)$$

From this equation, it is clear that in this scheme the term E_0 provides the first correction to the ground-state energy computed within the mean-field approach. As a bonus, the formalism allows to calculate the energy gap, Δ , between the two lowest energy levels. The term $\Delta a^\dagger a$ accounts for this lowest excitation produced in the system.

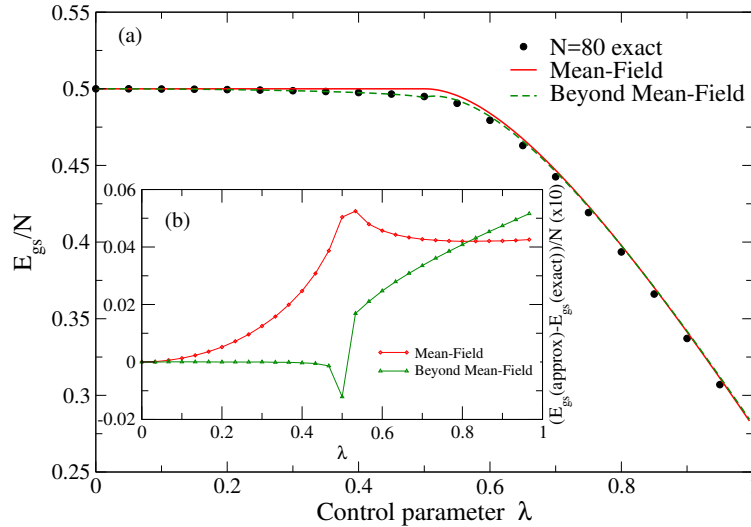


FIGURE 1. (Color online) In panel (a), the ground-state energy per particle E_{gs}/N is plotted as a function of the control parameter λ for the Tavis-Cummings model. Calculations are done for $\omega_0 = 1$, $\omega = 2$ and $J = 40$ ($N = 80$) (black full dots). Lines are for the mean-field result (full red line) and for the beyond mean-field approach (dashed green line). The inset graphic, panel (b), shows the difference between the ground-state energy per particle computed within the mean-field and the beyond mean-field approximations and the exact values obtained numerically.

In Figure 1, the ground-state energy per particle, E_{gs}/N , is plotted as a function of the control parameter λ . The system has a size of $N = 80$ with $\omega_0 = 1$ and $\omega = 2$. In the figure, the exact diagonalization (depicted with symbols) of the TC Hamiltonian, Equation 2, is compared to the results obtained by means of the mean-field (red full line) and beyond-mean field (dashed green line) approaches. First of all, we observe that the ground-state energy changes its behaviour at $\lambda = 0.5$, which corresponds to the critical value λ_c for the QPT. Secondly, the beyond-mean field approach fits better to the exact solution than the mean-field approach for a finite-size system. This is due to the fact that the mean-field approach is exact only in the thermodynamic limit, $J \rightarrow \infty$. In order to show how accurate are the two approximations performed with respect to the exact results, we present in panel (b) the difference between the ground-state energy per particle computed within the mean-field and the beyond mean-field approximations and the exact values obtained numerically. In general, we can see that the beyond mean-field calculation improves the mean field results. This validates the beyond mean-field formalism as a valuable tool for taking into account the finite-size effects in the system.

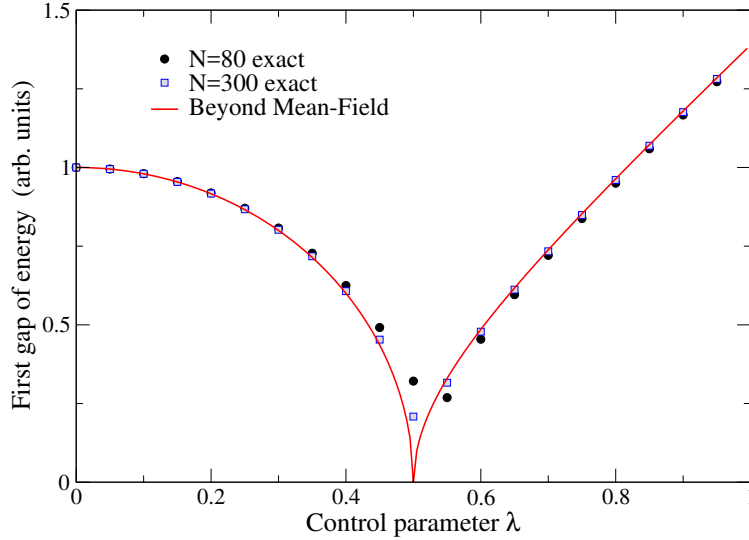


FIGURE 2. (Color online) Energy gap, Δ , between the ground-state and the first excited state as a function of the control parameter λ in the Tavis-Cummings model. The full red line gives the beyond mean-field results while exact calculations are presented for two system sizes: $J = 40$ ($N = 80$) represented by black dots and $J = 150$ ($N = 300$) represented by blue squares. All calculations are done with $\omega_0 = 1$, $\omega = 2$.

In Figure 2, the evaluated energy gap between the ground-state and the first excited state using the beyond mean-field approximation is plotted (full red line) together with the exact numerical results for two system sizes, black dot symbols for system with $N = 80$ and blue square symbols for $N = 300$. Again, $\omega_0 = 1$ and $\omega = 2$ are used. We observe that the beyond mean-field approach gives a very accurate description of the first excited state. There is only a small discrepancy around the critical point, $\lambda_c = 0.5$, but this is expected due to finite-size effects of the system. Furthermore, we can observe that the bigger the system is, the closer are the exact results to the beyond mean-field approach calculation. It should be noted, that the mean-field approach does not provide information about the gap energy, so the first approximation to this quantity is given by this beyond mean-field approach. This means that we need to compute the next order in the N expansion ($N^{-1/2}$) to observe finite size effects in the gap with the beyond mean-field approach. On the other hand, the fact that the energy gap, Δ , drops down to zero at the critical point is a consequence of the system undergoing a second order QPT and is nicely given by our calculation.

Conclusions

We have described the Tavis-Cummings model within a mean-field approach using a formalism of coherent states. In such a formalism, a bosonic coherent state and a spin coherent state are used for describing the radiation field and the atomic field, respectively. This allows to calculate the ground-state energy of the system by means of a variational procedure. In order to improve the mean-field description, we have performed a beyond-mean-field study. This task

has been possible using several canonical transformations on the system. Specifically, we have applied the Holstein-Primakoff followed by shift and, finally, Bogolibov transformations. In this way, we have been able to compute the first correction to the mean-field value for the ground-state energy. This new approach improves remarkably the results computed within the mean-field framework and fits pretty well with the exact numerical results. Finally, the new approach has allowed us to describe with good accuracy the behaviour of the first energy gap in the system.

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