Efficient basis for the Dicke model: I. Theory and convergence in energy

Miguel A Bastarrachea-Magnani and Jorge G Hirsch

Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México, Apartado Postal 70-543, Mexico DF, CP 04510, Mexico
E-mail: miguel.bastarrachea@nucleares.unam.mx

Received 12 September 2013
Accepted for publication 12 September 2013
Published 2 April 2014

Abstract
An extended bosonic coherent basis has been shown by Chen et al (2008 Phys. Rev. A 78 051801) and Liu et al (2009 Phys. Rev. A 80 165308) to provide numerically exact solutions of the finite-size Dicke model. The advantages in employing this basis, as compared with the photon number (Fock) basis, are exhibited to be valid for a large region of the Hamiltonian parameter space by analyzing the converged values of the ground state energy.

Keywords: Dicke model, efficient basis, numerical convergence

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

1. Introduction

The Dicke Hamiltonian describes a system of $N$ two-level atoms interacting with a single monochromatic electromagnetic radiation mode within a cavity [1]. The Hamiltonian is very simple but not exactly solvable, and continues to drive research into its properties. One of the most interesting is its quantum phase transition (QPT) in the thermodynamic limit [2, 3]. The interest in solving the Dicke Hamiltonian for a finite $N$ comes not only from the fact that it provides a good description for the systems manipulated in the laboratory but also for the close connection found between QPTs, entanglement and quantum chaos [4–6]. Further, Dicke-like Hamiltonians have attracted much attention because of the experimental realization of the superradiant phase transition in a Bose–Einstein condensate [7, 8].

The Dicke Hamiltonian is integrable for a finite $N$ in two limits: when the atom–field interaction or the atomic energy gap are zero. In both situations, the atomic sector is described in the angular momentum basis, which is finite with $j = N/2$. The no interaction case is diagonal in the photon number (Fock) basis, while the generalized bosonic coherent basis allows construction of analytic eigenstates of the Hamiltonian when the atomic excitation energy goes to zero [9, 10]. A reduction in the size of the truncated subspace by orders of magnitude can be obtained employing the coherent basis, which allows the achievement of easily converged values of the observables [9, 10].

The purpose of this work, and the accompanying one [11], is to show that the benefits of employing the coherent basis are valid for a large region of the Hamiltonian parameter space, for the ground state and for a significant part of the energy spectra. In this first part, the convergence in the energy is the criterion of choice.

2. The Dicke Hamiltonian and its integrable limits

The interaction between a system of $N$ two-level atoms and a single mode of a radiation field can be described by the Dicke Hamiltonian

$$H_D = \omega a^\dagger a + \omega_0 J^z + \frac{\gamma}{\sqrt{N}} (a + a^\dagger) (J'_x + J'_y).$$

The frequency of the radiation mode is $\omega$, which has an associated number operator $a^\dagger a$. For the atomic part $\omega_0$ is the excitation energy, meanwhile $J^z$, $J'_x$ and $J'_y$ are collective atomic pseudo-spin operators that obey the $SU(2)$ algebra. The subspace of interest is defined by $j = N/2$. In the thermodynamic limit the QPT takes place when the interaction parameter $\gamma$ reaches the critical value $\gamma_c = \sqrt{\omega_0 \omega}/2$. At zero interactions the eigenstates are the tensor products between photon numbers, Fock states $|n\rangle$ for the radiation modes and angular momentum eigenstates $|j, m\rangle$ for the atomic part, which we call the Fock basis.

When the atomic frequency goes to zero, we have another integrable limit. It is obtained performing a $-\pi/2$ rotation of the pseudospin operators around the $y$-axis $J'_x = -J_x$, $J'_y = J_y$ with $J_z = \frac{J_x J_y - J_y J_x}{2}$ and shifting the bosonic annihilation operator by $A = a + \frac{2\gamma}{\omega \sqrt{N}} J_z = a + G J_z$. Substituting both
transformations in the Hamiltonian we obtain
\[ H_D = \omega \left( A^\dagger A - G^2 J_2^2 \right) - \frac{\omega_0}{2} (J_+ + J_-). \] (2)

When \( \omega_0 \to 0 \) the Dicke Hamiltonian eigenstates are the tensor product between the number eigenstates \( |N⟩ \) of \( A^\dagger A \) and the angular momentum eigenstates \( |j, m⟩ \) of \( J \). \([9, 10]\)

The vacuum of \( A \) is an eigenstate of the annihilation operator \( a \) with eigenvalue \( \alpha = -Gm \). It is a coherent state seen in the Fock basis and the ground state of \( H_D \) when \( \omega_0 \to 0 \). We call them the coherent basis. In what follows we associate this basis with the use of a capital \( N \), while for the Fock basis we employ a small \( n \).

The coherent states depend on the angular projection eigenvalue \( m \) of the atomic state, and on the interaction parameter \( \gamma \) (\( G = 2\gamma / \omega \sqrt{N} \)). When the interaction becomes null, the exact solution in the zero interactions limit is recovered. It implies that the coherent basis contains as a particular case the Fock basis in the situation in which it is the exact solution.

In the next section we describe the numerical diagonalization.

3. Numerical diagonalization

While the Fock basis is commonly used to diagonalize the Hamiltonian, it becomes intractable in the strong coupling limit even for a few dozens of atoms \([9]\).

We compare the minimal truncation needed to obtain convergence of the solution, using the Fock and the coherent basis to diagonalize the Hamiltonian, truncating the bosonic sector up to \( n_{\text{max}} \) and \( N_{\text{max}} \), with energies \( E_F^N \) and \( E_C^N \) for the ground state, respectively. The convergence criteria are defined by using the upper limits \( n_{\text{max}} \) and \( N_{\text{max}} \), with some tolerance \( \epsilon \):

\[ \Delta E_F = |E_F^N(n_{\text{max}} + 1) - E_F^N(n_{\text{max}})| < \epsilon. \] (3)

We consider the solution converged if the above relation holds. The same goes for the coherent basis. The same criteria will be used to find the minimum values \( n_{\text{max}} \) and \( N_{\text{max}} \) for any excited level \( k \). In the next section, we compare \( n_{\text{max}} \) with \( N_{\text{max}} \) in order to analyze the truncation behavior and the advantages of each basis in different parameter regions.

3.1. Ground state energy

In what follows, we explore the truncation behavior for both basis in several parameter regions, principally for \( \gamma \) and \( \omega_0 \). A comparison between the truncation in both basis is shown, in the terms explained above, for different values of the interaction parameter \( \gamma \) and \( j \), in resonance \( \omega_0 = \omega = 1 \), for the ground state. In this case the critical value of the interaction parameter is \( \gamma_c = 0.5 \). The advantage of using the coherent basis becomes clear when the truncation is analyzed as a function of \( j = N/2 \), from 1 to 40. As the atomic number \( N \) increases, the minimum number of photons needed to obtain convergence in the strong coupling limit grows too, making the numerical diagonalization very difficult using the Fock basis. For two representative interaction parameters, \( \gamma = 0.5 \) and 1.0, we show the results in figure 1.

For the ultra-strong coupling \( \gamma = 1.0 \) it is very difficult to obtain the numerical solution using the Fock basis for \( j > 20 \) (\( N > 40 \)) because it requires extremely large computing resources. This is the major problem of using the Fock basis. On the other hand, for the coherent basis, the dimensionality necessary for convergence is small and decreases as \( j \) increases.

In figure 2 we show the behavior of \( n_{\text{max}} \) and \( N_{\text{max}} \) as functions of \( \gamma \), in resonance, for several representative values of \( j \). Again, \( \gamma_c = 0.5 \).

As we can see, meanwhile the value of \( N_{\text{max}} \) increases slowly with \( \gamma \), \( n_{\text{max}} \) increases rapidly, making very hard the numerical diagonalization with the Fock basis for \( j > 20 \) and \( \gamma \approx 1 \). While the truncation in both basis is almost the same as in the normal phase \( \gamma < \gamma_c = 0.5 \), in the superradiant phase \( n_{\text{max}} \) increases noticeably faster than \( N_{\text{max}} \).

Employing projected atomic \( SU(2) \) coherent states, an analytical expression for the lower bound of truncation, \( \langle n_{\text{max}} \rangle \), in the Fock basis, can be obtained \([12]\). It is built by taking the expectation values of \( \alpha^\dagger \alpha \), and adding five times its quadratic deviation. In the superradiant phase it reads

\[ \langle n_{\text{max}} \rangle = N\gamma^2 \left[ 1 - \left( \frac{\sqrt{\omega_0} \gamma}{2\gamma} \right)^4 \right] + 5 N\gamma^2 \left[ 1 - \left( \frac{\sqrt{\omega_0} \gamma}{2\gamma} \right)^4 \right]. \] (4)
In figure 3 we compare this expression with the \( n_{\text{max}} \) obtained numerically using the \( \Delta E \) convergence criteria. The agreement between the two curves is remarkably good. It points out that the \( \Delta E \) criteria are enough to obtain the right value of the truncation. The above expression describes the minimal dimension of the photon sector necessary to calculate the ground state energy with the desired precision, showing that it grows linearly with the number of atoms \( N \), and quadratically with the interaction strength \( \gamma \), as mentioned above.

3.2. Out of resonance

In order to analyze the truncation behavior out of resonance, we fix \( \omega = 1 \) and vary the value of \( \omega_0 \) for \( j = 20 \) and two values of \( \gamma \). In figure 4 we show the results for \( \gamma = 0.5 \) and 1.0, respectively. In this case the normal region is defined by \( \omega_0 > 4 \omega \gamma^2 \). It means that the superradiant region comprises \( \omega_0 < 1 \). In figure 4 (left) and \( \omega_0 < 4.0 \) in figure 4 (right).

As was pointed out above, when \( \omega_0 \to 0 \), for every \( \gamma \) and \( j \), the coherent basis is the best option to diagonalize the Hamiltonian because it is the exact solution. As \( \omega_0 \) increases, a crossing between the curves describing \( n_{\text{max}} \) and \( N_{\text{max}} \) as functions of \( \omega_0 \) can be observed. It takes place in the normal region, where \( \gamma \ll \gamma_c \), i.e. the coupling constant is very small compared with the atomic excitation energy. Only in this region does the Fock basis seem to require a truncation smaller than the coherent basis.
3.3. Precision versus truncation

It is possible to select the desired precision in the ground state energy by knowing how fast $\Delta E$ goes to zero in both bases as $n_{\text{max}}$ and $N_{\text{max}}$ increase. For several $j$ representatives and with $\gamma = 0.5$, in resonance, we show the results in figure 5. Working in this parameter region around the QPT region no preference is given to any of the two basis. Here $\Delta E_F$ and $\Delta E_C$ account for the Fock and coherent basis, equation (3).

As shown in figure 5, increasing the energy precision in the Fock basis demands a larger $N_{\text{max}}$, which grows also with $j$. In the coherent basis, left figure, the required values of $n_{\text{max}}$ are smaller, and seem to be quite independent of $j$ in the cases analyzed here.

A linear fit for $j = 40$ gives us the following relation between $N_{\text{max}}$ and $\Delta E_C$:

$$-\log_{10}(\Delta E_C) = 0.278 + 0.732n_{\text{max}} \Rightarrow 
\Delta E_C = 0.526 \times 10^{-0.732N_{\text{max}}}. \quad (5)$$

4. Conclusions

To obtain the eigenvalues and eigenvectors of the Dicke Hamiltonian for a finite number of atoms it is necessary to perform a numerical diagonalization, employing a truncated boson number space. Two bases, associated with the two integrable limits of the Hamiltonian, are used in this work. The Fock basis corresponding to the zero interaction limit is the most commonly used; however, it consumes a lot of computing resources and becomes impractical to study the superradiant region for more than a few dozens of atoms. In the present paper we have shown that, in most of the Hamiltonian’s parameter regions including the QPT, the coherent basis requires a significant smaller truncation. In the accompanying work [11] we present a similar analysis for a convergence criterion based on the wave function, and for excited states.

Acknowledgments

We thank O. Castaños, R. López-Peña and E. Nahmad for many useful and interesting conversations. This work was partially supported by CONACyT-México and PAPIIT-UNAM 102811.

References

[1] Dicke R H 1954 Phys. Rev. 93 99
[2] Hepp K and Lieb E H 1973 Ann. Phys. 76 360
[3] Wang Y K and Hioe F T 1973 Phys. Rev. A 7 831
[4] Emary C and Brandes T 2003 Phys. Rev. E 67 066203
[5] Lambert N, Emary C and Brandes T 2005 Phys. Rev. Lett. 92 073602
[6] Vidal J and Dusuel S 2006 Europhys. Lett. 74 817
[7] Baumann K, Guerlin C, Brennecke F and Esslinger T 2010 Nature 464 1301
[8] Nagy D, Kónya G, Szirmai G and Domokos P 2010 Phys. Rev. Lett. 104 130401
[9] Chen Q H, Zhang Y Y, Liu T and Wang K L 2008 Phys. Rev. A 78 051801
[10] Bastarrachea-Magnani M A and Hirsch J G 2011 Rev. Mex. Fis. 57 69
[11] Hirsch J G and Bastarrachea-Magnani M A 2014 Phys. Scr. T160 014018
[12] Castaños O, Nahmad-Achar E, López-Peña R and Hirsch J G 2011 Phys. Rev. A 84 013819