Efficient basis for the Dicke model: II. Wave function convergence and excited states

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1. Introduction

The Dicke Hamiltonian describes a system of $N$ two-level atoms interacting with a single monochromatic electromagnetic radiation mode within a cavity. It is described in the accompanying paper \[1\] and \[2\]. The purpose of this second part is to show that the benefits of employing the coherent basis are valid for a large region of the Hamiltonian parameter space and many excited states by analyzing the convergence in the wave functions.

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

$$H_D = \omega_0 a^\dagger a + \omega_0 J_0^z + \frac{\gamma}{\sqrt{N}} (a + a^\dagger) (J_+^z + J_-^z).$$

The frequency of the radiation mode is $\omega$, which has an associated number operator $a^\dagger a$. For the atomic part $a_0$ is the excitation energy, meanwhile $J_0^z$ and $J_0^x$ are collective atomic pseudo-spin operators that obey the $SU(2)$ algebra. It holds that if $j (j+1)$ is the eigenvalue of $J^2 = J_0^z J_0^x + J_0^z J_0^y$, then $j = N/2$ defines the symmetric atomic subspace which includes the ground state. The interaction parameter $\gamma$ depends principally on the atomic dipolar moment.

2. Numerical diagonalization

We compare the minimal truncation needed to obtain convergence of the solution, using the two bases defined in \[2\]: the coherent basis $|N; j, m\rangle$ and the Fock basis $|n; j, m\rangle.

The wave functions, expanded in the truncated Fock (F) and coherent (C) bases are, for a given $j = N/2$

$$|\Psi_X^j\rangle = \sum_{x=0}^{x_{\text{max}}} \sum_{m=-j}^j C_{m,x}^j |x; j, m\rangle,$$

where $x = n$ for $X = F$, and $x = N$ for $X = C$, and $k = 1, \ldots, (x_{\text{max}} + 1)(2j + 1)$ enumerates the eigenstates ordered by their energies $E_X^j$ with $k = 1$ assigned to the ground state.

2.1. The wave functions

The probability $P_n$ of having $n$ photons in the $k$th state in the Fock basis, or $P_N$ of having $N$ excitations in the coherent basis is

$$P_{x,n} = |\langle x | \Psi_X^j \rangle|^2 = \sum_m |C_{m,x}^j|^2.$$

where $x = n, N$ for $X = F, C$, respectively. The ground state probability distribution $P_k = P_{1,k}$ is shown as a function of $n$ or $N$ up to $n_{\text{max}}$ or $N_{\text{max}}$, for $\gamma = 0.5$ and $1.0$, and $j = 10$ in figures 1 and 2. Both wave functions were calculated with the truncation necessary to have the energy converged with $\Delta E < \epsilon = 1 \times 10^{-6}$. 

(Some figures may appear in color only in the online journal)
From figures 1 and 2 it is clear that many components that contribute very little to the wave function must be included in the calculations to obtain the desired precision in the ground state energy. It can also be observed in the figures that for \( \gamma = 0.5 \), which is \( \gamma_c \) in this case, the largest probability is to have no photons in the Fock basis, or no excitations in the coherent basis. The situation is different in the superradiant region, \( \gamma = 1 \), where in the Fock basis the distribution of photons resembles a Gaussian curve, with its maximum at a photon number proportional to the number of atoms, while in the coherent basis the probability of having zero excitations remains dominant. This is the power of the coherent basis, which allows exact ground state wave functions to be obtained numerically for numbers of atoms which are intractable in the Fock basis.

To study the convergence in the wave function we define its precision \( \Delta P_X \) [7] as

\[
\Delta P_X \leq \sum_{n=-j}^{j} \left| C_{n,n+1,m} (x_{\text{max}} + 1) \right|^2.
\]

where \( x = n, N \) for \( X = F, C \), respectively. This \( \Delta P \) criterion demands less computing resources than the \( \Delta E \) criterion [2, 7], because it requires only the information about one truncation value (\( x_{\text{max}} \)) instead of two.

Figure 3 displays the plots of \( -\log_{10}(\Delta P_F) \) as a function of \( n_{\text{max}} \), and of \( -\log_{10}(\Delta P_C) \) as a function of \( N_{\text{max}} \).

A linear fit, for \( j = 40 \), gives us the following relation between \( N_{\text{max}} \) and \( \Delta P_C \):

\[
-\log_{10}(\Delta P_C) = 1.45 + 0.811 N_{\text{max}}
\]

\( \Rightarrow \Delta P_C = 0.0354 \times 10^{-0.811 N_{\text{max}}} \). (5)

3. Numerically exact results for excited states

In this section we extend the analysis to the excited states. To accurately evaluate a significant part of the energy spectrum is a necessary ingredient in the study of quantum chaos [3] and of excited state quantum phase transitions (ESQPT) [5, 6].

In figure 4 we display plots of \( \Delta P \) as a function of the state \( k \), for \( j = 40, \gamma = 0.5, \omega_0 = 1.0, N_{\text{max}} = 20 \) and \( \epsilon = 1 \times 10^{-5} \). In the upper figures we show the \( \Delta P_F \) and in the lower ones \( \Delta P_C \). On the left the vertical scale is linear and all states are listed on the horizontal axis, while on the right hand side the vertical scale is logarithmic and only the 150 states with lower energies are included. The horizontal green line depicts the tolerance \( \epsilon \).

It is indeed remarkable to observe in figure 4 that a few hundred states calculated in the coherent basis have their wave function converged, and \( \Delta P_C \), for these states, grows in a smooth and nearly monotonic way as a function of the \( k \) index. This is not the case in the Fock basis, where \( \Delta P_F \) fluctuates by orders of magnitude between a given state and the following one. It is worth comparing the convergence criteria based on the wave function and described above, with the more standard convergence in energy, which was described in the previous paper [2]. In figure 5 we show \( \Delta P_C \) versus \( \Delta E_C \) for the first 250 excited states, \( k \), whose energies converged in the coherent basis with \( \Delta E < 1 \times 10^{-4} \).

A linear fit of these data results in

\[
-\log_{10}(\Delta P_C(k)) = 0.71077 - 1.10337 \log_{10}(\Delta E_C(k))
\]

\( \Rightarrow \Delta P_C = 0.19464 \times (\Delta E_C)^{1.10337}. \) (6)
The number of states whose $\Delta P$ is smaller than a tolerance $\epsilon$ for $j$ and $n_{\text{max}}$ given for the Fock basis and $N_{\text{max}}$ for the coherent basis is presented in table 1. The two tolerances selected are $\epsilon_1 = 1 \times 10^{-6}$ and $\epsilon_2 = 1 \times 10^{-4}$, with $\gamma = 0.5$ and $\omega_0 = 1$.

The advantages associated with the use of the coherent basis are even more clear in this case, because the number of states whose wave function has converged with the selected tolerance is larger than those whose energies have converged. It should be mentioned, however, that the tolerances in $\Delta P$ are absolute, because its best case value of a fully converged state is zero, and the worst situation, for completely different wave functions, is one. In contrast, the energy scale is arbitrary, and can have positive and negative values, even some levels with energies very close to zero. It makes the use of the relative error employed in [1, 7] dangerous when the reference energy is very small. But for excited states a fixed value of $\epsilon$ implies the need for more precise digits in the calculated energy, making the convergence more difficult for higher energies. For this reason our $\Delta E$ criterion is more stringent than the $\Delta P$ one: every excited state with converged energy has guaranteed the convergence of its wave function. As the coherent basis
provides many converged states with a single truncation value, it is promising to study the presence of ESQPT, predicted in Dicke-like systems and spin systems for \( \gamma \) values deeply in the superradiant phase \([5, 6]\).

### 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 basis, associated with the two integrable limits of the Hamiltonian, are used in this work. In the present paper we have shown that, in most of the Hamiltonian’s parameter regions including the ESQPT, the coherent basis requires a significantly smaller truncation. We extended the analysis to the convergence in the wave function, exhibiting both convergence criteria as equivalent, and presented the numerical relationships between them. The study of the probability distributions of the number of bosons was helpful in understanding the differences between the two bases, and the advantages of the coherent basis. The convergence of the energies and the wave functions was also investigated for the excited states, showing that the coherent basis is very powerful also in this case, allowing hundreds of converged states to be obtained with a single truncation value. This finding can be very useful in order to observe the presence of quantum chaos around the phase transition, as well as to study the ESQPT.

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