Energy spectra of a spin-$\frac{1}{2}$ XY spin molecule interacting with a single mode field cavity

H Tonchev, A A Donkov, H Chamati

Institute of Solid State Physics, Bulgarian Academy of Sciences,
72 Trarigradsko Chaussée, 1764 Sofia, Bulgaria
E-mail: htonchev@issp.bas.bg, aadonkov@issp.bas.bg, chamati@issp.bas.bg

Abstract. We report results from our continued investigations on a finite-size chain (molecule) of $L$ spin-$\frac{1}{2}$ spins with XY spin exchange interaction coupled at an arbitrary spin site to a single mode of an electromagnetic field via the Jaynes-Cummings model. Here we study the energy spectra in the case of an arbitrary photon fill number $n$, as compared to the $n=1$ limit in our previous work [J. Phys.: Conf. Ser. 682 (2016) 012032] and [J. Phys.: Conf. Ser. 764 (2016) 012017]. By building the appropriate combinations of basis product states involving the photon as well as the up down spins it is possible to simplify the systems that are necessary to diagonalize from $n \times 2^L$ to at most $2^L$. This results are in tune with those reported in the recent paper by N. Wu [Phys. Rev. B 97 (2018) 014301], and may prove to be useful for the quantum computing aficionados.

1. Introduction

The Jaynes-Cummings [1–3] model for the interaction of an atomic two level system with a quantized electromagnetic field has an exact solution, see, e.g., [4, 5] for the formulae. Extensions to a field coupled to $L$ 2-level non-interacting systems has also been studied, for example in [6, 7]. In our model consideration the Jaynes-Cummings term is interpreted as a coupling between the field and a spin, of value $\frac{1}{2}$, see [8] for some physical reasoning of such a possibility. Introducing more spins into the spin chain, and switching some kind of a spin-spin interaction between the spins, one can envisage an application of this model to bit manipulation [9].

One can start with an exactly solvable XY model [10], or use a more recent setting [11], and then study the effect of having an additional boson field linearly coupled to the spins, as is the Jaynes-Cummings term. From this point of view, it is useful to obtain some exact formulae for the combined model Hamiltonian. With the help of a transformation to fermion operators [12] this is achieved in [13]. Here, on the other hand, we look into the problem by using the original, spin up and spin down basis states on each site of the chain, “sift” the matrices through the invariant available in the model [14] and then focus also on the corresponding eigenvectors expressed in terms of this states.

Below, in Section 2, we set the Hamiltonian of the model, and consider the resulting more compact form of the matrices to be actually diagonalized, as obtained by the “sifting through” procedure, and show the results for a system of up to 2 spins, concluding with remarks, in Section 3.
2. Bosonic field coupled to a site on a spin chain

The Hamiltonian under consideration is:

\[
\hat{H} \equiv \hat{H}_{JC} + \hat{H}^{XY} = \omega_R \hat{S}_k^z + \omega_f (\hat{a}^\dagger \hat{a} + \frac{1}{2}) + G (\hat{a} \hat{S}_k^+ + \hat{a}^\dagger \hat{S}_k^-) + J \sum_{i} (\hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y),
\]  

which is assumed here without further justification to be applicable to a system of spins in a cavity with a laser field, so that we have one mode of frequency \(\omega_f\) of a laser field focused on one of the spins of the spin \(\frac{1}{2}\) chain of \(L\) sites, (e.g., \(L = 5\) in figure 1). The interaction \(G\) part is from the Jaynes-Cummings (JC) model for the photon (\(\hat{a}, \hat{a}^\dagger\)) interacting with a two level system (spin operator \(\hat{S}_k^i (i = x, y, z)\) on site \(k\), the term with \(J\) is the XY model of the spin-spin interaction between nearest-neighbour spins, and the index \(i\) is enumerating the sites along the spin molecule, \(i = 1, \ldots, L-1\) for open ended molecule, and \(i = 1, \ldots, L\) for a closed cyclic molecule using the convention \(\hat{S}_{L+1} \equiv \hat{S}_1\). Here we focus on the open ended configuration.

![Figure 1](image-url)  

Figure 1. (color online) A view of a spin system in a cavity with an electro-magnetic field of frequency \(\omega_f\) focused on a particular spin.

The spin basis is chosen as up, down for each site, \(|\uparrow_i\rangle\) and \(|\downarrow_i\rangle\), while the photon number states are \(|n\rangle\), with \(n = 0, 1, \cdots\). For example, the action of the Hamiltonian on the state with maximum spin \(M_z = L/2\) value we have:

\[
\hat{H}|n, \uparrow_1 \cdots \uparrow_k \cdots \uparrow_L\rangle = (\frac{1}{2} \omega_R + \omega_f (n + \frac{1}{2})) |n, \uparrow_1 \cdots \uparrow_k \cdots \uparrow_L\rangle + G \sqrt{n+1} |n+1, \uparrow_1 \cdots \downarrow_k \cdots \uparrow_L\rangle
\]  

and then for the connected state we get correspondingly:

\[
\hat{H}|n+1, \uparrow_1 \cdots \downarrow_k \cdots \uparrow_L\rangle = (\frac{1}{2} \omega_R + \omega_f (n + \frac{3}{2})) |n+1, \uparrow_1 \cdots \downarrow_k \cdots \uparrow_L\rangle + G \sqrt{n+1} |n, \uparrow_1 \cdots \downarrow_k \cdots \uparrow_{L-1} \uparrow_L\rangle + \frac{1}{2}J (|n+1, \uparrow_1 \cdots \downarrow_{k-1} \uparrow_k \cdots \uparrow_L\rangle + |n+1, \uparrow_1 \cdots \downarrow_k \uparrow_{k+1} \cdots \uparrow_L\rangle). 
\]  

A few comments are in order. From these expressions we can deduce that the \(G\) part mixes a state with \(|n = n_f, M_z = M\rangle\) with states \(|n_f + 1, M-1\rangle\) and \(|n_f - 1, M+1\rangle\) with appropriate factors, and the \(J\) part of the Hamiltonian rearranges the spins, without a change in the value of \(n\) and \(M_z\), individually, as expected [15, 16], and for their sum as well. This is one way of showing that there is an invariant, given by the value of the sum \(n + M_z\), since the mixed vectors belong to the same eigenvalue of this invariant. We will use this below to build the appropriate systems to obtain the eigenvalues. Another conclusion that can be drawn, is that when we truncate the series on \(n\), by assuming a given maximum value \(n_{\text{max}}\), this will introduce spurious zero matrix elements (zero value) of the Hamiltonian acting on the \(|n_{\text{max}}, M_z\rangle\) state, which can lead to overcounting of the existing dark modes, the modes with \(E = 0\), in the spectrum of the Hamiltonian, [17].

Now, looking back into equations (2) and (3), we see that for a given starting value \(n = n_f\), by continuing the above procedure of applying the Hamiltonian to the states that appear on the right side, we can build a closed system, which involves states with \(0, 1, 2, \cdots, L\) turned spins and correspondingly
increased values of \( n (n_f + 1, n_f + 2, \cdots, n_f + L/2) \), all the way to the \( |n_f + L/2, \downarrow_1 \cdots \downarrow_k \cdots \downarrow_L \rangle \) state. This produces a system of \( 1 + L + (L)(L - 1)/2 + \cdots + 1 = 2^L \) equations (by counting the ways to place 1 downward spin, 2 downward spins, and so on, on \( L \) sites). In this most general case with an invariant \( n_f + L/2, n_f \geq 0 \) to obtain the eigenvalues we need to diagonalize a \( 2^L \times 2^L \) matrix.

We can imagine now a state that initially has 1 turned downward spin somewhere in the chain, \( |n = n_f, M_z = L/2 - 1 \rangle \). The above procedure will still lead to a \( 2^L \) sized system of equations, with appropriate coefficients, for big enough \( n_f \). On the other hand, if we look at a state \( |n = 0, \downarrow_1 \cdots \downarrow_k \cdots \downarrow_L \rangle \), it is not possible to simultaneously turn one of the spins up and to decrease \( n \), as \( n \) is already at a minimum value. For this particular state, with an invariant value of \(-L/2\), we need to diagonalize a \( 1 \times 1 \) matrix, as it turns out to be an eigenstate. By doing the above algebra, we find that for all the values of the invariant that are less then \( L/2 \) we obtain system of equations with size that is less than \( 2^L \). The number of states with an invariant \(-L/2 + 1 = 1 + L\), with an invariant \(-L/2 + 2 \) this number is \( 1 + (\frac{1}{2}) + (\frac{3}{2}) \), and for the invariant \(-L/2 + m \) the subspace has the dimension of:

\[
Dim_m \equiv 1 + \binom{L}{1} + \binom{L}{2} + \cdots + \binom{L}{m}, \quad 0 \leq m \leq L.
\]

With this formula we count the states by first assigning \( n = m \), with all the spins downward (1 state), then \( n = m - 1 \) and 1 upward spin among \( L - 1 \) downward ones (\( L \) number of states), and so on. By extending the definition of \( Dim_m \), so that \( Dim_m = 2^L \), for \( m \geq L \), we can summarize the above discussion with the conclusion that for an invariant value \(-L/2 + m \) the corresponding eigenvalues problem requires a diagonalization of a \( Dim_m \times Dim_m \) matrix.

As concluding introductory remarks, we mention that the limiting cases, \( J = 0 \) or \( G = 0 \), of the Hamiltonian can be diagonalized analytically. For example, for the Jaynes-Cummings Hamiltonian \( H_{JC} \) the corresponding spectrum looks like (compare with, e.g., [5, 7]):

\[
H_{JC}|n = 0, \downarrow \rangle = E_{\text{gnd}}|n = 0, \downarrow \rangle, \quad H_{JC}(a_\pm|n, \uparrow \rangle + b_\pm|n + 1, \downarrow \rangle) = E_\pm(a_\pm|n, \uparrow \rangle + b_\pm|n + 1, \downarrow \rangle)
\]

where

\[
E_{\text{gnd}} = -\delta/2, \quad E_\pm = (n + 1)\omega_f \pm \Omega_n/2, \quad \Omega_n := \sqrt{\delta^2 + 4G^2(n + 1)}, \quad \delta := (\omega_R - \omega_f),
\]

and the normalized coefficients for the eigenvectors of the higher energy states:

\[
a_\pm = \pm \sqrt{(\Omega_n \pm \delta)/(2\Omega_n)}, \quad b_\pm = \pm \sqrt{(\Omega_n \mp \delta)/(2\Omega_n)}, \quad a_\pm^2 + b_\pm^2 = 1,
\]

and the quantum optics convention is used to denote with \( \delta \) the detuning and with \( \Omega_n \) the Rabi frequency.

For the pure \( H^K \) part, the energies are given by, e.g., [11]

\[
E_l = \frac{2J \sin(l\pi/L)}{L \sin(\pi/L)}, \quad 0 \leq l \leq L.
\]

The explicit form of the matrix elements of the Hamiltonian from equation (1) can be easily obtained, since the spin states correspond to spin 1/2, and it may be just harder to write conveniently the expression, then to derive it. It has the form (compare with [13]), where for convenience we have used the notations \( |\uparrow \rangle \equiv |+1/2\rangle \), \( |\downarrow \rangle \equiv |-1/2\rangle \), and \( \sigma_i = \pm 1/2 \):

\[
\hat{H}|n, \sigma_1 \cdots \sigma_k \cdots \sigma_L \rangle = \sum_{n' + \sum(\sigma'_i) = n + \sum(\sigma_i) \equiv -L/2 + m} H_{m \times m}^{|n', \sigma'_1 \cdots \sigma'_k \cdots \sigma'_L \rangle}(9)
\]
with the \( \text{Dim}_m \times \text{Dim}_m \) matrix \( H_m \) corresponding to the invariant value \(-L/2 + m\) is given by, \( \text{with the extended definition of} \ \text{Dim}_m = 2^L, m \geq L \):

\[
\langle n', \sigma'_1 \cdots \sigma'_k \cdots \sigma'_L \mid H \mid n, \sigma_1 \sigma_2 \cdots \sigma_k \cdots \sigma_L \rangle = \left( \frac{\omega_R}{2} \right)^\frac{L}{2} \delta_{\sigma_k, \pm 1/2} + \omega_f (n + \frac{1}{2}) \delta_{n', n} \prod_{i=1}^L \delta_{\sigma'_i, \sigma_i} + G \left( \sqrt{n} \delta_{n', n-1} \delta_{\sigma_k, -1/2} + \sqrt{n + 1} \delta_{n', n+1} \delta_{\sigma_k, +1/2} \right) \prod_{i=1, i \neq k}^L \delta_{\sigma'_i, \sigma_i} + \frac{J}{2} \sum_{i=1}^{L-1} \delta_{\sigma_i, -1/2} \delta_{\sigma_{i+1}, +1/2} + \delta_{\sigma_i, +1/2} \delta_{\sigma_{i+1}, -1/2} \right) \delta_{n', n} \prod_{j=1, j \neq i+1}^L \delta_{\sigma'_j, \sigma_j}.
\]

(10)

As an example, let's consider a system with two spins, and the Jaynes-Cummings term being coupled to site 1, this corresponds to \( k = 1, L = 2 \) in equation (1). We have two \(-1, 0\) special values of the invariant, in the form \(-L/2 + m\) this is \( m = 0, 1 \), with eigensystems of size \( \text{Dim}_m = 1, 3 \) correspondingly, and for the invariant values \( \geq 1 \), or \( m \geq 2 \) the corresponding matrix is of size \( 4 = 2^2 \). Explicitly, using equations (4) and (9), we have the matrices:

\[
H_{m=0}^{1 \times 1} = \frac{-\omega_R + \omega_f}{2}, \quad n = 0, -1/2, -1/2),
\]

(11)

and

\[
H_{m=1}^{3 \times 3} = \begin{pmatrix}
\frac{\omega_R + \omega_f}{2} & J/2 & G \\
J/2 & -\frac{\omega_R + \omega_f}{2} & 0 \\
G & 0 & -\omega_R + 3\omega_f
\end{pmatrix}
mixing \begin{pmatrix}
|n = 0, 1/2, -1/2), \\
|n = 0, -1/2, 1/2) \\
|n = 1, -1/2, -1/2)
\end{pmatrix}
\]

(12)

and

\[
H_{m=2}^{4 \times 4} = \begin{pmatrix}
\frac{\omega_R + \omega_f}{2} & 0 & G & 0 \\
0 & \frac{\omega_R + 3\omega_f}{2} & J/2 & G\sqrt{2} \\
G & J/2 & 0 & -\omega_R + 3\omega_f \\
0 & G\sqrt{2} & 0 & -\omega_R + 5\omega_f
\end{pmatrix}
mixing \begin{pmatrix}
|n = 0, 1/2, 1/2) \\
|n = 1, 1/2, -1/2) \\
|n = 1, -1/2, 1/2) \\
|n = 2, -1/2, -1/2)
\end{pmatrix}
\]

(13)

which can be obtained as a specific case with \( n_f = 0 \) from the general expression valid for all the invariant values \( \geq 1 \) \( (m \geq 2) \) with arbitrary \( n = n_f \):

\[
H_{m \geq 2}^{4 \times 4} = \begin{pmatrix}
\frac{\omega_R + (2n_f + 1)\omega_f}{2} & 0 & G/\sqrt{n_f + 1} & 0 \\
0 & \frac{\omega_R + (2n_f + 3)\omega_f}{2} & J/2 & G\sqrt{n_f + 2} \\
G/\sqrt{n_f + 1} & J/2 & 0 & -\omega_R + (2n_f + 3)\omega_f \\
0 & G/\sqrt{n_f + 2} & 0 & -\omega_R + (2n_f + 5)\omega_f
\end{pmatrix}
mixing \begin{pmatrix}
|n = n_f, 1/2, 1/2) \\
|n = n_f + 1, 1/2, -1/2) \\
|n = n_f + 1, -1/2, 1/2) \\
|n = n_f + 2, -1/2, -1/2)
\end{pmatrix}
\]

(14)

With the explicit expressions for the matrices, we can evaluate the spectra by considering the eigenvalues equations \( \det(H_m^{\text{Dim}_m \times \text{Dim}_m} - \lambda \text{ Identity}) = 0 \).
3. Conclusion
In this report we have shown analytical approach to obtain the energy spectra for arbitrary filling number of a one photon mode for Jaynes-Cummings model in an open spin molecule with XY type spin-spin interaction between the spin-$\frac{1}{2}$ sites.

Acknowledgments
The authors thank I. Boradjiev for pointing us to the reference [13] and N. B. Ivanov, E. Korutcheva, and B. Obreshkov for useful discussions. Support by the Bulgarian Science Foundation grant DN0818/14.12.2016 is gratefully acknowledged.

References
[1] Jaynes E and Cummings F 1963 Proc. IEEE 51 89
[2] Alperin M M, Klubis Y D and Khizhnyak A I 1987 Introduction to the Physics of Two-Level Systems (Kiev: Naukova Dumka)
[3] Gerry C and Knight P 2004 Introductory quantum optics (Cambridge: University Press)
[4] Scully M O and Zubairy M S 1997 Quantum Optics (Cambridge: University Press)
[5] Hur K L, Henriot L, Petrescu A, Plekhanov K, Roux G and Schirò M 2016 Compt. Rend. Phys. 17 808
[6] Tavis M and Cummings F W 1968 Phys. Rev. 170 379
[7] Scharf G 1970 Helv. Phys. Acta 43 806
[8] Boradjiev I et al 2018 In preparation
[9] Wang X 2001 Phys. Rev. A 64 012313
[10] Lieb E, Schultz T and Mattis D 1961 Ann. Phys. 16 407
[11] De Pasquale A and Paolo F 2009 Physical Review A 80 032102
[12] Jordan P and Wigner E 1928 Z. Phys. 47 631
[13] Wu N 2018 Phys. Rev. B 97 014301
[14] Juárez-Amaro R, Zúñiga-Segundo A and Moya-Cessa H M 2015 Appl. Math. Inf. Sci. 9 299–303
[15] Dirac P A M 1978 The Principles of Quantum Mechanics (Oxford University Press)
[16] Feynman R P 1972 Statistical Physics (Benjamin Press)
[17] Tonchev H, Donkov A A and Chamati H 2016 Jour. Phys.: Conf. Ser. 682 012032; ibid. 764 012017