PHYSICAL REVIEW VOLUME 188, NUMBER 2 10 DECEMBER 1969

Approximate Solutions for an N-Molecule–Radiation-Field Hamiltonian

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(Received 26 May 1969)

Three approximation schemes are discussed and compared with the exact solutions for a Hamiltonian describing the interaction of a single-mode quantized radiation field and N two-level "molecules," each resonant with the mode frequency. In particular, the approximation of treating the molecules as uncorrelated is found to be accurate when the system energy is several times larger than the cooperation number of the molecular system.

I. INTRODUCTION

In a previous publication,[1] we presented the exact solution for a Hamiltonian describing N identical two-level molecules (TLM) interacting with a single-mode quantized radiation field. The model Hamiltonian studied in Ref. 1 neglects "counter-rotating" interaction terms, and the TLM's are at resonance with the electromagnetic field and are all at equivalent-mode positions in the resonant cavity. In the present paper, we use these exact solutions to this idealized system as a basis of comparison with three different approximation schemes: (1) The exact difference equation is approximated by a differential equation, which is identical to the harmonic-oscillator equation. This approximation is valid for all values of the average system energy (the average system energy also being the uncoupled molecules-plus-field energy $=c$), but is only accurate for the ground and low-lying excited states. (2) The TLM's are considered as independent, in the sense that they interact with each other only through an "averaged" field. This approach is common and has been used, in essence, by Scully and Lamb[2] in their quantized field theory of laser operation. We find in what follows that this approach is appropriate for all eigenstates when $c \gtrsim r$, where r is the "cooperation number" analogous to the total angular momentum quantum number of a spin system, and c is again the average energy of the system (TLM plus field). This approximation is appropriate only for $c \gg 1$. (3) The third approximation scheme is appropriate when the system energy is highly negative, $c=-r+\epsilon$, where $0 \ll \epsilon \ll r$, and again gives accurate results in this regime for all states and eigenvalues.

We have not been able to find a suitable approximation for all eigenvalues and eigenvectors for the energy region $0 < c \lesssim r$.

II. REVIEW OF DIFFERENTIAL EQUATION APPROXIMATION

In this section, we begin by briefly reviewing the notation of Ref. 1. The Hamiltonian, divided by the mode frequency, is taken as

$$\mathcal{H}=R_3+a^\dagger a-\kappa a R_+-\kappa^* a^\dagger R_-\,, \tag{2.1}$$

where

$$[a,a^\dagger]=1,\quad [R_+,R_-]=2R_3,\quad \text{and}\quad \kappa=|\kappa|\,e^{i\phi_1}. \tag{2.2}$$

States of the noninteracting ($\kappa=0$) system are defined such that

$$R_3|r,m\rangle=m|r,m\rangle\,, \tag{2.3a}$$

$$R_\pm|r,m\rangle=e^{\pm i\phi_2}[r(r+1)-m(m\pm 1)]^{1/2}|r,\,m\pm 1\rangle\,, \tag{2.3b}$$

$$a|n\rangle=\sqrt{n}e^{i\phi_3}|n-1\rangle\,, \tag{2.3c}$$

$$\begin{aligned}R^2|r,m\rangle&=[R_3{}^2+\tfrac{1}{2}(R_+R_-+R_-R_+)]|r,m\rangle\\&=r(r+1)|r,m\rangle.\end{aligned} \tag{2.3d}$$

Here $m \le r \le \frac{1}{2}N$, r, m integer or half integer, and N is the total number of molecules. Since the cooperation[3] operator R^2 and the average energy operator $R_3+a^\dagger a$ both commute with the Hamiltonian (2.1), we label the eigenstates of $\mathcal{H}$ by the eigenvalues r and c, the eigenvalues of R^2 and $R_3+a^\dagger a$, respectively. An eigenstate of $\mathcal{H}$ is then

$$|r,c,j\rangle=\sum_{n=\max\binom{c-r}{0}}^{c+r} A_n{}^{(r,c,j)}|n\rangle|r,\,c-n\rangle\,, \tag{2.4a}$$

$$\mathcal{H}|r,c,j\rangle=\lambda_{rcj}|r,c,j\rangle. \tag{2.4b}$$

The $A_n{}^{(r,c,j)}$ satisfy the difference equation

$$\begin{aligned}-|\kappa|e^{-i\phi}(\sqrt{n})C_{r,c-n}A_{n-1}{}^{(r,c,j)}+(c-\lambda_{rcj})A_n{}^{(r,c,j)}\\-|\kappa|e^{i\phi}[\sqrt{(n+1)}]C_{r,c-n-1}A_{n+1}{}^{(r,c,j)}=0\,,\end{aligned} \tag{2.5a}$$

where

$$\phi=\phi_1+\phi_2+\phi_3$$

and

$$C_{r,c-n}=[r(r+1)-(c-n)(c-n+1)]^{1/2}. \tag{2.5b}$$

The $A_n{}^{(r,c,j)}$ satisfy the boundary conditions

$$A_{r+c+1}{}^{(r,c,j)}=A_{\max(-1,c-r-1)}{}^{(r,c,j)}=0.$$

It is convenient to define B_n so that

$$A_n=\frac{(qe^{-i\phi})^nB_n}{[\sqrt{(n!)}]C_{c-1}C_{c-2}\cdots C_{c-n}},\quad c<r \tag{2.6a}$$

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[1] M. Tavis and F. W. Cummings, Phys. Rev. **170**, 379 (1968).

[2] M. O. Scully and W. E. Lamb, Jr., Phys. Rev. **159**, A208 (1967).

[3] R. H. Dicke, Phys. Rev. **93**, 99 (1953).

and

$$A_n = \frac{(qe^{-i\phi})^n B_n}{[\sqrt{(n!)}]C_{r-1}C_{r-2}\cdots C_{c-n}}, \quad c \geq r \tag{2.6b}$$

where

$$q = (c-\lambda)/2|\kappa|. \tag{2.6c}$$

The superscripts (subscripts) (r,c,j) are suppressed for simplicity whenever this does not cause confusion; also the subscript r is suppressed in $C_{r,n}$. The B_n's then satisfy the difference equation

$$q^2 B_{n+1} - 2q^2 B_n + nC_{c-n}{}^2 B_{n-1} = 0. \tag{2.7}$$

The details of the exact solution of (2.7) and (2.5a) are given in Ref. 1.

Rewriting (2.7) as

$$B_{n+1} + B_{n-1} - 2B_n + [(nC_{n-1}{}^2 - q^2)/q^2]B_{n-1} = 0, \tag{2.8}$$

we can then approximate this difference equation by the differential equation

$$\frac{d^2 B_n}{dn^2} + \left(\frac{\alpha_1 - q^2}{q^2} - \frac{\alpha_2}{q^2}(n-n_0)^2\right)B_n = 0, \tag{2.9}$$

if we let

$$\Delta^2 B_n \equiv B_{n+2} + B_n - 2B_{n+1} \rightarrow d^2 B_n/dn^2 \tag{2.10}$$

as well as drop the cubic term in the square bracket of (2.8) expressed as a cubic polynomial in $(n-n_0)$. We have defined

$$\alpha_1 = n_0 C_{c-n_0}{}^2, \tag{2.11a}$$

$$\alpha_2 = [3r(r+1) + c(c+1) + 1]^{1/2}, \tag{2.11b}$$

$$n_0 = \tfrac{1}{3}(2c+1) + \tfrac{1}{3}[3r(r+1) + c(c+1) + 1]^{1/2}. \tag{2.11c}$$

The solutions to (2.9) are the familiar Hermite polynomials when the harmonic-oscillator boundary conditions are used. The eigenvalues are given by

$$q_j = -[\sqrt{(\alpha_2)}](j+\tfrac{1}{2}) + \sqrt{[(j+\tfrac{1}{2})^2\alpha_2 + \alpha_1]}, \quad j = 0, 1, \cdots, r. \tag{2.12}$$

When this approximation is compared with exact results, agreement is very good for all regions of c and r where the continuum approximation (2.10) is valid. The ground and first few excited states are reproduced well.

The dispersion in photon number in the ground state (for given r and c), $j=0$, in the differential equation approximation is

$$\sigma^2 = \langle (n-n_0)^2 \rangle = \sum_n |A_n{}^{(0)}|^2 (n-n_0)^2 / \sum_n |A_n{}^{(0)}|^2, \tag{2.13a}$$

where

$$|A_n{}^{(0)}|^2 \cong e^{-(n-n_0)^2\sqrt{\alpha_2}/q_0} \tag{2.13b}$$

(q_0 is the ground-state energy). Thus,

$$\sigma^2 = q_0/2\sqrt{\alpha_2}. \tag{2.14}$$

{This is given incorrectly in Ref. 1 as $\sigma^2 = n_0/[1+2(\sqrt{\alpha_2})n_0/q_0]$.} The dispersion in photon number is in every case smaller than (or equal to) $\frac{1}{2}n_0$. When the energy in the electromagnetic field greatly exceeds the maximum energy available to the molecular system, that is, $c \gg r$, then the dispersion is much less than $\frac{1}{2}n_0$ and is $\sim \frac{1}{2}r$.

III. AVERAGED FIELD APPROXIMATION

In this section, we discuss an approximate solution to the Hamiltonian (2.1) in which the TLM's are treated as uncorrelated in the sense that they interact with each other only through an "averaged field." This approximation is seen frequently in the literature, and its validity is assumed in a recent quantum analysis of the laser.[2] This approximation is valid, as we show in this section, in the region $c \geq r$; it is then not *a priori* clear that this approximation will lead to correct results in an analysis of the laser build up.

The averaged field approach may be motivated by the observation that as c becomes larger than r, the $\sqrt{n}$ term in the off-diagonal matrix element of $\mathcal{H}$ (2.1) may be approximated as a constant $= \sqrt{n_0}$, where n_0 is to be determined self-consistently. This becomes clear when one remembers that for a given c and r, n varies between the value $c+r$ and $c-r$.

We wish c and r to remain good quantum numbers, so that the Hamiltonian becomes

$$\mathcal{H}_f = R_3 + a^\dagger a - \kappa(\sqrt{n_0})\mathcal{L}R_+ - \kappa^*(\sqrt{n_0})\mathcal{L}^\dagger R_-, \tag{3.1}$$

where we have introduced photon raising and lowering operators

$$\begin{aligned} \mathcal{L}|n\rangle &= |n-1\rangle, \quad & n \geq 1 \\ &= 0, & n < 1 \end{aligned} \tag{3.2a}$$

$$\mathcal{L}^\dagger |n\rangle = |n+1\rangle. \tag{3.2b}$$

The matrix representation of H_f in the $|n\rangle|r,m\rangle$ bases is essentially the same as shown in Figs. 1 and 2 of Ref. 1 and differs only in the replacement of n by n_0 in the off-diagonal terms. We do not use the difference equation approach to find the exact solutions of (3.1) as this is an unnecessarily complicated method here. Instead, we make use of the independent molecule nature of the approximation and write

$$\mathcal{H}_f = \sum_{k=1}^{N} \left(\frac{a^\dagger a + R_3}{N} - \kappa(\sqrt{n_0})\mathcal{L}R_{+k} - \kappa^*(\sqrt{n_0})\mathcal{L}R_{-k} \right),$$

$$(N = \text{total number of molecules}) \tag{3.3}$$

where $R_{\pm k}$ are the raising (lowering) operators for the kth molecule. A more natural basis set now is the photon states $|n\rangle$ and the independent molecule "up" and "down" states $|\uparrow\rangle$ and $|\downarrow\rangle$, respectively. As an example, the submatrix of H_f for a given c and $N=2$ is shown in Fig. 1.

Now we note that if the photon states are ignored for the moment, this matrix can be written as the sum of direct matrix products for independent molecules,

$$\mathcal{H}_f^{(2)}=\mathbf{A}_1\otimes\mathbf{I}_2+\mathbf{I}_1\otimes\mathbf{A}_2\,, \tag{3.4}$$

where

$$\mathbf{A}_k=\begin{bmatrix}\frac{1}{2}c & -(\sqrt{n_0})\kappa\\ -(\sqrt{n_0})\kappa^* & \frac{1}{2}c\end{bmatrix},\quad \mathbf{I}_k=\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix},\quad k=1,2.$$

To take advantage of this, we introduce "pseudophoton" states in such a way as to conserve energy by denoting the basis of a single molecule-plus-field as

$$|\bar{c}-\tfrac{1}{2}\rangle|\uparrow\rangle_k \quad\text{and}\quad |\bar{c}+\tfrac{1}{2}\rangle|\downarrow\rangle_k\,, \tag{3.5}$$

where

$$\mathfrak{L}|\bar{c}+\tfrac{1}{2}\rangle=|\bar{c}-\tfrac{1}{2}\rangle,\quad R_{+k}|\downarrow\rangle_k=|\uparrow\rangle_k,\quad \text{etc.},$$

and $\bar{c}=c/N$. The eigenvalues and eigenstates for this single molecule $\mathbf{A}_k$ are then

$$\lambda_\pm=\bar{c}\pm(\sqrt{n_0})|\kappa|\,, \tag{3.6a}$$

$$|-\rangle=(\sqrt{2})^{-1}(|\bar{c}-\tfrac{1}{2}\rangle|\uparrow\rangle e^{i\phi}+|\bar{c}+\tfrac{1}{2}\rangle|\downarrow\rangle)\,, \tag{3.6b}$$

$$|+\rangle=(\sqrt{2})^{-1}(|\bar{c}-\tfrac{1}{2}\rangle|\uparrow\rangle+e^{i(\pi-\phi)}|\bar{c}+\tfrac{1}{2}\rangle|\downarrow\rangle)\,. \tag{3.6c}$$

The eigenstates of H_f, denoted by $|r,c,j\rangle_f$, are now constructed from the $|\pm\rangle$ states by the observation that the exact solution to (2.1) expressed as a linear combination of $|n\rangle|r,m\rangle$ states is independent of N, except for the constraint $r\leq\frac{1}{2}N$. That is, if one considers a Hamiltonian describing, say, four molecules or two molecules interacting with a field, one finds the same states and eigenvalues for $r=1$ for these two problems. For convenience, then, in constructing states of H_f which are eigenstates of r and c we choose $r=\frac{1}{2}N$ without loss of generality. Thus, we construct normalized $|rcj\rangle_f$ states from the ground state by application of the raising operator,[3] i.e.,

$$|r,c,j\rangle_f=\{[R^2-R_3(R_3+1)]^{-1/2}R_+\}^j\prod_{k=1}^{N}|-\rangle_k\,, \tag{3.7}$$

where R_+ is the sum of individual pseudomolecule raising operators, that is,

$$R_{+k}|-\rangle_k=|+\rangle_k\,. \tag{3.8}$$

We can also express this as

$$|r=\tfrac{1}{2}N,\,c,\,j\rangle_f=\frac{1}{[N!/j!(N-j)!]^{1/2}}\times\sum_{\mathcal{P}}\Big(\prod_{k=1}^{j}|+\rangle_k\Big)\Big(\prod_{k'=1}^{N-j}|-\rangle_{k'}\Big)\,, \tag{3.9}$$

where $\mathcal{P}$ means a permutation between the $|+\rangle$ and $|-\rangle$ states, but not between the individual $|+\rangle$ or $|-\rangle$ states alone. Substituting into (3.9) from (3.6), we find, after considerable rearrangement and care to preserve the normalization of the $|r,m\rangle$ states,

$$|r,c,j\rangle_f=\sum_{n=c-r}^{c+r}D_n^{(r,c,j)}|n\rangle|r,\,c-n\rangle\,, \tag{3.10}$$

where

$$D_n^{(r,c,j)}=\left[2^r\left(\frac{(2r)!}{j!(2r-j)!}\right)^{1/2}\right]^{-1}\left(\frac{(2r)!}{L!(2r-L)!}\right)^{1/2}e^{i(2r-j-L)\phi}\times{\sum_{L'=d}^{u}}'\frac{e^{\frac{1}{2}(L+L')\pi i}L!(2r-L)!}{[\frac{1}{2}(L+L')]![\frac{1}{2}(L-L')]![j-\frac{1}{2}(L+L')]![2\mathrm{r}-j-\frac{1}{2}(L-L')]!}\,, \tag{3.11}$$

where

$$L\equiv r-c+n\,,$$
$$d\equiv\max[-L,\,L+2j-4r]\,,$$
$$u\equiv\min[L,\,2j-L]\,,$$

and the prime on the summation indicate that L' ranges over integer values such that the factorials are also integers, that is, only every other value of L' starting from $L'=d$ is taken in computing the sum.

From the expression for the eigenstates (3.9), we easily obtain the eigenvalues as the sum of the eigenvalues (3.6a) of the $|\pm\rangle$ states, namely,

$$\lambda_j^{(f)}=c-2(r-j)|\kappa|\sqrt{n_0}\,. \tag{3.12}$$

Equations (3.10) and (3.12) are valid for general values of r, and not only $r=\frac{1}{2}N$.

The ground state is particularly simple, i.e.,

$$D_n^{(r,c,0)}=\frac{1}{2^r}\left[\frac{(2r)!}{(r+c-n)!(r+n-c)!}\right]^{1/2}e^{-in\phi}\,,$$

and the probability for finding n photons in the ground state is simply a binomial distribution with $\langle n\rangle=c$. This can be approximated for $c\gg1$ as a Gaussian centered at $n=c$, with a dispersion $\sigma^2=\frac{1}{2}r$ in agreement with the differential equation approximation. The excited states also have $\langle n\rangle=c$ and are very similar in appearance to the eigenstates of the harmonic oscillator. By comparison with the exact solutions to (2.1),[4] it is found that for $c>5r$ the eigenvalues (3.12) with $n_0=c$ agree with

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[4] M. Tavis, thesis, University of California, Riverside, 1968 (unpublished).

$\lvert c-1\rangle\lvert\uparrow\rangle\lvert\uparrow\rangle$	$\lvert c\rangle\lvert\uparrow\rangle\lvert\downarrow\rangle$	$\lvert c\rangle\lvert\downarrow\rangle\lvert\uparrow\rangle$	$\lvert c+1\rangle\lvert\downarrow\rangle\lvert\downarrow\rangle$
c	$-\sqrt{n_0}\kappa$	$-\sqrt{n_0}\kappa$	
$-\sqrt{n_0}\kappa^*$	c		$-\sqrt{n_0}\kappa$
$-\sqrt{n_0}\kappa^*$		c	$-\sqrt{n_0}\kappa$
	$-\sqrt{n_0}\kappa^*$	$-\sqrt{n_0}\kappa^*$	c

FIG. 1. A submatrix of H_f for a given c and for 2 TLM's ($N=2$).

the exact eigenvalues to within three significant figures, with correspondingly good agreement with the exact average photon number and dispersion.

IV. AVERAGED TLM APPROXIMATION

In this section, we discuss an approximation to the solution of (2.1) which is valid when $c<0$. The exact results again yield a linear eigenvalue spectrum, as in the region $c>r$. If we examine the matrix elements of the interaction in the Hamiltonian (2.1) in the $|n\rangle|r,m\rangle$ bases, the off-diagonal elements have a magnitude proportional to $\sqrt{n}\sqrt{[(r-m)(r+m+1)]}$, where n varies between zero and $c+r$ for $c<0$. Since $m=c-n$, m varies between c and $-r$. Define $r'=\frac{1}{2}(c+r)$, then $m'=r'-n$ varies between r' and $-r'$. Then

$$\sqrt{[n(r-m)(r+m+1)]}=\sqrt{[(r'-m')]}\times\sqrt{\{[2r-(r'+m')][r'+m'+1]\}}, \quad (4.1)$$

and since $r'\ll r$, we can approximate this as

$$\sqrt{[n(r-m)(r+m+1)]}\approx\sqrt{[(r'-m')(2r)(r'+m'+1)]}. \quad (4.2)$$

This has the same form as for the case discussed above, $c>r$, with $2r$ replacing n_0 of Sec. III. However, in this case we cannot factor the resulting approximate Hamiltonian into a sum of direct products of individual molecule matrices as was done in Sec. III. Instead we take over directly the expressions for the eigenvalues and eigenvectors of H_f by replacing r by r' in those expressions (3.10) and (3.12), except n now runs between zero and $c+r$ instead of $c-r\rightarrow c+r$, and r is not replaced by r' in the $|r,m\rangle$ states. Then,

$$\lambda_j^{(m)}=c-(c+r-2j)\sqrt{(2r)}\,|\kappa| \quad (4.3)$$

and

$$|r,c,j\rangle_m=\sum_{n=0}^{c+r}F_n^{(r,c,j)}|n\rangle|r,\,c-n\rangle, \quad (4.4)$$

where

$$F_n^{(r,c,j)}=\{2^{(c+r)/2}\sqrt{[(c+r)!/j!(c+r-j)!]}\}^{-1}\left(\frac{(c+r)!}{n!(c+r-n)!}\right)^{1/2}$$

$$\times e^{-i(c+r-j-n)\phi}\sum_{n'=d}^{u}{}'\frac{e^{i(n+n')\pi/2}n!(c+r-n')!}{[\frac{1}{2}(n+n')]![\frac{1}{2}(n-n')]![j-\frac{1}{2}(n+n')]![c+r-j-(\frac{1}{2}n-n')]!} \quad (4.5)$$

and

$$d=\max[-n,\,n-2(c+r-j)],$$

$$u=\min[n,\,2j-n],$$

and the definition of the prime on the summation is the same as below (3.11).

The average value of photon number is $\langle n\rangle=\frac{1}{2}(c+r)$ in the ground state, and the dispersion in photon number $\sigma^2=\frac{1}{2}\langle n\rangle$. This agrees with the results of the differential equation approximation of Sec. II. This approximation for $5(c+r)<r$ is accurate to three significant figures when compared with the exact results for the eigenvalues, average values of photon number, and dispersion.