A variational estimate of the lowest eigenvalue of the multiatom, multimode Hamiltonian of quantum optics

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Abstract. In those cases where a direct diagonalization of the energy matrix is not attempted because of insuperable practical difficulties of computation, it is always possible to estimate the gamut of the eigenvalue spectrum by a variational method. A trial state function similar in some respects to a Glauber state is employed. Certain asymptotically exact results due to Tavis and Cummings are recovered. Finally, ways in which the accuracy might be improved are outlined.

1. Introduction

In nonlinear optics, a system of N two-level atoms interacting with a finite set of electromagnetic field modes $\{k\}$ has been described by the Hamiltonian (Swain 1972):

$$H = \sum_{\{k\}} \omega_k a_k^\dagger a_k + \omega_0 R_3 + \sum_{\{k\}} g a_k R^{(+)} + g^* a_k^\dagger R^{(-)}. \tag{1}$$

Here, a_k is the photon annihilation operator, $R^\pm$, R_3 are the usual angular momentum operators with

$$R^2 = R_1^2 + R_2^2 + R_3^2 = \tfrac{1}{2}(R^+ R^- + R^- R^+) + R_3^2$$
$$[R^+, R^-] = 2R_3 \qquad [R_3, R^\pm] = \pm R^\pm. \tag{2}$$

The wavevectors k are such that $|k|$ is close to ω_0, the atomic level spacing. On this understanding, the k dependence of the coupling constant g is ignored. Interaction terms $a_k R^{(-)}$, $a_k^\dagger R^{(+)}$ and the phase factors are also suppressed (Jaynes and Cummings 1963). Constants of the motion are R^2 and the 'excitation number', that is

$$C = \sum_{\{k\}} a_k^\dagger a_k + R_3. \tag{3}$$

It is convenient to treat just $H - \omega_0 C$, that is

$$\sum_{\{k\}} \omega_{k0} a_k^\dagger a_k + g a_k R^{(+)} + g^* a_k^\dagger R^{(-)}$$

where $\omega_{k0} \equiv \omega_k - \omega_0$.

The eigenvalues of R^2 have the form $r(r+1)$, r taking an integer or half-integer value chosen from

$$N/2 \,;\, N/2 - 1 \,;\, \ldots \,; \qquad \ldots 0 \text{ or } \tfrac{1}{2}.$$

Dicke called r the cooperation number since $2r$ is the number of atoms participating collectively in the quantum processes. The operator $(R_3 + r)$ measures the number of cooperating atoms in their upper state.

A model Hamiltonian of this sort is reportedly relevant to a theory of Josephson junctions, and to the theory of phonon assisted phase transitions in certain vanadate crystals, as well as giving a description of frequency conversion in lasers. Generalizations of the model to include multiphoton interactions have lately been presented by Walls (1971).

Many interesting attacks on the problem of finding the stationary states and eigenvalues of H have been made (Tavis and Cummings 1968, Mallory 1969, Walls and Barakat 1970, Swain 1972) and while formal solutions have been given, closed expressions can be obtained only in special cases. Several treatments of the time evolution problem exist (eg Bonifacio and Preparata 1970, Walls and Barakat 1970, Pike and Swain 1971). It is well known that the basis states for the system will be finite in number and consequently the Schrödinger equation for the stationary states reduces to the finite matrix eigenvalue problem. Since Swain has summarized this there would appear to be nothing more to add. However, the practical diagonalization of a matrix is nontrivial when the number of rows and columns exceeds 70 or so. It is beyond the resources of most computers when this figure enters the hundreds. Matrices exceeding this size are met with quite modest systems. For example, suppose we have 16 atoms cooperating fully ($r = 8$). Taking $c = 0$ so that the photon number may take values from 0 to 8, we will suppose that the photons can go into six modes. With these quantum numbers the number of basis states depends on the 'compositions' of $8, 7, 6, \ldots, 2, 1, 0$ into 6 parts and is 3003. Diagonalization of the associated matrix is out of the question. In these cases I believe that a less ambitious program can be justified beginning with an estimation of the range of the energy spectrum using a variational method. (The highest eigenvalue of H is the lowest eigenvalue of $-H$.) This is the subject of the present article.

The quality of a variational approximation depends on how closely the trial function represents the true ground state. Since the general form of the eigenfunctions is known (see Swain 1972) one could construct a trial function as a linear combination of a small number of simultaneous eigenstates of R^2 and C. These would have to be selected so as to be somehow representative of the basis set. It is not clear how this could be done. An alternative approach makes use of the observation (Tavis and Cummings 1968, Walls and Barakat 1970) that the ground state apparently has properties similar to the coherent states (Glauber 1963). This idea will be developed to construct a simple trial function for the system consisting of the product of a matter part and a photon occupation part, being an eigenstate of R^2 and having the correct expectation value of C. Conditions under which the stationary expectation value of H gives an upper bound on the ground state energy are established and discussed. A particularly satisfactory feature of the calculation is that in the case of interactions with photons in one resonance mode, the asymptotically exact results of Tavis and Cummings are recovered.

2. A trial ground state

Of the set $\{k\}$ there will be a vector $\boldsymbol{\kappa}$, or possibly several $\{\kappa\}$ corresponding to photons of lowest energy $\omega(\kappa)$. Let us assume that $\omega_\kappa < \omega_0$; then if $g = 0$, the state of lowest energy is the one in which all excitations are in the electromagnetic mode κ, all atoms being in their lower state ($R_3 = -r$). If the coupling is turned on, excitations leave the

softest mode to partially populate the upper atomic levels and (in second order perturbation theory) photons appear in other modes, but always so that the value of the operator C is preserved. Lee *et al* (1953) have given us a method of constructing a state containing an indefinite number of bosons, in their polaron theory (see also Pines 1963). This device, known as the displaced oscillator transformation, is of fundamental importance for the discussion of coherent states (Glauber 1963).

The state $S(k)|0_{\{k\}}\rangle$, where $|0_{\{k\}}\rangle$ is the photon vacuum and

$$S(k) = \exp(f^*(k)a_k - f(k)a_k^\dagger) \tag{4}$$

is a unitary operator, has the property

$$\langle n_k \rangle = |f(k)|^2. \tag{5}$$

Hence the state

$$\exp n_\kappa^{1/2}(a_\kappa - a_\kappa^\dagger) \prod_{k \neq \kappa} S(k)|0_{\{k\}}\rangle \equiv U_1|0_{\{k\}}\rangle \tag{6}$$

gives for the expectation value of the total photon number

$$n_\kappa + \sum_{k \neq \kappa} |f(k)|^2.$$

By analogy it can be seen that if $|-r\rangle$ is the matter ground state when $g = 0$, then a state of indefinite excitation is

$$U_2|-r\rangle \equiv \exp(\beta R^{(+)} - \beta^* R^{(-)})|-r\rangle \tag{7}$$

where β, like f, is at our disposal. From the Baker–Hansdorf formula and the canonical commutation relations, it is quite straightforward to show that

$$U_2^{-1} R_i U_2 = \sum_{j=1}^{3} T_{ij} R_j \qquad (i = 1, 2, 3) \tag{8}$$

T_{ij} being an orthogonal matrix expressible in terms of β. I shall not give this in full, since only the third column is needed:

$$T_{13} = \cos \phi \sin \theta \qquad T_{23} = \sin \phi \sin \theta \qquad T_{33} = \cos \theta$$
$$\theta = 2|\beta| \qquad \phi = -\arg \beta. \tag{9}$$

It should be said that the rotation associated with this canonical transformation is not the most general, since the third Euler angle ψ is not assigned independently. An immediate result is that the expectation value of R_3 in the state $U_2|-r\rangle$ is $-r\cos\theta$. As a trial function, we take the product state

$$\Psi \equiv U_1 U_2|-r\rangle . |0_{\{k\}}\rangle \tag{10}$$

which is automatically an eigenstate of R^2, although not an eigenstate of C. However, we can impose the constraint

$$n_\kappa + \sum_{k \neq \kappa} |f(k)|^2 - r\cos\theta = c \tag{11}$$

on any variation of the parameters where c is the appropriate eigenvalue of C so that

$$(\Psi, C\Psi) = c. \tag{12}$$

Because Ψ is not an eigenstate of C, care must be exercised in formulating a variational

principle. It is reassuring to note that the dispersion of the c values in the state Ψ is roughly Poisson in type, tending to the Poisson value in the limit $c \gg r$; so this defect of the trial function becomes relatively unimportant in this limit. There is a parallel with thermodynamics, where a variational calculation of the free energy may violate certain sum-rules, notably the 'response-fluctuation identity'.

3. Variational equations

The remaining transformed operators are:

$$U_1^{-1} a_k U_1 = S^\dagger(k) a_k S(k) = a_k - f(k)$$

$$U_1^{-1} a_k^\dagger U_1 = a_k^\dagger - f^*(k).$$

Also

$$\langle -r | U_2^{-1} R^\pm U_2 | -r \rangle = -r \, e^{\pm i\phi} \sin \theta. \tag{13}$$

Hence

$$(\Psi, (H - \omega_0 C)\Psi) \equiv E_0$$

$$= \omega_{\kappa 0} n_\kappa + r \sin \theta b^{1/2} n_\kappa^{1/2} (g \, e^{i\phi} + g^* \, e^{-i\phi})$$

$$+ \sum_{k \neq \{\kappa\}} (\omega_{k0} |f(k)|^2 + 2r \sin \theta \, \text{Re} \, g \, e^{i\phi} f(k)). \tag{14}$$

The possibility that there may be b photons in $\{\kappa_i\}$ is allowed for. Because the interaction is isotropic, n_{κ_i} depends only on $|\kappa_i|$ and equation (11) still applies if

$$n_\kappa = \sum_{\{\kappa_i\}} n_{\kappa_i}. \tag{15}$$

The parameters θ, ϕ and $f(k)$ are now determined by the condition

$$\delta E_0 = 0$$

or

$$\frac{\delta E_0}{\delta f(k)} = \frac{\delta E_0}{\delta f^*(k)} = \frac{\partial E_0}{\partial \theta} = \frac{\partial E_0}{\partial \phi} = 0$$

leading to the three independent equations:

$$(\omega_\kappa - \omega_k - r \sin \theta b^{1/2} n_\kappa^{-1/2} \, \text{Re} \, g \, e^{i\phi}) f^*(k) + r \sin \theta g \, e^{i\phi} = 0 \tag{16}$$

$$\omega_{\kappa 0} \sin \theta - \left(2n_\kappa^{1/2} \cos \theta - r \sin^2 \theta \, n_\kappa^{-1/2} + 2 \cos \theta \sum_{k \neq \kappa} f(k) \right) \text{Re} \, g \, e^{i\phi} = 0 \tag{17}$$

$$\text{Im} \left\{ g \, e^{i\phi} \left(n_\kappa^{1/2} + \sum_{k \neq \kappa} f(k) \right) \right\} = 0. \tag{18}$$

From (16) the product $f(k) g \, e^{i\phi}$ is real, hence (18) reduces to

$$\phi + \arg g = 0 \text{ or } \pi. \tag{19}$$

Consideration of the weak coupling limit shows that the choice π rather than 0 in (19) gives the lower energy. Further, $f(k)$ is real and depends only on $|k|$. If max $|\omega_{k0}| = \delta$, equations (16), (17) and (11) may be solved by iteration in powers of $|g|\delta^{-1}$ or $|g|^{-1}\delta$ whichever is appropriate.

4. Examples

4.1. Interaction with one mode κ at resonance

On setting $\omega_{\kappa 0} = 0$ and $f(k) = 0$, we find

$$E_0 = -2|g|r \sin \theta (c + r \cos \theta)^{1/2} \tag{20}$$

where

$$3r \cos^2\theta + 2c \cos \theta - r = 0. \tag{21}$$

It follows that:

$$n_\kappa = \tfrac{1}{3}\{2c + (c^2 + 3r^2)^{1/2}\} \tag{22}$$

which in the limit $r \gg 1$, $c \gg 1$ coincides with equation (4.4) of Tavis and Cummings (1968). Their asymptotically exact energy formulae are easily found from (20) and (21); for example if $c = 0$ we find $\cos \theta = 3^{-1/2}$ and hence

$$E_0 = -2|g|r^{3/2}2^{1/2}3^{-3/4}.$$

Again, if $c \gg r$, $\cos \theta \simeq 0$ and $E_0 \simeq -2|g|rc^{1/2}$, in accord with the intuitive picture of a macroscopic dipole moment $2|g|r$ interacting with an electric field $c^{1/2}$.

Some numerical results for $r = c$ are compared in table 1 with exact energies taken from the literature or calculated by the author. An isolated result concerning 24 atoms ($r = 12$, $c = 36$) is $E_0/|g|$ (exact) $= -146.64$ (Walls and Barakat 1970). The variational estimate is -145.90 which is in error by approximately $\tfrac{1}{2}\%$.

Table 1.

$r\,(= c)$	$-E_0/|g|$ exact		Estimate	$-\%$ error
$\tfrac{1}{2}$	1		0·77	23
1	$\sqrt{6}$	⎫	$(8/9)\sqrt{6}$	11
$\tfrac{3}{2}$	4·31	⎬ Mallory (1969)	4	7·2
2	6·50	⎭	6·17	5·1
$\tfrac{5}{2}$	8·979		8·606	4·2
3	11·71		11·31	3·4
$\tfrac{7}{2}$	14·69		14·26	2·9
12	91·23	Walls and Barakat (1970)	90·50	0·8

4.2. Interaction with several modes at resonance

Very few exact results are available when $b > 1$, probably reflecting the fact that the number of basis states, namely

$$\sum_{n=\min(0,c-r)}^{c+r} \frac{(n+b-1)!}{n!(b-1)!}$$

rapidly increases with b and gives the cumbersome matrices noted in §1. Table 2 summarizes the work in this case. The figures suggest that the estimates are upper bounds on the lowest eigenvalues, the relative discrepancy tending to zero as r and c increase.

Table 2.

r	c	b	$-E_0/|g|$ exact	Estimate	$-\%$ error
$\frac{1}{2}$	$\frac{1}{2}$	b	$b^{1/2}$	$0{\cdot}77\,b^{1/2}$	23
$\frac{1}{2}$	$\frac{3}{2}$	2	2	1·77	11
1	0	2	2 (Swain 1972)	1·75	12
2	0	2	5·29	4·96	6
3	0	2	9·51	9·12	4

4.3. Interaction of one atom with one mode κ

On putting $r = \frac{1}{2}$, $\omega_{\kappa 0} = -\delta$ and $f(k) = 0$, the variational equations are readily solved in powers of $|g|\delta^{-1}$ giving

$$E_0 = (c+\tfrac{1}{2})\left\{-\delta - \frac{|g|^2}{\delta} + \frac{|g|^4}{\delta^3}\left(c+\frac{3}{2}\right)\ldots\right\}. \tag{23}$$

This is greater than the exact expression (Jaynes and Cummings 1963) which in the weak coupling limit is

$$(c+\tfrac{1}{2})\left\{-\delta - \frac{|g|^2}{\delta} + \frac{|g|^4}{\delta^3}\left(c+\frac{1}{2}\right)\ldots\right\}. \tag{24}$$

In terms of $|g|^{-1}\delta$ these formulae appear as:

$$-c\delta - c^{1/2}|g|\{1 + (4c)^{-1}|g|^{-2}\delta^2\ldots\} \qquad \text{(estimate)} \tag{25}$$

$$-c\delta - (c+\tfrac{1}{2})^{1/2}|g|\{1 + (8c+4)^{-1}|g|^{-2}\delta^2\ldots\} \qquad \text{(exact)}. \tag{26}$$

It is clear that the relative error vanishes as $c \to \infty$.

4.4. $r = 1$, $c = 0$; two-off-resonance modes

This example has been discussed by Swain (1972). We set $\omega_{\kappa 0} = -\delta$, $\omega_{k0} = +\delta$ and, for simplicity, assume that $|g|\delta^{-1}$ is small. One finds

$$f(k) \simeq |g|^2\delta^{-2}n_\kappa^{1/2}$$

$$\sin\theta = 2|g|\delta^{-1}(1 - 4|g|^2\delta^{-2}\ldots)$$

$$n_\kappa = 1 - 2|g|^2\delta^{-2} + 13|g|^4\delta^{-4}\ldots$$

giving

$$E_0 = -\delta - 2|g|^2\delta^{-1} + 4|g|^4\delta^{-3}\ldots. \tag{27}$$

This exceeds the exact result by $2|g|^4\delta^{-3}$, to fourth order.

5. Validity of the method

In the usual derivation of the energy variational principle, the trial function is expanded in terms of the eigenfunctions of the Hamiltonian. These will be simultaneous eigenfunctions of R^2 and C, ψ_{lc_i} say, where l labels the functions belonging to excitation

number c_i (the r label is suppressed). The range of the l suffix depends of course, on c and r. We can write

$$\Psi = \sum_{l,c_i} a_{lc_i} \psi_{lc_i} \tag{28}$$

where the distribution of c_i values is peaked about some value c with variance

$$c + \tfrac{1}{2} r (\sin^2 \theta + 2 \cos \theta). \tag{29}$$

If the energy of the state ψ_{lc_i} is $E(l, c_i)$ and

$$|a_{lc_i}|^2 = p_{lc_i}$$

then

$$(\Psi, H\Psi) \equiv \langle H \rangle = \sum_{l,c_i} p_{lc_i} E(l, c_i)$$

$$= E(0, c) + \sum_{l,c_i} p_{lc_i} \{ (E(l, c_i) - E(0, c_i)) + (E(0, c_i) - E(0, c)) \}. \tag{30}$$

Suppose that for each c_i, $E(0, c_i)$ is the lowest eigenvalue, it follows that:

$$\langle H \rangle \geqslant E(0, c) + \sum_{l,c_i} p_{lc_i} (E(0, c_i) - E(0, c)). \tag{31}$$

There is a smooth function $E(0, x)$ which coincides with $E(0, c_i)$ for integer (or half-integer) values of x. By the second mean value theorem

$$E(0, x) = E(0, c) + (x - c) E'(0, c) + \tfrac{1}{2} (x - c)^2 E''(0, \zeta)$$

with

$$\zeta = c + (x - c) \bar{\theta} \qquad 0 < \bar{\theta} < 1.$$

Hence

$$\langle H \rangle \geqslant E(0, c) + \tfrac{1}{2} \sum_{l,c_i} p_{lc_i} E''(0, \zeta_i) (c - c_i)^2. \tag{32}$$

For values of $c \gtrsim r$, the c dispersion of Ψ is roughly of Poisson type, and so only values of c_i within about $c^{1/2}$ of c will contribute to the sum in (32). In order to establish the variational principle it is sufficient that $E''(0, x)$ is positive for x in the neighbourhood of c. We may then assert that

$$\langle H \rangle = E_0 + \omega_0 c > E(0, c). \tag{33}$$

Just beyond the region of linear optics, when $c \gtrsim -r$ one might expect that the binding energy would be proportional to the number of excitations, that is, $c + r$. This would imply a zero value for $E''(0, c)$ in this region. Tavis and Cummings have shown that on resonance $E''(0, c)$ is positive for $c > -r$ and $r \gg 1$. Continuity arguments suggest that this 'curvature' remains positive when the off-resonance parameter δ is nonzero provided $\delta/|g|$ is small. Examination of particular exact results for $r = \tfrac{1}{2}$, 1 strengthens the view that $E''(0, c)$ is positive in general; for example, when $r = 1$, $E(0, c) = -2|g|(c + \tfrac{1}{2})^{1/2}$ so that

$$E''(0, c) = \tfrac{1}{2} |g| (c + \tfrac{1}{2})^{-3/2} > 0.$$

6. Conclusion

Although the results described are quite accurate when r and c are large, there is room for improvement when either r is small, or when both r and c are small. Pines (1963) has noted that the variational method is equivalent to a canonical transformation on H, the ground state then being the vacuum state of the 'new' particles. Corrections to this ground state energy can then be found by perturbation theory on the new Hamiltonian.

Alternatively, we can attempt to improve the trial function of § 2; an obvious generalization of the unitary operators based on the forms:

$$\exp(\beta R^{(+)} - \beta^* R^{(-)} + \gamma R_3)$$

and

$$\exp(f(k)a_k - f^*(k)a_k^\dagger + i\alpha(k)a_k^\dagger a_k)$$

introduces extra parameters γ and $\alpha(k)$ but unfortunately leads to no essential changes. A more interesting line of attack seeks to reduce the c dispersion of Ψ. We can use the following theorem.

Suppose Ψ is not an eigenstate of C, but $(\Psi, C\Psi) = c$. If $F(x)$ is everywhere positive and

$$F'(c) = 0 \qquad F''(c) < 0$$

then the c dispersion of $(F(C)\Psi, F(C)\Psi)^{-1/2} F(C)\Psi$ is less than that of Ψ.

I shall not give the proof of this result. It may suffice to remark that the procedure implicit in the theorem is analogous to the process in algebra for finding approximations to the largest eigenvalue of a matrix by repeatedly applying it to a (trial) column vector.

Acknowledgments

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