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On a Quantum Mechanical Maser Model[1])

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(4. VI. 70)

Summary. A system of N two-level molecules interacting with one mode of the radiation field is treated quantum mechanically with exact methods. The interaction is taken from electric and magnetic dipole coupling where antiresonant terms are neglected. The eigenvalue spectrum of the Hamiltonian is discussed in detail and asymptotic expressions for the eigenvalues (for large N) are derived. The eigenvalues are approximately equidistant with a distance between successive eigenvalues proportional to $N^{1/2}$. This leads to oscillations of the number of photons in time with a period proportional to $N^{-1/2}$, as it is observed in the pulsation of laser output.

1. Introduction

One of the many surprising facts of the laser phenomenon is the complicated time behavior of the radiation output. Looking at an oscillogramm of the output of a pulsed ruby laser, one sees that the radiation is emitted in a series of μsec pulses. Under pure experimental conditions (single-mode operation) one finds regular pulsation of the radiation with a period of about 2×10^{-6} sec. Moreover, in multi-mode operation picosecond pulses have been observed. On the other hand, the relevant excited state of Cr^{3+} in ruby has a life time of about 3×10^{-3} sec.

Comparing these numbers, it is clear that N optically active molecules in a laser cavity behave radically different as N independent molecules. The laser phenomenon is essentially a many-body problem. Hence, for a complete understanding, a full quantum mechanical treatment of a system of N molecules coupled by the radiation field is necessary. At first sight, such a program might appear very ambitiously, but compared with other many-body systems, the laser is simple for the following reasons: (i) The particles are simple because for the basic mechanism it is good enough to describe them by two-level molecules. Indeed, in a pulsed laser only the levels of the laser transition are important, the pumping levels are only necessary for the preparation of the very uncommon initial state. (ii) The interaction is simple because, as the use of the cavity shows, only modes of the radiation field with frequencies within a small intervall are essential. Furthermore, it is possible to control the modes [1] so that only a few or even one can oscillate. The latter is most the case in masers and we consider this situation here.

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We study a system of N molecules interacting with one mode of the radiation field described by the Hamiltonian

$$H = \sum_{i=1}^{N} b_i^+ \, b_i + a^+ a + \sum_{i=1}^{N} (g \, a^+ b_i + \bar{g} \, b_i^+ a) = H_0 + H_I \, . \tag{1.1}$$

The photon operators a, a^+ satisfy

$$a \, a^+ - a^+ a = 1 \, , \tag{1.2}$$

and the molecules are assumed to exist in two states only, so that we take

$$b_i^+ = \frac{1}{2} \, \sigma_i^+ = \frac{1}{2} \, (\sigma_i^1 + i \, \sigma_i^2) \, , \quad b_i = \frac{1}{2} \, \sigma_i^- = \frac{1}{2} \, (\sigma_i^1 - i \, \sigma_i^2) \, , \; i = 1, 2, \ldots N \tag{1.3}$$

where σ^1, σ^2, $\sigma^\pm$ are the Pauli matrices. In particular, we have

$$[b_i \, , b_j] = [b_i \, , b_j^+] = [b_i^+ \, , b_j^+] = 0 \, , \quad i \neq j \tag{1.4}$$

and

$$b_i^2 = (b_i^+)^2 = 0 \, . \tag{1.5}$$

The interaction term H_I in equation (1.1) results from electric (g real) and magnetic dipole coupling (g imaginary) where antiresonant terms $a^+ b_i^+$, $b_i a$ have been neglected.

The Hamiltonian (1.1) has the property that the interaction term commutes with the free Hamiltonian

$$[H_0 \, , H_I] = 0 \tag{1.6}$$

which seems to have been overlooked in earlier studies [2–4]. This property which makes an exact analysis possible holds in the multimode case too. We shall consider this more general problem elsewhere. If antiresonant terms are included, equation (1.6) is no longer true, but these terms can be treated by perturbation theory in contrast to the resonant terms.

The eigenvalues of the free Hamiltonian H_0 are

$$E_r = r \, , \quad r = 0, 1, 2 \ldots \tag{1.7}$$

each of which is 2^N-fold degenerate. The degeneracy is removed by the interaction, so that the eigenvalues of H must be of the form

$$E_{r,n} = r + |g| \, \varepsilon_{r,n} \, , \quad n = 1, 2 \ldots 2^N \tag{1.8}$$

where the $\varepsilon_{r,n}$ are determined by an *algebraic* eigenvalue problem. In order to formulate this, a concrete representation of the Hamiltonian (1.1) must be chosen. This is done in the next section, using the Hilbert space of analytic functions introduced by Bargmann [5], which is the very natural space in problems with Bose operators.

In the third section, the 2^N-dimensional algebraic eigenvalue problem is reduced utilizing the invariance of H with respect to permutations of the molecules. In the following sections, the resulting $(N+1)$-dimensional eigenvalue problem is studied and asymptotic expressions for the eigenvalues (for large N) are derived. The eigenvalue spectrum found has interesting physical consequences which are discussed in the last section. It turns out, for example, that the number of photons oscillates in time with a period (strictly speaking a quasi-period)

$$T = \frac{1}{|g|} \frac{\log E + c}{E^{1/2}}$$

where c is a constant depending on the number of photons n_0 at time $t = 0$, $E = 1/2\,(N + R + 2)$ and $R = N + n_0$. This gives an explanation for the pulsation of laser output mentioned above. However, for a complete theory of laser pulsation, losses must be included in the model.

2. Concrete Representation of the Problem

As a first step in the analysis of the Hamiltonian (1.1), we choose a Schrödinger representation in some concrete Hilbert space. The representation of the operators b_i, b_i^+ by tensor products of 2×2 matrices is straightforward:

$$b_i^+ = \mathbf{1} \otimes \ldots \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}_i \otimes \ldots \mathbf{1}\,, \tag{2.1}$$

$$b_i = \mathbf{1} \otimes \ldots \otimes \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_i \otimes \ldots \mathbf{1}\,. \tag{2.2}$$

To represent the photon operators a, a^+ we use the Hilbert space $\mathfrak{F}$ of analytic functions introduced by Bargmann [5]. This space consists of complex functions $f(z)$ analytic in the whole of $\mathbf{C}$ and satisfying

$$\int |f(z)|^2 \, d\mu(z) < \infty \tag{2.3}$$

with

$$d\mu(z) = \frac{1}{\pi} e^{-|z|^2} \, dx \, dy\,, \qquad z = x + i\,y\,.$$

The inner product in $\mathfrak{F}$ is defined by

$$(f, g) = \int \bar{f}(z)\, g(z) \, d\mu(z) \tag{2.4}$$

and we have the following complete orthonormal system

$$f_n(z) = \frac{z^n}{\sqrt{n!}}\,, \qquad n = 0, 1, 2 \ldots \tag{2.5}$$

The operators a, a^+ are represented in $\mathfrak{F}$ by

$$a^+ \to z\,, \qquad a \to \frac{\partial}{\partial z}\,. \tag{2.6}$$

One notes that the commutation relation (1.2) holds and the correspondence between $\mathfrak{F}$ and the ordinary Fock space is given by

$$f = \sum_n \frac{c_n}{\sqrt{n!}} (a^+)^n \,|0\rangle \to f(z) = \sum_n \frac{c_n}{\sqrt{n!}} z^n \in \mathfrak{F}\,.$$

Now, the Hamiltonian H of our system operates in the Hilbert space

$$\mathcal{H} = \mathfrak{F} \otimes \mathbf{C}^2 \otimes \dots \otimes \mathbf{C}^2 = \mathfrak{F} \otimes \mathbf{C}^{2^N} . \tag{2.7}$$

The elements $\varphi \in \mathcal{H}$ are tensores $\varphi = \{\varphi_{n_1 \cdots n_N}(z)\}$, $n_i = 0,1$, the components of which $\varphi_{n_1 \cdots n_N}(z)$ are analytic functions $\in \mathfrak{F}$. Using the definitions (2.1), (2.2) and (2.6), the time independent Schrödinger equation for the system takes the following form

$$\begin{aligned}(H\,\varphi)_{n_1 \cdots n_N} &= \nu\,(n_1, \dots n_N)\,\varphi_{n_1 \cdots n_N} + z\,\frac{\partial}{\partial z}\,\varphi_{n_1 \cdots n_N} \\ &\quad + g\,z \sum_i \delta_{n_i,1}\,\varphi_{n_1 \cdots \underset{i}{0} \cdots n_N} + \bar{g}\,\frac{\partial}{\partial z} \sum_i \delta_{n_i,0}\,\varphi_{n_1 \cdots \underset{i}{1} \cdots n_N} = E\,\varphi_{n_1 \cdots n_N}\end{aligned} \tag{2.8}$$

where $\nu(n_1, \dots n_N)$ is the number of zeros$'_s$ in the index set $\{n_1, \dots n_N\}$ or, physically speaking, the number of excited molecules.

For illustration, let us consider the case of only one molecule. A state of this system is simply given by $\varphi = \{\varphi_0(z), \varphi_1(z)\}$, and the Schrödinger equation (2.8) reads

$$\varphi_0 + z\,\varphi_0' + \bar{g}\,\varphi_1' = E\,\varphi_0\,, \quad z\,\varphi_1' + g\,z\,\varphi_0 = E\,\varphi_1\,. \tag{2.9}$$

This linear system of ordinary differential equations can be solved by the ansatz

$$\varphi_0(z) = e_0\,\frac{z^{R-1}}{\sqrt{(R-1)!}}\,, \quad \varphi_1(z) = e_1\,\frac{z^R}{\sqrt{R!}}\,. \tag{2.10}$$

Inserting this in equation (2.9), we get the following algebraic equations

$$e_0 + (R-1)\,e_0 + \bar{g}\,\sqrt{R}\,e_1 = E\,e_0\,, \quad g\,\sqrt{R}\,e_0 + R\,e_1 = E\,e_1\,, \tag{2.11}$$
$$(e_0, e_1) \in \mathbf{C}^2\,.$$

For the eigenvalues and eigenfunctions, we obtain

$$E_{R\pm} = R \pm |g|\,\sqrt{R}\,, \quad R = 0, 1, 2 \dots \tag{2.12}$$

and

$$\varphi_{R\pm} = \frac{1}{\sqrt{2}}\left(\frac{z^{R-1}}{\sqrt{(R-1)!}}\,,\ \pm\frac{z^R}{\sqrt{R!}}\right), \quad R \geqslant 1\,, \quad \varphi_0 = (0, 1)\,. \tag{2.13}$$

According to equation (2.12), the double eigenvalues $E_R = R$, $R \geqslant 1$ of the free Hamiltonian are split into two simple eigenvalues $E_{R\pm}$. Since the corresponding eigenfunctions (2.13) form a complete system in $\mathcal{H}$, the spectrum of H consists of the point spectrum (2.12) only. Taking an initial state ψ_0 of $R-1$ photons and the molecule in the excited state

$$\psi_0 = \frac{z^{R-1}}{\sqrt{(R-1)!}}\,(1, 0) = \frac{1}{\sqrt{2}}\,(\varphi_{R+} + \varphi_{R-})\,,$$

we obtain for the state ψ_t at time t

$$\psi_t = e^{-iHt}\,\psi_0 = e^{-iRt}\left(\frac{z^{R-1}}{\sqrt{(R-1)!}}\,\cos|g|\,\sqrt{R}\,t,\ -i\,\frac{z^R}{\sqrt{R!}}\,\sin|g|\,\sqrt{R}\,t\right).$$

Hence, the system oscillates between the states with $R-1$ photons present and the molecule in the upper state and R photons and the molecule in the lower state.

In the general case of N molecules, we proceed in the same lines. The system (2.8) is solved by the following ansatz

$$\varphi = \left(\begin{array}{l} e_{00}\cdots \dfrac{z^{R-N}}{\sqrt{(R-N)!}} \\[2ex] \left.\begin{array}{l} e_{100}\cdots \\ e_{010}\cdots \\ \cdots\cdots \end{array}\right\} \dfrac{z^{R-N+1}}{\sqrt{(R-N+1)!}} \\[2ex] \cdots\cdots\cdots\cdots\cdots \\[2ex] e_{11}\cdots \dfrac{z^{R}}{\sqrt{R!}} \end{array}\right) \begin{array}{c} \binom{N}{0} \\[6ex] \binom{N}{1} \\[6ex] \binom{N}{N} \end{array} \tag{2.14}$$

where $R \geqslant N$ is assumed, otherwise we actually have a problem for smaller N. Since

$$\binom{N}{0} + \binom{N}{1} + \cdots \binom{N}{N} = 2^N$$

the components $(e_{00\ldots}, e_{10\ldots}, e_{01\ldots}, \ldots) = e$ really form a vector $e \in \mathbf{C}^{2^N}$.

Using the ansatz (2.14) in equation (2.8) we obtain an algebraic eigenvalue problem in $\mathbf{C}^{2^N}$

$$M_1\, e = E\, e \tag{2.15}$$

with

$$M_1 = \begin{pmatrix} R_0 & A_1 & 0 & \ldots & \\ B_1 & R_1 & A_2 & 0\ldots & \\ 0 & B_2 & R_2 & A_3 & \\ \cdots & \cdots & & & \\ & & & & R_N \end{pmatrix}. \tag{2.16}$$

Here

$$R_n = R \times \mathbf{1}\,,$$

$\mathbf{1}$ is the $\binom{N}{n}$ dimensional unit matrix. The submatrices A_n are $\binom{N}{n-1} \times \binom{N}{n}$ rectangular matrices which cause transitions from states with $(N-n+1)$ excited molecules and $(n-1)$ molecules in the lower state to states with $(N-n)$ excited molecules and n molecules in the lower state. They have the following form

$$A_n = g\sqrt{R-N+n}\; P_n\,. \tag{2.17}$$

The root arises from the normalization factors in equation (2.14) and P_n is a $\binom{N}{n-1} \times \binom{N}{n}$ matrix formed according to the following rule: we number the rows of P_n by the $\binom{N}{n-1}$ permutations of $(n-1)$ ones and $(N-n+1)$ zeros and the columns by the $\binom{N}{n}$ permutations of n ones and $(N-n)$ zeros; if it is possible to change the permutation numbering the row into the permutation numbering the column by the substitution of one 0 by 1, then the corresponding matrix element is 1, otherwise 0. For instance, for $N = 4$ we have

$$P_2 = \begin{array}{cccccc|l} 1100 & 1010 & 1001 & 0110 & 0101 & 0011 & \\ 1 & 1 & 1 & 0 & 0 & 0 & 1000 \\ 1 & 0 & 0 & 1 & 1 & 0 & 0100 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0010 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0001\,. \end{array}$$

For later use, we note that the matrices P_n contain n ones in each column. This is due to the fact that the n ones in each column permutation can be changed into a zero according to the rule. In the same way, we see that each row contains $(N-n+1)$ ones. The submatrices B_n are the hermitian conjugates

$$B_n = A_n^+ \,.$$

3. Reduction of the Problem

At first, we remove the diagonal part in the matrix M_1 (2.16), considering instead of M_1 the matrix

$$M_2 = M_1 - R \times \mathbf{1} \tag{3.1}$$

where $\mathbf{1}$ is a 2^N-dimensional unit matrix. The hermitian matrix M_2 is proportional to $|g|$, we therefore write

$$M_3 = |g|\, M_2\,. \tag{3.2}$$

Supposed we have solved the hermitian eigenvalue problem for M_3

$$M_3\, e = \varepsilon\, e \tag{3.3}$$

then the eigenvalues of M_1 or H are given by

$$E_{R,n} = R + |g|\, \varepsilon_{R,n}\,, \quad n = 1, 2, \ldots 2^N\,. \tag{3.4}$$

From now on, we consider a fixed $R \geqslant N$. The matrix M_3 which we have to study has a similar structure as M_1. The difference is only that the A_n's (2.17) have a phase factor $e^{i\alpha}$ in front instead of

$$g = |g|\, e^{i\alpha}$$

and that the main diagonal of M_3 is 0.

Since the Hamiltonian H is invariant under permutations of the molecules, the matrices M_1 and M_3 commute with these permutations. Hence, the eigenvalues $E_{R,n}$ or $\varepsilon_{R,n}$ can be classified according to representations of the symmetric group S_N.

In order to find how to do this, let us consider the case $g = 0$ at first. In this case, we have the 2^N-fold degenerate eigenvalue $E_R = R$ and the corresponding eigenspace carries a tensor representation of the unitary group $U(2)$ namely the identical representation of

$$U(2) \otimes U(2) \otimes \ldots \otimes U(2)\,, \quad N \text{ factors.} \tag{3.5}$$

This, at the same time, is a representation D of S_N of degree 2^N which is reducible. Now, for $g \neq 0$ the eigenvalue $E_R = R$ splits into as many eigenvalues $E_{R,n}$ (3.4) as there are irreducible components in D (we have no accidental degeneracy). Exactly this situation occurs in Weyl's theory of representations of the unitary group $U(n)$ [6], with the only difference that we are interested in the irreducible representations of S_N contained in (3.5), while in Weyl's theory one looks for representations of $U(n)$. Using the duality of Weyl's theory between the unitary and the symmetric groups, we have the following answer to the reduction problem in question: Let us reduce (3.5) with respect to $U(2)$

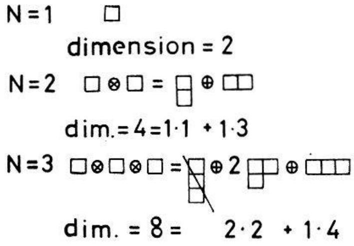
$$U(2)^{\otimes N} = f_1\,F_1 \oplus f_2\,F_2 \oplus \ldots \oplus f_i\,F_i \tag{3.6}$$

where the F_k are irreducible representations of $U(2)$ of degree n_k and multiplicity f_k. Then the reduction of D into irreducible representations of S_N is given by

$$D = n_1\,D_1 \oplus n_2\,D_2 \oplus \ldots \oplus n_i\,D_i \tag{3.7}$$

where the D_k are irreducible representations of S_N of degree f_k and multiplicity n_k.

The reduction (3.6) can be carried out by means of Young diagrams [7]. It is very easy to proceed successively in $N = 1, 2, 3 \ldots$; the first steps are:



Therefore, we have: for $N = 1$,2 single eigenvalues, for $N = 2$,1 + 3 single eigenvalues, for $N = 3$,2 double eigenvalues and 4 single eigenvalues, etc.

In addition to the multiplicities of the eigenvalues, the Young diagrams give us the symmetry classes of the tensor indeces of the corresponding eigenfunctions. One symmetry class is of particular interest, namely the symmetric class, which corresponds to the horizontal diagram of N squares (the last diagram in the above examples). This diagram occurs exactly once in (3.6) and has the $U(2)$-dimension $(N + 1)$. Therefore, there are $(N + 1)$ simple eigenvalues corresponding to symmetric eigenfunctions. From now on, we restrict our attention to this symmetric $(N + 1)$-dimensional subspace of $\mathbf{C}^{2^N}$. The physical reason for this is not the Pauli principle, of course, but the fact that the initial state with all molecules excited, which is interesting for the laser problem, lies in this subspace.

The projection onto the symmetric subspace is achieved by the projector

$$P = \begin{pmatrix} P_0 & & 0 \\ & P_1 & \\ & \cdots & \\ 0 & & \\ & & P_N \end{pmatrix} \text{ with } P_n = \frac{1}{\binom{N}{n}} \begin{pmatrix} 1 & 1 & \ldots & 1 \\ 1 & 1 & \ldots & 1 \\ \cdots & & & \end{pmatrix}$$

where P_n is a $\binom{N}{n} \times \binom{N}{n}$ matrix with all elements $= 1$, apart from the factor in front. We get

$$M_4 = P\,M_3 = P\,M_3\,P = \begin{pmatrix} 0 & A_1' & 0 & \\ B_1' & 0 & A_2' & \\ & B_2' & 0 & A_3' \\ \cdots & & & \end{pmatrix} \tag{3.8}$$

with

$$A_n' = B_n'^{+} = P_{n-1}\,A_n = e^{i\alpha} \frac{n}{\binom{N}{n-1}} \begin{pmatrix} 1 & 1 & \ldots & 1 \\ 1 & 1 & \ldots & 1 \\ \cdots & & & \end{pmatrix}, \quad n = 1, \ldots N$$

where the last matrix now has $\binom{N}{n-1}$ rows and $\binom{N}{n}$ columns. Next we make an orthogonal transformation using

$$O = \begin{pmatrix} O_0 & & 0 \\ & O_1 & \\ \cdots & & \\ 0 & & O_N \end{pmatrix} \text{ with } O_n = \frac{1}{\sqrt{\binom{N}{n}}} \begin{pmatrix} 1 & 1 & \ldots & 1 \\ & \times & & \end{pmatrix}$$

where the last matrix is an $\binom{N}{n} \times \binom{N}{n}$ orthogonal matrix with the elements in the first row $= 1$ and the other rows arbitrary.

We then arrive at the matrix

$$M_5 = O\,M_4\,O^{-1}$$

which has the same structure as (3.8) but with

$$A_n'' = B_n''^{+} = O_{n-1}\,A_n'\,O_n^T = \begin{pmatrix} a_n'' & 0 & 0 & \ldots \\ 0 & 0 & 0 & \ldots \\ \cdots & & & \end{pmatrix}$$

instead of A_n', where

$$a_n'' = e^{i\alpha}\, n \sqrt{R - N + n} \sqrt{\frac{\binom{N}{n}}{\binom{N}{n-1}}} = e^{i\alpha} \sqrt{(R - N + n)\, n\, (N - n + 1)}\,. \tag{3.9}$$

The matrix M_5 defines a hermitian transformation of the $(N+1)$-dimensional symmetric subspace and annihilates its orthogonal complement. Now we consider the symmetric subspace only, then instead of M_5 we must study the $(N+1) \times (N+1)$ hermitian tridiagonal matrix M_6 with a''_n above and $\bar{\ }''_n$ below the main diagonal and 0 otherwise. Next, we make an unitary transformation to remove the phase factor in (3.9). This can be done using

$$U = \begin{pmatrix} 1 & & & \\ & e^{i} & 0 & \\ & & e^{2i} & \\ 0 & & & \\ \cdots & & & \\ & & & e^{Ni} \end{pmatrix},$$

then

$$M_7 = U \, M_6 \, U^{-1}$$

is a real symmetric tridiagonal matrix, the elements a''''_n of which are given by (3.9) without the phase factor. Finally, let us invert the order of the matrix elements

$$a_n = a''''_{N+1-n} = \sqrt{(R+1-n)\,(N+1-n)\,n} \;, \quad n = 1, \dots N \,, \tag{3.10}$$

so that the tridiagonal matrix M to be analysed is

$$M = \begin{pmatrix} 0 & a_1 & & & \\ a_1 & 0 & a_2 & & \\ & a_2 & 0 & a_3 & \\ & & \cdots & & \\ & & & 0 & a_N \end{pmatrix} . \tag{3.11}$$

4. Determination of the Eigenvalues

Although there are powerful numerical methods to determine the eigenvalues of a symmetric tridiagonal matrix, the physical problem cannot be solved in this way, because the number of molecules N, say $10^{16} - 10^{23}$, is too big for any computer. For an analytical treatment, we convert the algebraic eigenvalue problem

$$M \, e = \varepsilon \, e \tag{4.1}$$

into a difference equation

$$a_n \, e_{n-1} + a_{n+1} \, e_{n+1} = \varepsilon \, e_n \,, \quad n = 0, 1, \dots N \,. \tag{4.2}$$

Equation (4.2) is readily obtained by writing equation (4.1) in components. For equation (4.2) we define

$$a_0 = a_{N+1} = 0$$

in accordance with (3.10).

The difference equation (4.2) remains fulfilled if we substitute

$$\varepsilon \to -\varepsilon \,, \quad e_{2i+1} \to -e_{2i+1} \,, \quad e_{2i} \to e_{2i} \,, \quad i = 0, 1, \dots \tag{4.3}$$

Hence, with ε also $-\varepsilon$ is an eigenvalue, the $N+1$ eigenvalues lay symmetrically around 0. For even N the eigenvalue $\varepsilon = 0$ must occur. Because of this, it is sufficient to determine the positive eigenvalues. An eigenvalue problem for the $1/2\,(N+1)$ (for odd N) or $1/2\,N$ positive eigenvalues (for even N) alone can be obtained by considering M^2 instead of M. Writing

$$M^2\, e = \varepsilon^2\, e$$

in components, the even and odd components decouple and the problem splits into two eigenvalue problems having the half dimensions. This is useful for numerical calculations, but for the analytical treatment we use equations (4.1), (4.2).

Let us recall that the components e_n in (4.2) determine the eigenstate φ of the system in the symmetric subspace $\mathcal{H}^s$ of the Hilbert space $\mathcal{H}$ completely according to

$$\varphi = \left(e_0\, \frac{z^R}{\sqrt{R!}},\ e_1\, \frac{z^{R-1}}{\sqrt{(R-1)!}},\ \dots\ e_N\, \frac{z^{R-N}}{\sqrt{(R-N)!}}\right). \tag{4.4}$$

Now we make a linear transformation of the components e_n:

$$e'_n = e_n \sqrt{\frac{\binom{N}{n}}{(R-n)!}} \tag{4.5}$$

where the normalization factor of the photons and a weighting factor due to the permutations of the molecules are enclosed. In the new components e'_n the difference equation (4.2) takes a rational form

$$(R+1-n)\,(N+1-n)\,e'_{n-1} + (n+1)\,e'_{n+1} = \varepsilon\, e'_n\,, \quad n = 0, 1, \dots N \tag{4.6}$$

where we must set

$$e'_{-1} = e'_{N+1} = 0\,. \tag{4.7}$$

We convert equation (4.6) into a differential equation using the characteristic function $f(z)$

$$f(z) = \sum_{n=0}^{N} e'_n\, z^{R-n}\,. \tag{4.8}$$

Multiplying (4.6) by z^{R-n} and summing over $n = 0, 1, \dots N$ we get

$$z\, f''(z) + (N+1-R)\, f'(z) - z^2\, f'(z) + R\, z\, f(z) = \varepsilon\, f(z) \tag{4.9}$$

where the primes denote differentiation with respect to z. Instead of equation (4.9) we can also write an equation of motion for the time dependent characteristic function $f(z, t)$

$$f(z,t) = \sum_{n=0}^{N} e'_n(t)\, z^{R-n} \tag{4.11}$$

substituting $E = R + |g|\,\varepsilon$ in equation (4.9) by $i\,\partial/\partial t$:

$$i\, \frac{\partial f}{\partial t} = R\, f + |g|\,(z\, f'' + (N+1-R)\, f' - z^2\, f' + R\, z\, f)\,. \tag{4.12}$$

Since the characteristic function f is an element of the Hilbert space $\mathfrak{J}$ of the photons, one may ask how it is related to the state of the radiation field. The latter is obtained by reduction of the whole state of the system (2.14) to the Hilbert space $\mathfrak{J}$. In that way, we obtain the following mixed state

$$W = \sum_{n=0}^{N} \binom{N}{n} |e_n|^2 \left(\frac{z^{R-n}}{\sqrt{(R-n)!}}, \cdot \right) \frac{z^{R-n}}{\sqrt{(R-n)!}}$$
$$= \sum_{n=0}^{N} |e'_n|^2 \, (z^{R-n}, .) \, z^{R-n} . \tag{4.13}$$

The expectation value of a photon operator A is then given by

$$\langle A \rangle_{\mathfrak{J}} = \mathrm{Tr}\, W A = \sum_{n=0}^{N} |e'_n|^2 \, (z^{R-n}, A \, z^{R-n}) . \tag{4.14}$$

On the other hand we have

$$(f, A\, f)_{\mathfrak{J}} = \sum_{n,m} \bar{e}'_n \, e'_m \, (z^{R-n}, A \, z^{R-m}) ,$$

and this is equal to (4.14) for all operators A commuting with the photon number operator

$$a^+ a = z \frac{\partial}{\partial z} .$$

Therefore, as far as observables like the photon number, the fluctuation of the photon number are concerned, we may interpret (4.11) as the state of the radiation field. In this sense, the molecules have been eliminated in equation (4.12). The interaction operator on the right hand side of equation (4.12) is no longer hermitian in $\mathfrak{J}$, it annihilates (first two terms) and creates photons (last two terms). But in addition, $f(z, t)$ determines the state of the molecules, too, because there is a one-to-one correspondence between equation (4.4) and (4.8). No information is lost going from equation (4.4) to (4.8), in contrast to the reduction (4.13) where the phases of the $e'_n(t)$ have been dropped out.

Now we return to equation (4.9). By the substitution

$$f(z) = y(z) \, z^l \, e^{\frac{1}{4} z^2} \tag{4.15}$$

where

$$2\, l = R - N - 1 \tag{4.16}$$

we remove the terms with f' and get

$$- y'' + \left[\frac{l\,(l+1)}{z^2} + \frac{z^2}{4} + \frac{\varepsilon}{z} \right] y = \left(R - l + \frac{1}{2} \right) y . \tag{4.17}$$

This is just the radial Schrödinger equation for a particle moving in an oscillator plus a Coulomb potential. The eigenvalue ε now enters as the ‘charge’, the energy

$$E = R - l + \frac{1}{2} = \frac{1}{2} (R + N) + 1 \tag{4.18}$$

being given. Since we look for a polynomial solution $f(z)$ (4.15), the corresponding eigenfunction $y(z)$ of (4.17) must be an ordinary $L^2(0, \infty)$ eigenfunction. The coincidence with the radial Schrödinger equation has no deeper physical reason; we remark in particular that l may be half integer according to equation (4.16). For the special case $\varepsilon = 0$ which occurs for even N we can immediately write down the solution $y(z)$ of equation (4.17)

$$y(z) = e^{-\frac{1}{4} z^2} z^{l+1} L_{N/2}^{(l+\frac{1}{2})} \left(\frac{z^2}{2}\right)$$

where $L_n^{(a)}$ is the generalized Laguerre polynomial [9]. With (4.15) we obtain

$$f(z) = z^{2l+1} L_{N/2}^{(l+\frac{1}{2})} \left(\frac{z^2}{2}\right)$$

and we see that indeed $f(z)$ is a polynomial in z even for half integer l if N is an even number. In the general case $\varepsilon \neq 0$ the equation (4.17) seems not to have been solved exactly, although it may be of some interest in other branches of physics, for instance in nuclear physics.

As a first step in the analysis of the eigenvalue spectrum, let us estimate the largest eigenvalue ε_{max}. Denoting the 'potential' in equation (4.17) by

$$V(z) = \frac{L^2}{z^2} + \frac{z^2}{4} + \frac{\varepsilon}{z} \tag{4.19}$$

where

$$L^2 = l\,(l+1)\,, \tag{4.20}$$

we must have for any eigenvalue

$$V(z_0) \leqslant E\,, \tag{4.21}$$

where $V(z_0)$ is the minimum of the potential. The position of the minimum z_0 is determined by

$$V'(z_0) = 0 = -\frac{2\,L^2}{z_0^3} + \frac{z_0}{2} - \frac{\varepsilon}{z_0^2} \tag{4.22}$$

or

$$\frac{L^2}{z_0^2} + \frac{\varepsilon}{z_0} = \frac{z_0^2}{2} - \frac{L^2}{z_0}\,.$$

Inserting this in equation (4.21) we get

$$V(z_0) = \frac{3}{4} z_0^2 - \frac{L^2}{z_0^2} \leqslant E$$

or

$$z_0 \leqslant \left(\frac{2}{3} E + \sqrt{\frac{4}{9} E^2 + \frac{4}{3} L^2}\right)^{1/2}.$$

Now, from (4.22) we obtain

$$\varepsilon = \frac{1}{2} z_0^3 - \frac{2\,L^2}{z_0} \leqslant \frac{1}{2} \left(\frac{2}{3} E + \frac{2}{3} E \sqrt{1 + \frac{3\,L^2}{E^2}}\right)^{3/2}$$

$$\varepsilon_{max} \leqslant \frac{1}{2} \left(\frac{4}{3} E + \frac{L^2}{E}\right)^{3/2}. \tag{4.23}$$

For lower estimates, a variation principle for the hermitian algebraic eigenvalue problem (4.1) can be used. Let $N + 1 = 2m$ be even and take the following sequence of m orthogonal trial vectors

$$e^1 = \frac{1}{\sqrt{2}}(1, 1, 0, 0, \ldots) ,$$

$$e^3 = \frac{1}{\sqrt{2}}(0, 0, 1, 1, 0, \ldots) ,$$

$$\cdots\cdots$$

$$e^N = \frac{1}{\sqrt{2}}(0, \ldots \quad 1, 1) .$$

Then we get for the quadratic form

$$(e^i, M e^i) = 2 \sum_{n=1}^{N} a_n e^i_{n-1} e^i_n = a_i .$$

If $\alpha_1 < \alpha_3 < \ldots \alpha_N$ is the sequence of the a_i in the order of increasing magnitude, we obtain lower estimates for the m positive eigenvalues $\varepsilon_1 < \varepsilon_3 \ldots < \varepsilon_N$, namely

$$\alpha_n \leqslant \varepsilon_n . \tag{4.24}$$

For the special case $R = N$, the largest a_i in (3.10) is

$$a_{max} = \frac{2}{9} \sqrt{3} (N + 1)^{3/2} .$$

With (4.23), noting $L^2 = -1/4$, $E = N + 1$, this gives

$$\frac{2}{9} \sqrt{3} (N + 1)^{3/2} \leqslant \varepsilon_{max} \leqslant \frac{4}{9} \sqrt{3} (N + 1)^{3/2} . \tag{4.25}$$

Hence, the largest eigenvalue ε_{max} really increases like $N^{3/2}$. We discuss this result in the next section.

Now let us derive asymptotic expressions for the eigenvalues for large N or large E (4.18). For this purpose, it is very appropriate to apply the JWKB method to equation (4.17). There are two positive classical turning points z_1, z_2 and the WKB integral takes the following form

$$\int_{z_2}^{z_1} dz \sqrt{E - \frac{L^2}{z^2} - \frac{z^2}{4} - \frac{\varepsilon}{z}} = \int_{z_2}^{z_1} dz \frac{E z - \frac{1}{4} z^3 - \varepsilon - \frac{L^2}{z}}{\sqrt{-\frac{1}{4} z^4 + E z^2 - \varepsilon z - L^2}}$$

$$= \frac{1}{4} \int_{z_2}^{z_1} dz \frac{2 E z - z^3 - \varepsilon}{\sqrt{-\frac{1}{4} z^4 + E z^2 - \varepsilon z - L^2}} + \int_{z_2}^{z_1} dz \frac{E z - \frac{3}{2} \varepsilon - \frac{2 L^2}{z}}{\sqrt{-z^4 + 4 E z^2 - 4 \varepsilon z - 4 L^2}}$$

$$= \left(n + \frac{1}{2}\right) \pi . \tag{4.26}$$

The first integral is 0 and the second one can be transformed by means of complete elliptic integrals. By the standard substitution [10]

$$z = \frac{z_2 (z_1 - z_3) - z_3 (z_1 - z_2) \sin^2\Phi}{(z_1 - z_3) - (z_1 - z_2) \sin^2\Phi}$$

where $z_1 > z_2 > z_3 > z_4$ are the four real zeros of the quartic form under the root, we get

$$\begin{aligned}\left(n + \frac{1}{2}\right) \pi = \mu\, K(k) & \left(E\, z_3 - \frac{3}{2}\, \varepsilon_n - \frac{2\, L^2}{z_3}\right) \\ & + \mu\, \Pi \left(\frac{z_1 - z_2}{z_1 - z_3}, k\right) E\, (z_2 - z_3) \\ & - \mu\, \Pi \left(\frac{z_3}{z_2} \frac{z_1 - z_2}{z_1 - z_3}, k\right) 2\, L^2\, \frac{z_3 - z_2}{z_2\, z_3}\,. \end{aligned} \tag{4.27}$$

Here

$$\mu = \frac{2}{\sqrt{(z_1 - z_3)(z_2 - z_4)}}\,, \qquad k^2 = \frac{z_3 - z_4}{z_3 - z_1} \cdot \frac{z_2 - z_1}{z_2 - z_4} \tag{4.28}$$

and K and Π are the complete elliptic integrals of the first and third kind respectively. Expanding the elliptic integrals in equation (4.27) for large N, which is done in the Appendix, we arrive at the following equation for the positive eigenvalues ε_n

$$\varepsilon_n = 2\,\pi\, \frac{\frac{1}{2}\, E^{3/2} - \left(n + \frac{1}{2}\right) E_0^{1/2} - E^{1/2}\, L \left(1 - \frac{2}{\pi} \arcsin\beta\right)}{1 + \log(16\, E^{3/2}) - \frac{1}{2} \log(\varepsilon_n^2 + 4\, L^2\, E)} \tag{4.29}$$

where

$$E_0 = E + \frac{3}{2} \frac{L^2}{E}$$

$$\beta = \left(\frac{1}{2} + \frac{1}{2\sqrt{1 + 4\, L^2\, \frac{E}{\varepsilon^2}}}\right)^{1/2}$$

and

$$n = 0, 1, 2, \ldots \begin{array}{ll} \frac{1}{2} N & \text{if } N \text{ even} \\ \frac{1}{2} (N - 1) & \text{if } N \text{ odd}, \end{array}$$

the largest n gives the lowest eigenvalue. Equation (4.29) holds good for

$$\Delta_1 = \frac{\sqrt{3}}{2} \frac{\varepsilon_n}{E^{3/2}} \ll 1\,, \tag{4.30}$$

that means in the lower part of the spectrum. As we shall see in the next section, this is just the interesting part in the laser problem.

The equation (4.29) is of the following form

$$\varepsilon = \frac{b - g_1(\varepsilon)}{a - g_2(\varepsilon)} \tag{4.31}$$

where $g_1(\varepsilon)$ is a positive decreasing function and $g_2(\varepsilon)$ is a positive increasing function of ε. It is easy to solve (4.31) for ε by a method of bisection, utilizing the fact that for an $\varepsilon' \gtrless \varepsilon$ the right hand side in (4.31) is $\lessgtr \varepsilon'$. A considerable improvement in the accuracy of equation (4.29) is obtained substituting

$$L^2 = l\,(l+1)\ (4.20)\ \text{ by }\ L^2 = \left(l + \frac{1}{2}\right)^2 . \tag{4.32}$$

This substitution due to Kramers [11] is very appropriate here, because in order to get the correct behaviour of the solution for smal z the centrifugal barrier must be modified according to (4.32). In addition, with (4.32) the equation (4.29) can be used also in the case $R = N$, which now corresponds to $L = 0$. With the old definition (4.20) of L^2 we would have $L = -1/2$; this gives no classical turning point z_2, so that the application of the JWKB method would be doubtful. In Table 1 we have compared the results for various eigenvalues calculated from equation (4.29) with the exact results for $N = 2001$, $R = 2002$. We see that the formula (4.29) is good in the lower half of the spectrum.

Table 1
Comparison between the exact and the JWKB eigenvalues for $N = 2001$, $R = 2002$.

n	JWKB	exact	n	JWKB	exact	n	JWKB	exact
1000	13.570	13.716	800	9357.7	9353.3	600	21709.	21663.
999	41.107	41.424	799	9413.6	9409.2	599	21776.	21729.
998	69.471	69.806	798	9469.6	9465.1	598	21844.	21796.
997	98.694	98.990	797	9525.6	9521.0	597	21911.	21863.
996	128.69	128.95	796	9581.7	9577.1	596	21978.	21930.
995	159.39	159.60	795	9637.9	9633.1	595	22045.	21997.
994	190.70	190.88	794	9694.2	9689.3	594	22113.	22064.
993	222.56	222.73	793	9750.5	9745.5	593	22180.	22131.
992	254.94	255.09	792	9806.8	9801.8	592	22248.	22198.
991	287.79	287.92	791	9863.3	9858.2	591	22315.	22265.

The functions $g_1(\varepsilon)$, $g_2(\varepsilon)$ in equation (4.31) are slowly varying functions of ε. Therefore, if a not too big part of the spectrum is considered, the eigenvalues are approximately equidistant. For the distance of successive eigenvalues $\varepsilon_{n-1} - \varepsilon_n$ we get a simple asymptotic expression by going back to the WKB condition (4.26). Considering the n on the right hand side as a function of ε, $n(\varepsilon)$, we differentiate

$$-\int_{z_2}^{z_1} \frac{dz}{\sqrt{-z^4 + 4\,E\,z^2 - 4\,\varepsilon\,z - 4\,L^2}} = \pi\,\frac{dn(\varepsilon)}{d\varepsilon} .$$

The left hand integral is $= \mu K(k)$. The function $n(\varepsilon)$ is approximately linear as we just have seen, therefore

$$\frac{dn(\varepsilon)}{d\varepsilon} \approx \frac{1}{\varepsilon_n - \varepsilon_{n-1}} .$$

Then we get

$$\frac{\pi}{\varepsilon_{n-1} - \varepsilon_n} = \mu K(k) \tag{4.33}$$

or axpansion for large N (see Appfter eendix)

$$\varepsilon_{n-1} - \varepsilon_n = \frac{2 \pi E_0^{1/2}}{\log(16 E^{3/2}) - \frac{1}{2} \log(\varepsilon_n^2 + 4 L^2 E)} . \tag{4.34}$$

5. Physical Discussion

First let us return to the estimates (4.25) for the largest eigenvalue ε_{max}. At first sight, this result looks very strange. Since the eigenvalues are distributed symmetrically around 0, there is the negative eigenvalue $-\varepsilon_{max}$ which decreases like $-N^{3/2}$. Then the ground state energy (3.4)

$$E_0 = N - |g| \varepsilon_{max} \tag{5.1}$$

decreases like $-N^{3/2}$ and therefore the system seems to be unstable in the thermodynamic limit. For a fixed coupling constant g this is the case, indeed. But in reality g is volume-dependent according to

$$g = \mu \sqrt{\frac{2 \pi \omega}{\hbar V}} \tag{5.2}$$

where the dipole moment μ and the frequency ω are constants. Taking this volume-dependence into account, the term $|g| \varepsilon_{max}$ is proportional to V or N as it must be. Then the ground state energy is

$$E_0 = \text{const}\, N \tag{5.3}$$

and the system is stable. If the constants μ and ω in (5.2) are large enough, the second term in equation (5.1) can overcompensate the first and the constant in equation (5.3) can become negative. In this case, a 'phase transition' occurs in the sense that the ground state is not a state with $E_0 = 0$ without photons and all molecules in the lowest state, but some state with spontaneously excited molecules. This fact is not very surprising because the interaction has an extreme long-range character.

The most interesting feature of the model in connection with the laser problem is the fact that the eigenvalues are approximately equidistant (4.34). Hence, over not too large time intervals the relevant quantities, like the photon number $n(t)$, must oscillate in time with a period

$$T = \frac{2 \pi}{\varepsilon_{n-1} - \varepsilon_n} . \tag{5.4}$$

This can be illustrated by numerical examples. In Figure 1 we have a typical picture: for $N = 100$, $R = 110$, $g = 1$ we have calculated the photon number $n(t)$ numerically, taking all molecules in the upper state at $t = 0$ and $n(0) = 10$; we have plotted $n(t)$ in Figure 1 normalized according to

$$r(t) = \frac{n(t) - n(0)}{R - n(0)}, \tag{5.5}$$

which is a number between 0 and 1.

Let us suppose now that only the eigenstates with eigenvalues in the neighbourhood of some effective eigenvalue ε_{eff} contribute to our initial state of all molecules in the upper state. That this is the case indeed, emerges from numerical calculations (see below), and it will be investigated analytically in a subsequent paper by the analysis of the eigenfunctions. Let us write

$$\varepsilon_{eff} = a\, E^{\gamma}\,. \tag{5.6}$$

Such a rough expression is good enough because ε enters on the right of equation (4.34) only in the slowly varying function $\log(\varepsilon^2 + 4\, L^2\, E)$. Then we get from (4.34) for the period of the radiation oscillations in the case $L = 0$, i.e. $R = N$,

$$T\sqrt{E} = \log 16 - \log a + \frac{3}{2} \log E - \gamma \log E$$

that means $T\sqrt{E}$ must be a linear function of $\log E$. This is nicely confirmed by the numerical results (Fig. 2), the exponent γ in equation (5.6) turns out to be $\gamma = 1/2$. This is also found for other R ($R = N + 5$, $R = N + 10$) so that the general expression for T is given by

$$\begin{aligned} T\sqrt{E_0} &= \log 16 + \frac{3}{2} \log E - \frac{1}{2} \log\,(\varepsilon_{eff}^2 + 4\, L^2\, E) \\ &= \log 16 - \frac{1}{2} \log\,(a^2 + 4\, L^2) + \log E\,. \end{aligned} \tag{5.7}$$

On the left hand side E_0 can be changed into E in the order of N^{-1} considered here. The result $\gamma = 1/2$ in equation (5.6) is important, because it shows that ε_{eff} lies in the lower part of the spectrum where the JWKB method is well applicable.

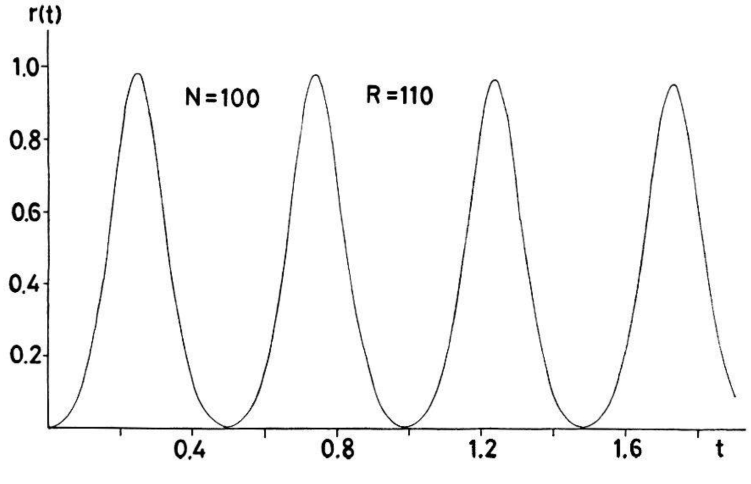


Figure 1
Pulsations of the radiation power.

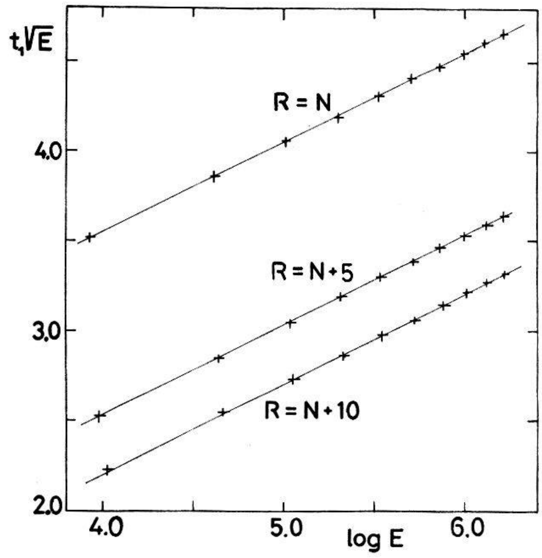


Figure 2
Linear behavior of $T\sqrt{E}$ as a function of $\log E$.

The numerical calculations leading to equation (5.7) were performed in the following way. The system

$$i\,\frac{\partial e(t)}{\partial t} = M\,e(t)$$

was integrated from $t = 0$ to the first maximum of the number of photons (5.5). The initial state $e(0) = (1, 0, 0, \ldots)$ was taken, what means that all molecules are initially in the upper state. In Table 2, the results for the position t_1 and the magnitude r_1 of the first maximum are given for various N and R. We see at first that the magnitude r_1 converges for increasing N to a limit which is already reached for values of N of ~ 500. The limit values are strongly dependent on R (especially for small R), that means on the number of photons being present at $t = 0$. This gives the reason why the laser can be used as an amplifier. Secondly, taking the position t_1 of the first maximum for $1/2\ T$, we have plotted in Figure 2 $1/2\ T\sqrt{E}$ as a function of $\log E$. We find the linear behavior expressed by equation (5.7). The factor a in equation (5.6) turns out to be $a = 0.72,\ 2.10,\ 3.79$ for $R = N$, $R = N + 5$, $R = N + 10$ respectively. Hence, ε_{eff} lies in the neighbourhood of the first, second and forth eigenvalue respectively.

Table 2
Position t_1 and magnitude r_1 of the first radiation maximum.

N	$R = N$		$R = N + 5$		$R = N + 10$	
	t_1	r_1	t_1	r_1	t_1	r_1
50	0.4928	0.7874	0.3449	0.9632	0.2978	0.9815
100	0.3839	0.7851	0.2802	0.9610	0.2471	0.9796
150	0.3304	0.7844	0.2459	0.9603	0.2190	0.9789
200	0.2954	0.7839	0.2235	0.9599	0.1996	0.9784
250	0.2720	0.7837	0.2071	0.9596	0.1860	0.9782
300	0.2540	0.7836	0.1944	0.9595	0.1752	0.9781
350	0.2389	0.7835	0.1841	0.9593	0.1668	0.9780
400	0.2271	0.7834	0.1757	0.9593	0.1596	0.9779
450	0.2170	0.7833	0.1685	0.9592	0.1532	0.9779
500	0.2082	0.7833	0.1622	0.9591	0.1475	0.9778

Summing up, the period of the radiation oscillations in physical units is given by

$$T_0 = \frac{1}{g} \frac{\log E + c}{E^{1/2}}, \quad E = \frac{1}{2} (N + R) + 1 \tag{5.8}$$

with (5.2)

$$g = \mu \sqrt{\frac{2 \pi \omega}{\hbar V}} .$$

The dipole moment μ can be obtained from the natural line width $\Delta\omega$ or the radiative life time $\tau = 2 \pi / \Delta\omega$ of the laser transition

$$\Delta\omega = \frac{4}{3} \left(\frac{2 \pi}{\lambda} \right)^3 \frac{\mu^2}{\hbar} .$$

Setting $R = N$, $E = N + 1 \approx N$ and neglecting the constant c in the numerator of equation (5.8), we get

$$T_0 = \sqrt{\frac{4 V \tau}{3 c \lambda^2}} \frac{\log N}{N^{1/2}} . \tag{5.9}$$

An inverse square root dependence $N^{-1/2}$ has also been found by Birnbaum, Stocker and Welles [14, 15] in their phenomenological theory. The decrease of T_0 with increasing N (increasing pumping power), as it is predicted by equation (5.9), has been observed experimentally [14]. But it seems not to be simple to check equations (5.9) or (5.8) quantitatively with experiments. The reason is that for a pulsed laser the number of photons and the number N of excited molecules at $t = 0$ are not accurately known. Especially the latter is quite uncertain because only a part of the active molecules is excited, and furthermore one must imagine that only some portion acts cooperatively at times. For a complete quantitative theory of the out-put pulsations the losses must be also included in the model.

Note added in proof: After this was written the papers by M. Tavis and F. W. Cummings [20] and by R. Bonifacio and G. Preparata [22] came to our attention, where the present model is treated by different methods. See also D. F. Walls and R. Barakat [21], W. R. Mallory [23].

Appendix

We must calculate the roots of

$$z^4 - 4 E z^2 + 4 \varepsilon z + 4 L^2 = 0 . \tag{A.1}$$

The cubic resolvent

$$x^3 - 2 E x^2 + (E^2 - L^2) x - \frac{\varepsilon^2}{4} = 0 \tag{A.2}$$

is transformed to the normal form

$$y^3 + 3 p y + 2 q = 0 \tag{A.3}$$

by means of

$$x = y + \frac{2}{3} E . \tag{A.4}$$

In equation (A.3) we have the casus irreducibilis $q^2 + p^3 \leqslant 0$, and we get

$$p = -\frac{1}{9}(E^2 + 3\,L^2) \overset{\text{def}}{=} -\frac{1}{9}\,E_0 \tag{A.5}$$

$$q = \frac{1}{27}\,E^3 - \frac{1}{3}\,E\,L^2 - \frac{\varepsilon^2}{8}$$

$$\cos\varphi = -\sqrt{\frac{q^2}{p^3}} = -\frac{\frac{1}{27}\,E^3 - \frac{1}{3}\,E\,L^2 - \frac{\varepsilon^2}{8}}{\left[\frac{1}{9}(E^2 + 3\,L^2)\right]^{3/2}}\,. \tag{A.6}$$

Expanding the denominator for

$$E \gg L \tag{A.7}$$

we have

$$\cos\varphi = -1 + \frac{27}{2}\,\frac{L^2}{E^2} + \frac{27}{8}\,\frac{\varepsilon^2}{E^3} - \frac{3^5}{16}\,\frac{\varepsilon^2\,L^2}{E^5} \overset{\text{def}}{=} -1 + \delta\,. \tag{A.8}$$

Then for $\delta \ll 1$, that means

$$E^3 \gg \varepsilon^2 \tag{A.9}$$

in addition to (A.7), we get

$$\varphi = \pi - (2\,\delta)^{1/2} - \frac{1}{24}\,(2\,\delta)^{3/2} + \dots \tag{A.10}$$

$$\overset{\text{def}}{=} \pi - 3\,\Delta - \frac{27}{24}\,\Delta^3$$

with

$$2\,\delta = 9\,\Delta^2$$

that is

$$\Delta^2 = \frac{3}{4}\,\frac{\varepsilon^2}{E^3} + 3\,\frac{L^2}{E^2} - \frac{27}{8}\,\frac{\varepsilon^2\,L^2}{E^5}\,. \tag{A.11}$$

Now the solutions of equation (A.3) are given by

$$y_1 = \frac{2}{3}\,E_0 \cos\frac{1}{3}\,\varphi = \frac{1}{3}\,E_0 + E_0\,\frac{\Delta}{\sqrt{3}} - E_0\,\frac{\Delta^2}{6}$$

$$y_2 = \frac{2}{3}\,E_0 \cos\frac{1}{3}\,(\varphi + 2\,\pi) = -\frac{2}{3}\,E_0 + E_0\,\frac{\Delta^2}{3}$$

$$y_3 = \frac{2}{3}\,E_0 \cos\frac{1}{3}\,(\varphi + 4\,\pi) = \frac{1}{3}\,E_0 - E_0\,\frac{\Delta}{\sqrt{3}} - E_0\,\frac{\Delta^2}{6}$$

and with (A.4) using $E_0 = E + 3/2\, L^2/E$, $E_1 = 2/3\, E + 1/3\, E_0$

$$x_1 = E_1 + E_0 \frac{\Delta}{\sqrt{3}} - E_0 \frac{\Delta^2}{6}$$

$$x_2 = \frac{2}{3}(E - E_0) + E_0 \frac{\Delta^2}{3} = \frac{1}{4} \frac{\varepsilon^2}{E^2} - \frac{3}{4} \frac{\varepsilon^2 L^2}{E^4} \overset{\text{def}}{=} \frac{1}{3} E \Delta_1^2$$

$$x_3 = E_1 - E_0 \frac{\Delta}{\sqrt{3}} - E_0 \frac{\Delta^2}{6} .$$

Then we obtain for the roots of (A.1)

$$z_1 = \sqrt{x_1} - \sqrt{x_2} + \sqrt{x_3} = 2\sqrt{E_1} - \sqrt{E} \left(\frac{\Delta^2}{4} + \frac{\Delta_1}{\sqrt{3}} \right)$$

$$z_2 = \sqrt{x_1} + \sqrt{x_2} - \sqrt{x_3} = \sqrt{E} \left(\frac{\Delta}{\sqrt{3}} + \frac{\Delta_1}{\sqrt{3}} \right)$$

$$z_3 = -\sqrt{x_1} + \sqrt{x_2} + \sqrt{x_3} = -\sqrt{E} \left(\frac{\Delta}{\sqrt{3}} - \frac{\Delta_1}{\sqrt{3}} \right)$$

$$z_4 = -\sqrt{x_1} - \sqrt{x_2} - \sqrt{x_3} = -2\sqrt{E_1} + \sqrt{E} \left(\frac{\Delta^2}{4} - \frac{\Delta_1}{\sqrt{3}} \right) . \tag{A.12}$$

From equation (A.12) we get all parameters required in equation (4.26):

$$\mu = \frac{2}{\sqrt{(z_1 - z_3)(z_2 - z_4)}} = \frac{1}{\sqrt{E_0}} \left(1 - \frac{\Delta}{2\sqrt{3}} \right)$$

$$k^2 = \frac{z_3 - z_4}{z_3 - z_1} \cdot \frac{z_2 - z_1}{z_2 - z_4} = 1 - 2 \frac{\Delta}{\sqrt{3}} + \frac{2}{3} \Delta^2$$

$$E\, z_3 - \frac{3}{2} \varepsilon - \frac{2 L^2}{z_3} = E^{3/2} \frac{\Delta}{\sqrt{3}} - \frac{9}{4} \varepsilon \frac{L^2}{E^2} + \frac{3}{4} \frac{\varepsilon^2}{E^3} \frac{\Delta + \Delta_1}{\sqrt{3}}$$

$$E\,(z_2 - z_3) = E^{3/2} \left(\frac{2\Delta}{\sqrt{3}} + 0(\Delta^3) \right)$$

$$2 L^2 \frac{z_3 - z_2}{z_2 z_3} = E^{3/2} \frac{4\Delta}{\sqrt{3}} \left(1 + \frac{3}{8} \frac{\varepsilon^2}{E^3} \right)$$

$$\frac{z_1 - z_2}{z_1 - z_3} \overset{\text{def}}{=} n = 1 - \frac{\Delta}{\sqrt{3}} - \frac{\Delta \Delta_1}{3} + \frac{\Delta^2}{6}$$

$$\frac{z_3}{z_2} \frac{z_1 - z_2}{z_1 - z_3} = - \frac{\Delta - \Delta_1}{\Delta + \Delta_1} (1 + 0(\Delta)) . \tag{A.13}$$

At first, let us expand the complete elliptic integrals of the third kind in equation (4.27). For the first integral, being of the circular case, we get [16]

$$\Pi(n, k) = K(k) + \frac{\pi}{2} \delta_2 [1 - \Lambda_0(\varepsilon, k)] \tag{A.14}$$

where

$$\delta_2 = \sqrt{\frac{n}{(1-n)\,(n-k^2)}} = \frac{\sqrt{3}}{\Delta}\left(1 + \frac{\Delta}{2\sqrt{3}}\right)$$

$$\varepsilon = \text{arc sin}\sqrt{\frac{1-n}{1-k^2}} = \frac{\pi}{4} + \frac{\Delta_1}{2\sqrt{3}} + \frac{\Delta}{4\sqrt{3}}$$

and $\Lambda_0(\varepsilon, k)$ is Heumann's Lambda function. The second one must be transformed according to [17]

$$\Pi(n', k) = a_1\,\Pi(n'', k) + a_2\,K(k) \tag{A.15}$$

with

$$a_1 = -\frac{n'\,(1-k^2)}{(1-n')\,(k^2-n')} = \frac{\Delta^2 - \Delta_1^2}{2\sqrt{3}}\,(1 + 0(\Delta))$$

$$a_2 = \frac{k^2}{k^2 - n} = \frac{\Delta + \Delta_1}{2\Delta}\,(1 + 0(\Delta))$$

$$n'' = \frac{k^2 - n}{1 - n} = 1 - \frac{\Delta + \Delta_1}{\sqrt{3}} > k^2\,.$$

The remaining elliptic integral of the third kind is expanded in the same way as (A.14), giving

$$\Pi(n'', k) = K(k) + \frac{\pi}{2}\,\delta_2'\,[1 - \Lambda_0(\varepsilon', k)]$$

where

$$\delta_2' = \sqrt{\frac{n''}{(1-n'')\,(n''-k^2)}} = \sqrt{\frac{3}{\Delta^2 - \Delta_1^2}} = \frac{E}{L}$$

$$\varepsilon' = \text{arc sin}\sqrt{\frac{1-n''}{1-k^2}} = \text{arc sin}\sqrt{\frac{\Delta + \Delta_1}{2\Delta}}\,.$$

Inserting all this in equation (4.27), taking μ to the left, we get

$$\begin{aligned}\left(n + \frac{1}{2}\right)\pi\sqrt{E_0}\left(1 + \frac{1}{2}\,\frac{\Delta}{\sqrt{3}}\right) &= E^{3/2}\,\frac{\Delta}{\sqrt{3}}\,K(k)\\ &+ E^{3/2}\,\frac{2\Delta}{\sqrt{3}}\left[K(k) + \frac{\pi}{2}\,\frac{\sqrt{3}}{\Delta}\left(1 + \frac{\Delta}{2\sqrt{3}}\right)(1 - \Lambda_0(\varepsilon, k))\right]\\ &- E^{3/2}\,\frac{4\Delta}{\sqrt{3}}\left\{K(k)\,\frac{\Delta + \Delta_1}{2\Delta} + \frac{\Delta^2 - \Delta_1^2}{2\sqrt{3}\,\Delta}\left[K(k) + \frac{\pi}{2}\,\frac{E}{L}\,(1 - \Lambda_0(\varepsilon', k))\right]\right\}.\end{aligned}$$

We collect terms proportional to $E^{3/2}\,\Delta$ or ε:

$$\begin{aligned}\pi\left(1 + \frac{1}{2}\,\frac{\Delta}{\sqrt{3}}\right)\left[\left(n + \frac{1}{2}\right)E_0^{1/2} - (1 - \Lambda_0(\varepsilon, k))\,E^{3/2}\right]\\ = K(k)\,E^{3/2}\,\frac{\Delta - 2\Delta_1}{\sqrt{3}} - \pi\,E^{1/2}\,L\,(1 - \Lambda_0(\varepsilon', k))\,.\end{aligned} \tag{A.15}$$

For Heumann's Lambda function, we use the expansion [18]

$$\Lambda_0(\varepsilon, k) = \frac{2}{\pi}\left[\varepsilon + k'^2\,\frac{1}{2}\left(\log\frac{4}{k'} - \frac{1}{2}\right)\sin\varepsilon\,\cos\varepsilon\right] + \dots$$

where

$$k'^2 = 1 - k^2 = 2 \frac{\Delta}{\sqrt{3}}$$

giving

$$\Lambda_0(\varepsilon, k) = \frac{1}{2} + \frac{1}{\pi} \left(\frac{\Delta_1}{\sqrt{3}} + \frac{\Delta}{2\sqrt{3}} \log \frac{8\sqrt{3}}{\Delta} \right)$$

and

$$\Lambda_0(\varepsilon', k) = \frac{2}{\pi} \varepsilon' = \frac{2}{\pi} \arcsin \sqrt{\frac{\Delta + \Delta_1}{2\Delta}} .$$

The elliptic integral of the first kind has the well known expansion [19]

$$K(k) = \log \frac{4}{k'} = \frac{1}{2} \log \frac{8\sqrt{3}}{\Delta} . \tag{A.16}$$

Using this in equation (A.15), we obtain

$$\pi \left(1 + \frac{1}{2} \frac{\Delta}{\sqrt{3}}\right) \left[\frac{1}{2} E^{3/2} - \left(n + \frac{1}{2}\right) E_0^{1/2}\right] = E^{3/2} \frac{\Delta_1}{\sqrt{3}} \left(1 + \log \frac{8\sqrt{3}}{\Delta}\right) + \pi E^{1/2} L \left(1 - \frac{2}{\pi} \arcsin \sqrt{\frac{\Delta + \Delta_1}{2\Delta}}\right). \tag{A.17}$$

Since the difference in the square brackets on the left hand side is $0(E^{1/2})$, the first bracket can be set = 1. Then after small modifications we arrive at equation (4.29).

The expression (4.34) is readily obtained from (4.33) by means of equation (A.16).

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