

Superradiance: A numerical study

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The full set of Weisskopf-Wigner equations describing the spontaneous radiative decay of a system of up to four excited two-level atoms and many field modes is integrated numerically. Measures of collimation and of photon-photon directional correlation are evaluated and demonstrate the tendency of the photons to form a single ray. Decay rates of the initial state are found to be proportional to the number of atoms, as expected from analytical work.

I. INTRODUCTION

The radiative decay of systems of atoms prepared in various excited states is a fundamental process that has been much studied. The one-atom system was described by Weisskopf and Wigner¹ in their famous paper of 1930. The result is that over the time interval of most interest the atom decays exponentially and the emitted photon has a Lorentzian frequency distribution about the atomic frequency as center. At very short times the probability of finding the system atom-plus-field not in the initial state grows quadratically with time, as required by time-reversal invariance. The angular distribution of the radiation is that typical of dipole radiation. For a $\Delta m = 0$ transition involving only the z component of the atomic dipole moment the intensity $I(\theta) \propto \sin^2\theta$.

Stephen² studied the two-atom case in which one atom is initially excited and the other is in its ground state. If the atoms are close together, this leads to a 50% chance of the radiation being trapped in exchanges between the two atoms. At large separations it leads to two alternative modes of radiation with distinct lifetimes.

Dicke³ studied the N -atom case where the atoms are closely spaced relative to the atomic radiation's wavelength, and introduced the concept of superradiance as the accelerated radiation resulting from the coherent addition of atomic dipole moments. He also considered cases of partial and complete radiation trapping or subradiance. For an extended set of atoms he showed the existence of directional correlations between emitted photons. Ernst and Stehle⁴ applied the original Weisskopf-Wigner approach to a system of N atoms distributed with uniform density but without positional correlations over the volume of an ellipsoid. The Weisskopf-Wigner equations here become very complicated and numerous, so that a solution as good as Weisskopf and Wigner's for the one-atom system cannot be obtained analytically. An ansatz for the form of the desired amplitudes could be shown to satisfy the equations in a combinatorial sense, e.g., in the sense that $n! \approx n^n$, or perhaps even $n! \approx (n/e)^n$, but no better than this.

The results of this analysis showed two striking effects: (i) The lifetime of the system is shorter than that of independently decaying atoms, but the spectrum is narrower. (The final state is an N -photon state so this does

not contradict the uncertainty principle.) (ii) The emitted photons are strongly correlated in direction also, forming a diffraction-limited ray, the diffraction pattern corresponding to an aperture with the shape of the ellipsoid cross section perpendicular to the direction of the ray, most probably along the longest axis of the ellipsoid. These results are very similar to those of Rehler and Eberly⁵ obtained later using a much simpler semiclassical model which, however, required an initial prod to radiate, as a system of atoms all in their excited state has no electric dipole moment to act as a source of a classical field. Other aspects of this problem have been studied, for example Watson *et al.*⁶ and by MacGillivray and Feld.⁷ Watson *et al.* used the three-dimensional coupled semiclassical Maxwell-Bloch equations, simulating the spontaneous initiation of the superfluorescent pulse by a randomly chosen initial polarization of the inverted medium, and reached a good agreement with experiments. The treatment of the pulse initiation is, however, somewhat *ad hoc*. In the present treatment the entire course of the evolution of the state of the system is done completely quantum mechanically using the Weisskopf-Wigner method.

Experiments were done to see if these predicted effects could be observed in the laboratory. Vehrens, Hickspoor, and Gibbs⁸ studied the superradiance of cesium vapor. They found accelerated emissions and considerable collimation of the radiation, but they always observed radiation from both ends of a pencil-shaped volume, and these rays were not diffraction limited, but more or less filled the geometric opening angle as seen from the center of the volume.

The situation concerning superradiance being so ambiguous, it seems worthwhile to exploit the possibility of obtaining numerical solutions of the Weisskopf-Wigner equations for systems as large as the available computing resources will allow. The limiting factor is the large numbers of field states needed to show any photon-photon correlations that do develop. If n_k modes are used, and if states containing N photons must be included, as is the case if the initial state contains N excited atoms, then there are $\binom{n_k + N - 1}{N}$ states of the field. Initially and finally the atomic state is unique, but if N_g atoms are in the ground state and N_g photons are therefore present, there are $\binom{N}{N_g}$ atomic states for each field state. For example, with five frequencies in each of 328 directions, there are

1640 modes, and the total number of states included in the Weisskopf-Wigner calculation for two atoms is 1 348 901. For the two-atom system the analytical solution for large times is obtainable, and the numerical solution can be compared with it. This is done below, and the two are seen to be in good agreement.

For four atoms it is clearly impossible to use as many modes of the field, as the combinations lead to enormous numbers of states. The restriction to three frequency bins helps, but the number of directions must also be reduced. Work on the four-atom system is described in Sec. IV.

II. A NUMERICAL APPROACH TO QUANTUM-MECHANICAL TIME EVOLUTION

In many complex systems the accurate computation of the quantum-mechanical time-evolution operator e^{-iHt} (or, in the interaction picture, $T \exp[-i \int H_I^{\text{int}}(t) dt]$) is of crucial importance. In such systems, one typically must deal with a state space of high dimension, and direct diagonalization of the Hamiltonian is impractical. In the superradiance problems discussed in this paper, for example, the combined atomic-radiation-field state space has a dimensionality between 1×10^6 and 2×10^6 .

We have chosen instead an approach that makes maximal use of the properties of vector machines with large quantities of fast memory (such as the CRAY-XMP). The only operations performed correspond to matrix multiplication on a large state vector, which is a completely vectorizable procedure.

For a system of N two-states atoms interacting with the radiation field in Weisskopf-Wigner approximation, the interaction Hamiltonian may be written

$$H_I^{\text{int}}(t) = g \sum_{j,k} (b_j a_k^\dagger e^{i\mathbf{k} \cdot \mathbf{R}_j} e^{i(\omega - \omega_0)t} + \text{H.c.}) . \quad (2.1)$$

In (2.1), g is a coupling constant, essentially the dipole strength, with dimensions of energy. The exact dipole coupling contains the angular dependence resulting from the scalar product $\mathbf{E} \cdot \mathbf{d}$, but for the purposes of this work this dependence is suppressed. b_j is the deexcitation operator for atom j , a_k^\dagger the creation operator for a photon of momentum \mathbf{k} , \mathbf{R}_j the location of the j th atom, ω the frequency ($= |\mathbf{k}|$) of the emitted photon, and ω_0 the energy difference between the two atomic states ($\hbar=1$ throughout).

The state space is a direct product of atomic states with multiphoton states. We imagine the system contained in a box of finite volume V so that the photon momenta \mathbf{k} are discrete. In practice, we take n_k modes consisting of n_ω frequency bins and n_k/n_ω directions (more on angular coverage below). Thus there are Nn_k single-photon states, $[N(N-1)/2]n_k(n_k+1)/2$ two-photon states, etc. The total dimensionality is

$$D(N, n_k) = \sum_{r=0}^N \binom{N}{r} \binom{n_k + r - 1}{r} . \quad (2.2)$$

For example, for a two-atom system with 1640 photon modes, $D=1\,348\,901$, while for a four-atom system with

72 photon modes, $D=1\,490\,803$.

The calculation of the time evolution proceeds as follows. The time-evolution operator (in interaction picture) for the desired finite interval is broken up into a large number of small time steps

$$T \left[\exp \left[-i \int_0^t H_I^{\text{int}}(t') dt' \right] \right] = \prod_{i=1}^M \exp[-iH_I^{\text{int}}(t_i)\Delta t] , \quad (2.3)$$

where $M\Delta t = t$.

Then we approximate each unitary operator in the product by a truncation of the exponential expansion, expressed as a factorized product of linear terms

$$\begin{aligned} e^{-iH_I^{\text{int}}(t_i)\Delta t} &\simeq \sum_{m=1}^p \frac{1}{m!} \{[-iH_I^{\text{int}}(t_i)\Delta t]\}^m \\ &= [1 + \alpha_1 H_I^{\text{int}}(t_i)] [1 + \alpha_2 H_I^{\text{int}}(t_i)] \\ &\quad \times [1 + \alpha_p H_I^{\text{int}}(t_i)] . \end{aligned} \quad (2.4)$$

For example, for $p=2$, one takes $\alpha_1 = -i\Delta t(1+i)/2$, $\alpha_2 = -i\Delta t(1-i)/2$, and in general the expansion of the series of p complex time evolutions is equivalent to a single real-time evolution with a loss of unitarity at the H^{p+1} level. The advantage of the form (2.4) is simply that linear operations involving (2.1) are readily expressed in fully vectorized code. We have used (2.4) with $p \leq 6$ in the two-atom case to check that unitarity is indeed preserved to one part in 10^9 over the full evolution of the state. For the four-atom case, we have taken only the linear approximation ($p=1$) because it permits much more efficient use of the memory available (in this case, we do not need to keep a copy of the old state vector while forming the new one). This results in a loss of unitarity (over the whole time evolution) on the order of a few percent for the time interval used.

As a check on the numerical results, we note here some simple analytical features of the time-evolution generated by (2.1), in the one-atom case. For small time t , the probability of the one-photon state increases quadratically with time as $g^2 n_k t^2$ — or equivalently, the initial state (with the atom “up” and no photons present) decays as $1 - g^2 n_k t^2$. For somewhat larger times, the Fermi golden rule gives an exponential decay $e^{-\Gamma t}$ for the initial state with

$$\Gamma = 2\pi g^2 \frac{dn}{dk} . \quad (2.5)$$

For a discrete set of n_k momentum modes distributed over n_ω frequency bins of width $\Delta\omega$, $dn/dk \simeq n_k / (n_\omega \Delta\omega)$. We have checked that the discretization does not do violence to the physics by varying g, n_k, n_ω while keeping Γ fixed (see below).

III. ONE AND TWO ATOMS

For one- and two-atom systems good analytic solutions exist. Comparison of the numerical results with the ana-

lytic ones provides a check on the algorithm and the code, and further validates the discrete mode structure of the field used in the code.

The one-atom case leads to results shown in Fig. 1. Here the probability of finding the atom excited at time t when it was prepared at time 0 in its excited state shows the expected features; it begins to decrease quadratically, then decreases exponentially. The deviations for large times are caused by the discrete mode structure. There is a nonzero minimum difference between adjacent frequencies so for times greater than $1/\Delta\omega$ oscillations will appear. Only when $\Delta\omega \rightarrow 0$ does the emission become irreversible. The value of g_0 used is 0.345 (in these units). Thus according to Weisskopf-Wigner theory, $\Gamma = 2\pi(0.345)^2 = 0.75$. Fitting the third through the eleventh points plotted in Fig. 1 for the one-atom case to the best straight line, a value of $\Gamma = 0.79$ is obtained. These are close enough to indicate the one-atom mode structure is adequate. Doing the same for the four-atom system yields a value $\Gamma(4) = 2.92 = 4 \times 0.73$, another good check on the overall time evolution.

The decay of the initial state of a two-atom system is shown in Fig. 1 with two different mode structures. One structure has 7 frequency bins and 248 solid angle cells; the other has 5 frequency bins and 248 solid angle cells. The coupling strength g is adjusted as described in Sec. II. This should keep the rate of decay of the initial state the same in the two situations, and the figure shows that it does. Again there is a quadratic time dependence at the start changing to an exponential decay. The rate of this latter is twice that for the one-atom case, there now being twice as many ways for the system to leave the initial state. The four-atom case is plotted also. The rate of decay of the initial state is now very nearly 4 times that of the one-atom system. The rate of decay of the various

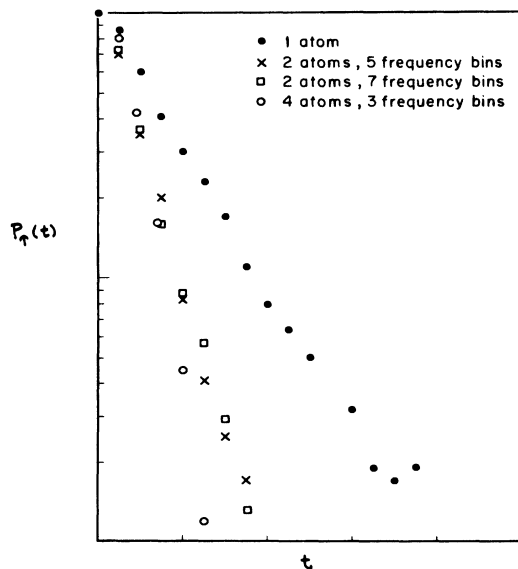


FIG. 1. Initial state decay for (a) one-atom system, (b) two-atoms (5 frequency bins), (c) two-atoms (7 frequency bins), (d) four-atoms.

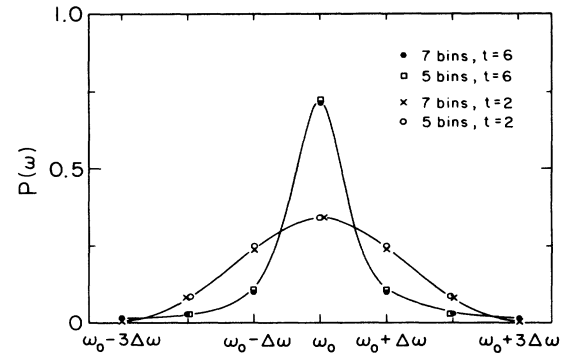


FIG. 2. Photon line shape (two atoms, 5 and 7 frequency bins).

systems thus scales properly with the number of atoms, and is independent of the mode structure used provided that g , the coupling of the atoms to each mode, is scaled with the number of modes so that $g^2 n_k$ is kept unchanged.

The time development of the frequency distribution of the photons emitted by the two-atom system is shown in Fig. 2. The calculations are done using mode structures including 5 frequency bins or 7 frequency bins. The narrowing of the line with increasing time is evident. The shape of the line does not depend noticeably on the number of bins aside from the missing wings in the 5-bin case where the extreme bins have been excluded as possible modes. The area under the curve thus excluded appears as a very slight increase in the height of the central portion.

Figure 3 shows the time dependence of the probabilities of finding 0, 1, or 2 photons in the two-atom system. The complication in the shapes of the curves at large times is due, as discussed above, to the discrete mode structure which prevents the emission from being truly irreversible.

The state of the two-atom system at large times contains two photons. If the atoms radiated independently, these two photons would not be correlated in direction or in frequency. The atoms are, however, coupled to the same radiation field, and the time evolution of the system includes processes in which a photon emitted by one atom is absorbed by the other. This produces a correlation be-

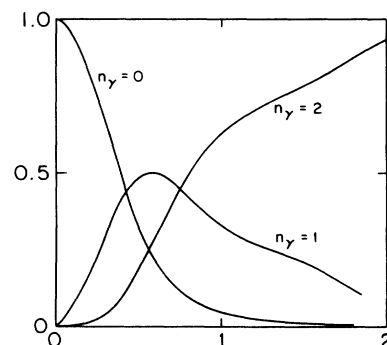


FIG. 3. Photon multiplicities vs time (two atoms).

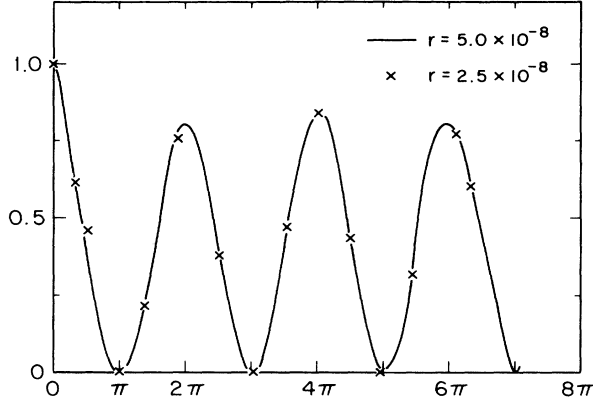


FIG. 4. Angular correlation $\langle (\mathbf{k}_1 - \mathbf{k}_2)(\mathbf{R}_1 - \mathbf{R}_2) \rangle$ for the two-photon final state.

tween the two photons relative to the independent emission by the two atoms which is shown in Ref. 1 to have the form

$$R(\mathbf{k}_1, \mathbf{k}_2) = 1 + \cos[(\mathbf{k}_1 - \mathbf{k}_2)(\mathbf{R}_1 - \mathbf{R}_2)] \quad (3.1)$$

to good accuracy in the cases studied here. To extract this correlation from the numerical results, the following procedure is used.

(a) The difference of the \mathbf{k} 's in the same solid angle cell but in distinct frequency bins is ignored.

(b) For given $\mathbf{R}_1 - \mathbf{R}_2 = D\hat{z}$ taken along the z axis, the range of values of $(\mathbf{k}_1 - \mathbf{k}_2)(\mathbf{R}_1 - \mathbf{R}_2) = (k_{1z} - k_{2z})D$ extending from 0 to $2kD$ is divided into bins, and the number of possible final states given the value of D and the chosen mode structure corresponding to each bin is found. Many bins contain no final states.

(c) The sum of the probabilities of the final states lying within each occupied bin is found and divided by the number of such states. This gives the ratio $R(\mathbf{k}_1, \mathbf{k}_2)$ aside from an overall normalization which is chosen to make it unity at $\mathbf{k}_1 = \mathbf{k}_2$.

The result of this procedure is shown in Fig. 4 for two values of D . The abscissa is the argument of the cosine. The range of the curves depends on the value of kD . The whole range of the curve for the greater separation is not shown.

The comparison of results obtained analytically and numerically gives confidence in the method of numerical computation. There is good reason, therefore, to believe the results obtained in more complicated cases where the analytical solution is not available.

IV. FOUR ATOMS

Four atoms can be arranged in many ways. Here essentially linear arrangements are considered as these are expected to radiate primarily along their axis. Because four-photon states occur, of which there are many more per mode than there are two-photon states, it is necessary to reduce the number of modes drastically in order to be able to follow the time evolution of the system. It was

seen above that a reduction from 7 to 5 frequency bins had little effect on the calculated results. For the four-atom system the number of frequency bins is further reduced to 3. The number of solid angle cells is also reduced. Instead of distributing these modes uniformly over the sphere, they are confined to polar caps around the axis, and are distributed uniformly within these caps. This can have the effect of causing the expected axial radiation pattern, but it will be seen that measures can be devised to detect photon-photon correlations which are independent of this mode structure. Note that the mode structure is symmetric on reflection in the origin so that no directionality along a line is built in.

The solid angle cells are specified by unit vectors. For each polar cap there is one along the axis. If there are n_1 in a ring of polar angle θ_1 , n_2 in a ring of polar angle θ_2 , etc., then these numbers are chosen so that

$$\frac{1 - \cos\theta_i}{1 + n_1 + \cdots + n_i} = \frac{1 - \cos\theta_1}{1 + n_1} \quad (4.1)$$

The azimuths in each ring are equally spaced. For most of the calculations reported here, $n_1 = 4$, $n_2 = 7$, and $\theta_1 = \tan^{-1}0.2 = 11.3^\circ$. There are 12 cells per cap, 3 frequency bins per cell, for a total of 72 modes. This leads to 1 490 803 states to be included in the Weisskopf-Wigner approximation.

To extract useful information from the large number of amplitudes, several quantities are defined and calculated every tenth time interval. They are the following.

(a) The total probability of finding the system in some state, a check on unitarity.

(b) The total probability of finding 0, 1, 2, 3, or 4 photons present.

(c) The unijet J , a measure of the presence of a ray in the emitted radiation. $J(1111)$ is defined as the expectation value of the square of the total momentum in states where no two photons are in the same mode, in units of ω_0^2 . $J(211)$, $J(31)$ are defined analogously where two or three photons are in the same mode. $J(4)$ is identically unity. This value is to be compared with the correspond-

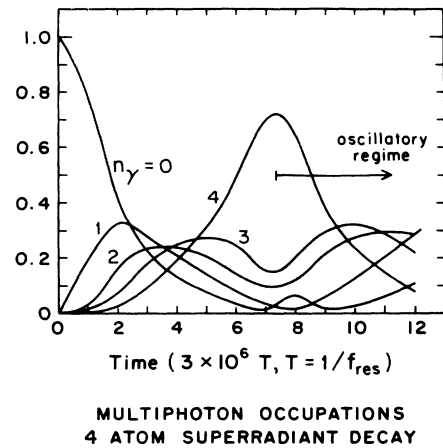


FIG. 5. Photon multiplicities vs time (four atoms).

TABLE I. Atomic coordinates ($\lambda_0=2\pi/\omega_0=3$).

Case	x's	y's	z's	$c(1111)$	$J(1111)$
A	0,0,0	0,0,0	15,-5,5,15	0.934	0.757
B	0,0,0	0,0,0	-15,-7,7,15	0.937	0.582
C	0,0,0	0,0,0	-15,-3.5,3.5,15	0.924	0.433
D	0,0,0	0,0,0	-15,-3.5,6.5,15	0.924	0.387
E	0,0,0	0,2.5,-2.5,0	-15,-3.5,6.5,15	0.931	0.356
F	0,0,0	0,2.5,2.5,0	-15,-3.5,6.5,15	0.928	0.373

ing values J_I calculated for independently emitted photons, equally likely to be in any mode, $J_I(1111) = [1 - 3/(n_k - 1)]/4$.

(d) The collimation value C , a measure of the concentration of the emission along the axis of the atomic distribution. It is the sum of the squares of the axial components of the photon momenta, $C(1111)$ when all photons are in distinct modes, $C(211)$ when two are in the same mode, etc., measured in units of ω_0^2 . Its values are compared with the corresponding values for independent emission.

The results of the computation in the four-atom case can be summarized as follows.

(1) The rate of decay of the initial state is very nearly 4Γ where Γ is the single atom rate, despite the drastic change in the mode structure.

(2) The multiphoton state probabilities behave as expected up to a time of order $2\pi/\Delta\omega$, when oscillatory behavior sets in due to the discreteness of the modes (see Fig. 5).

(3) There is an unambiguous tendency for the emitted photons to go in a common direction. The value of the unijet J depends in as yet obscure ways on the details of the atomic locations and the mode, but is always greater than that given by statistically distributed photons. This tendency is established very early in the time evolution and remains essentially unchanged throughout.

Table I lists six sets of atomic positions. The first four are all on a line; the last two include transverse displacements. In Table I, we show the measured values for the collimation and unijet parameters $C(1111)$ and $J(1111)$

for the four (distinct) photon state after 10 time steps (these quantities change very little in the subsequent evolution). The statistically expected values for $C(1111)$ and $J(1111)$, obtained by assigning equal *a priori* probabilities to each available final state, are 0.9391 and 0.2395, respectively. The unijet parameter is in each case larger (sometimes substantially) than the statistical value, indicating a tendency for the photons to emerge on the same side. The collimation parameter $C(1111)$, ranges from 0.9237 to 0.9368, all values close to, but slightly smaller than, the statistical value 0.9391 (this is necessarily close to one because the modes included are at most 0.3-radians polar angle). Similar results are obtained for the other collimation and unijet parameters $C(211)$, $J(211)$, etc.

In conclusion, our preliminary results show a strong tendency for one-sided emission at the four-atom level when the atoms are coupled to photon modes in polar caps aligned with the atoms, but no strong evidence for tight collimation of the outgoing jet. It remains to be seen how these results are modified by the inclusion of more atoms and/or more photon modes. The large SSD memory (128 MW) available on the Pittsburgh CRAY-XMP will allow a factor of 50 increase in dimensionality of the state space over the situations described here. Thus we shall be able to examine five-atom systems ($n_k \leq 72$) or four-atom systems (with n_k up to ~ 150). Another issue which will be explored more fully is the question of sensitivity to the initial state—in particular, to the presence of photons and/or unexcited atoms at $t=0$. Work along these lines is in progress.

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