Eur. Phys. J. D **23**, 279–284 (2003)
DOI: 10.1140/epjd/e2003-00033-9

THE EUROPEAN PHYSICAL JOURNAL D

Spontaneous emission of an excited two-level atom without both rotating-wave and Markovian approximation

C.-Q. Cao[1,a], C.-G. Yu[1], and H. Cao[2]

[1] Department of Physics, Peking University, Beijing 100871, P.R. China
[2] Department of Physics and Astronomy, Northwestern University, Evanston, IL 60208-3112, USA

Received 10 July 2002 / Received in final form 12 November 2002
Published online 4 February 2003 –

Abstract. The spontaneous emission of an excited atom is analyzed by quantum stochastic trajectory approach without both rotating-wave approximation and Markovian approximation. The atom finite size effect is also taken into account. We show by an example that the correction due to the counter-rotating wave term is rather small, even for the largest atomic number of real nuclei.

PACS. 42.50.Ct Quantum description of interaction of light and matter; related experiments – 42.50.Lc Quantum fluctuations, quantum noise, and quantum jumps

1 Introduction

The spontaneous emission of an excited atom is an old question of quantum theory. The first important progress in this respect is the proposition and evaluation of the Einstein A coefficient γ_A, which gives the spontaneous emission rate. It is well known that γ_A is proportional to d^2, where d denotes the electric-dipole transition moment. The next important progress is the formulation of Weisskopf-Wigner theory. It takes γ_A as the percentage decay rate of the upper-level population N_2 during the whole emission process, leading to an exponential decay of N_2 and consequently a Lorentzian line profile in the atomic spectrum. This treatment actually contains two approximations. One is the neglect of the finite size effect on the electric-dipole transition along with the omission of the contribution from all possible higher multipole transitions, caused by the replacement of the plane wave factor $e^{i\mathbf{k}\cdot\mathbf{x}}$ by 1 in the transition matrix element evaluation. Another is the so-called Markovian approximation on the reduced equations of the atomic variables derived by eliminating the photon variables. They are differential-integral equations with correlation functions to denote the memory effect. The Markovian approximation neglects this memory effect and hence changes them to simple differential equations.

The Weisskopf-Wigner theory applies well for the emission of outer-shell electron or inner-shell electron of light nuclei. But in the case of inner-shell electron emission of heavy nuclei, it may lead to obvious deviation, since (1) ω_0 is proportional to Z_{eff}^2 (where $Z_{\text{eff}}e$ is the charge of the atomic core felt by the emitting electron), and the radius a of the electron cloud is proportional to $1/Z_{\text{eff}}$, leading to a linear increase of $k_0 a = \omega_0 a/c$ with Z_{eff}. This makes the pointlike electric-dipole approximation (neglecting the factor $e^{i\mathbf{k}\cdot\mathbf{x}}$ in the integral) poorer for large Z_{eff}. (2) During the emission process, the frequency of the emitted photon does not need to be ω_0 (such photon is the so-called virtual photon) and the finite size correction will become larger for large ω. As to the Markov approximation, in the usual estimation, the characteristic correlation time is of order $2\pi/\omega_0$, while the decay time of the atomic variable is of order $1/\gamma_A$. Hence, the validity of the Markovian approximation requires $2\pi/\omega_0$ much smaller than $1/\gamma_A$, namely $2\pi\gamma_A/\omega_0 \ll 1$. It can be shown that γ_A/ω_0 increases as Z_{eff}^2, hence large Z_{eff} disadvantages the Markovian approximation.

Later on, some people considered the correction to the Weisskopf-Wigner theory [1–4]. But, as far as we know, all of them applied the Laplace transform to solve the resultant differential-integral equation, and various kinds of approximations were used in the inverse transform. Some papers even take the radiating atom as a pointlike electric dipole, so that the corresponding correlation spectrum diverges linearly with ω, and in the subsequent treatment an artificial cutoff of frequency is needed. Besides, majority of them only considers the case of $Z = 1$.

In a preceding paper [5], two of us with other coworkers restudied this problem by a totally different approach. The stochastic quantum trajectory formulation [6] is applied for this investigation, and the non-Markovian correction to the decay of upper-level population is taken into account by introduction of additional fictitious oscillators [7,8]. However, the counter-rotating wave interaction is still not taken into account. Now we will release this limitation to include the counter-rotating wave term in the interaction, since its effect also becomes larger for stronger coupling [9]. In this case there are two correlation

[a] e-mail: cqcao@pku.edu.cn

spectra, hence more fictitious oscillators are needed to simulate them. Moreover, in the case of the rotating-wave approximation, the total quanta of the fictitious oscillators is either one or zero, while the counter-rotating wave interaction puts no limitation on the quanta numbers. Both of these will increase the amount of numerical calculation.

In Section 2 the relevant differential-integral equation for the atom operators is given, with the two correlation spectra explicitly derived. The same hydrogen-like example as that of reference [5] is numerically studied for comparison. In Section 3 the quantum stochastic trajectory analysis [6] of the enlarged system [7,8] is carried out to give the time decay of the upper-level population. We see by this example that the correction due to counter-rotating wave term is rather small (except the end stage of decay) even for the largest atomic number Z of hydrogen-like atom, as conjectured by the usual estimation.

2 The spectra of correlation functions for spontaneous emission of a two-level atom

The $\mathbf{A}\cdot\mathbf{P}$ type $\hat{H}_{\rm int}$ for the spontaneous emission of a two-level atom is known as

$$\hat{H}_{\rm int}(t)=\mathrm{i}\hbar\sum_{\mathbf{k},j}\Big[g_{\mathbf{k}j}\hat{\sigma}_+(t)\hat{a}_{\mathbf{k}j}(t)-g^*_{\mathbf{k}j}\hat{\sigma}_-(t)\hat{a}^\dagger_{\mathbf{k}j}(t)+\bar{g}_{\mathbf{k}j}\hat{\sigma}_+(t)\hat{a^\dagger}_{\mathbf{k}j}(t)-\bar{g}^*_{\mathbf{k}j}\hat{\sigma}_-(t)\hat{a}_{\mathbf{k}j}(t)\Big] \quad (1)$$

with counter-rotating wave terms included, where $\hat{a}_{\mathbf{k}j}$ ($\hat{a}^\dagger_{\mathbf{k}j}$) is the photon annihilation (creation) operator of mode $(\mathbf{k},j)$, $\hat{\sigma}_\pm$ are atom-level change operators ($\hat{\sigma}_+$ corresponds to upward change and $\hat{\sigma}_-$ downward change), $g_{\mathbf{k}j}$ and $\bar{g}_{\mathbf{k}j}$ are coupling constants for rotating-wave term and counter-rotating wave term respectively,

$$g_{\mathbf{k}j}=-\frac{e}{m}\sqrt{\frac{2\pi\hbar}{Vkc}}\boldsymbol{\varepsilon}_{\mathbf{k}j}\cdot\mathbf{G}_{\mathbf{k}}, \quad (2a)$$

$$\mathbf{G}_{\mathbf{k}}=\int \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\Psi_2^\dagger(\mathbf{x})\nabla\Psi_1(\mathbf{x})\mathrm{d}^3\mathbf{x},$$

$$\bar{g}_{\mathbf{k}j}=-\frac{e}{m}\sqrt{\frac{2\pi\hbar}{Vkc}}\boldsymbol{\varepsilon}_{\mathbf{k}j}\cdot\bar{\mathbf{G}}_{\mathbf{k}}, \quad (2b)$$

$$\bar{\mathbf{G}}_{\mathbf{k}}=\int \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\Psi_2^\dagger(\mathbf{x})\nabla\Psi_1(\mathbf{x})\mathrm{d}^3\mathbf{x}$$

in which $\boldsymbol{\varepsilon}_{\mathbf{k}j}$ is the polarization vector of photon mode $(\mathbf{k},j)$, $\Psi_2(\mathbf{x})$ and $\Psi_1(\mathbf{x})$ are the upper level and lower level wave function respectively. They are two-component spinor functions. It is seen from equation (2) that when $\Psi_2(\mathbf{x})$ and $\Psi_1(\mathbf{x})$ have the same parity, $\bar{\mathbf{G}}_{\mathbf{k}}=-\mathbf{G}_{\mathbf{k}}$; when $\Psi_2(\mathbf{x})$ and $\Psi_1(\mathbf{x})$ have the opposite parity, $\bar{\mathbf{G}}_{\mathbf{k}}=\mathbf{G}_{\mathbf{k}}$; and similar relations for $g_{\mathbf{k}j}$ and $\bar{g}_{\mathbf{k}j}$.

The dynamical equations for both atom and photon operators are readily deduced from $\hat{H}_{\rm int}$. Eliminate the operators $\hat{a}_{\mathbf{k}j}$ and $\hat{a^\dagger}_{\mathbf{k}j}$by taking the electromagnetic (e.m.) field as reservoir, the resultant differential-integral equations are given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\sigma}_-(t)=\int_0^t[u_1(t-t')-\bar{u}_1(t-t')]\hat{\sigma}_3(t)\hat{\sigma}_-(t')\mathrm{d}t'+\mathrm{e}^{2\mathrm{i}\omega_0 t}\int_0^t[u_2(t-t')-\bar{u}_2(t-t')]\hat{\sigma}_3(t)\hat{\sigma}_+(t')\mathrm{d}t'-\hat{\sigma}_3(t)\left[\hat{\Sigma}_1(t)+\hat{\Sigma}_2^\dagger(t)\right] \quad (3a)$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\sigma}_3(t)=-2\int_0^t[u_1(t-t')-\bar{u}_1(t-t')]\hat{\sigma}_+(t)\hat{\sigma}_-(t')\mathrm{d}t'-\mathrm{e}^{2\mathrm{i}\omega_0 t}\int_0^t[u_2(t-t')-\bar{u}_2(t-t')]\hat{\sigma}_+(t)\hat{\sigma}_+(t')\mathrm{d}t'+2\hat{\sigma}_+(t)\left[\hat{\Sigma}_1(t)+\hat{\Sigma}_2^\dagger(t)\right]+\mathrm{h.c.} \quad (3b)$$

where $\hat{\sigma}_3$ is the atom population-difference operator and $\hat{\Sigma}_j(t)$'s are fluctuation operators defined in equation (5). There are totally four correlation functions in the above differential-integral equations:

$$u_1(t-t')=\sum_{\mathbf{k}j}|g_{\mathbf{k}j}|^2\mathrm{e}^{-\mathrm{i}(\omega-\omega_0)(t-t')}\equiv\int_0^\infty R_1(\omega)\mathrm{e}^{-\mathrm{i}(\omega-\omega_0)(t-t')}\mathrm{d}\omega, \quad (4a)$$

$$\bar{u}_1(t-t')=\sum_{\mathbf{k}j}|\bar{g}_{\mathbf{k}j}|^2\mathrm{e}^{\mathrm{i}(\omega+\omega_0)(t-t')}\equiv\int_0^\infty R_1(\omega)\mathrm{e}^{\mathrm{i}(\omega+\omega_0)(t-t')}\mathrm{d}\omega, \quad (4b)$$

$$u_2(t-t')=\sum_{\mathbf{k}j}g_{\mathbf{k}j}\bar{g}_{\mathbf{k}j}\mathrm{e}^{\mathrm{i}(\omega-\omega_0)(t-t')}\equiv\int_0^\infty R_2(\omega)\mathrm{e}^{\mathrm{i}(\omega-\omega_0)(t-t')}\mathrm{d}\omega, \quad (4c)$$

$$\bar{u}_2(t-t')=\sum_{\mathbf{k}j}g_{\mathbf{k}j}\bar{g}_{\mathbf{k}j}\mathrm{e}^{-\mathrm{i}(\omega+\omega_0)(t-t')}\equiv\int_0^\infty R_2(\omega)\mathrm{e}^{-\mathrm{i}(\omega+\omega_0)(t-t')}\mathrm{d}\omega, \quad (4d)$$

since $|g_{\mathbf{k}j}|^2=|\bar{g}_{\mathbf{k}j}|^2$. The correlation spectrum $R_1(\omega)$ is expressed by

$$R_1(\omega)=\frac{V}{(2\pi)^3}\frac{\omega^2}{c^3}\int\mathrm{d}\Omega_k\sum_j|g_{\mathbf{k}j}|^2=\frac{\mathrm{e}^2\hbar\omega}{4\pi^2m^2c^3}\int\mathrm{d}\Omega_k\left[|G_{\mathbf{k}}|^2-|\mathbf{n}_{\mathbf{k}}\cdot\mathbf{G}_{\mathbf{k}}|^2\right]. \quad (4e)$$

Similar expression for $R_2(\omega)$ can be written out directly. The $\mathbf{n}_{\mathbf{k}}$ in equation (4e) is the unit vector in the direction of $\mathbf{k}$. We see that there are two spectral functions $R_1(\omega)$ and $R_2(\omega)$, not just only one spectral function as in the references [1–5].

The two quantum fluctuation forces are expressed by

$$\hat{\Sigma}_1(t) = \sum_{\mathbf{k}j} g_{\mathbf{k}j}\hat{a}_{\mathbf{k}j}(0)\mathrm{e}^{-\mathrm{i}(\omega-\omega_0)t}, \tag{5a}$$

$$\hat{\Sigma}_2^\dagger(t) = \sum_{\mathbf{k}j} \bar{g}_{\mathbf{k}j}\hat{a}_{\mathbf{k}j}^\dagger(0)\mathrm{e}^{\mathrm{i}(\omega+\omega_0)t}. \tag{5b}$$

As a first step we calculate the coupling constant $\bar{\mathbf{G}}_\mathbf{k}$ and $\mathbf{G}_\mathbf{k}$. For simplicity, we omit the spin of the electron. Substituting the wave function of hydrogen-like atom

$$\Psi_1(\mathbf{x}) = f_1(r)Y_{l_1m_1}(\theta\ \varphi),\ \ \Psi_2(\mathbf{x}) = f_2(r)Y_{l_2m_2}(\theta\ \varphi) \tag{6}$$

and also the expansion formula of plane wave by spherical waves into equation (2a) and making use of the formula of $\nabla\Psi_1(\mathbf{x})$, one gets $\mathbf{G}_\mathbf{k}$ as in [5]

$$\begin{aligned}\mathbf{G}_\mathbf{k} = (-1)^{m_2}&\sqrt{\frac{4\pi(2l_2+1)}{2l_1+1}}\sum_{lm\mu}\frac{\mathrm{i}^l}{\sqrt{2l+1}}Y_{lm}(\theta_k\varphi_k)\\ &\times[-\sqrt{(l_1+1)(2l_1+3)}\{A_l(\omega)-l_1B_l(\omega)\}\\ &\times C(l_1+1,1,l_1;m_1-\mu,\mu,m_1)\\ &\times C(l_1+1,l_2,l;m_1-\mu,-m_2,m)\\ &\times C(l_1+1,l_2,l;0,0,0)+\sqrt{l_1(2l_1-1)}\{A_l(\omega)\\ &+(l_1+1)B_l(\omega)\}C(l_1-1,1,l_1;m_1-\mu,\mu,m_1)\\ &\times C(l_1-1,l_2,l;m_1-\mu,-m_2,m)\\ &\times C(l_1-1,l_2,l;0,0,0)]\mathbf{n}_\mu\end{aligned} \tag{7}$$

in which $C(l_1+1,1,l_1;m_1-\mu,\mu,m_1)$ etc are Clebasch-Gordan coefficients, $\mathbf{n}_\mu(\mu=+1,0,-1)$ are spherical bases,

$$\begin{aligned}\mathbf{n}_{+1} &= \frac{1}{\sqrt{2}}(\mathbf{n}_1+\mathrm{i}\mathbf{n}_2),\\ \mathbf{n}_0 &= \mathbf{n}_3,\\ \mathbf{n}_{-1} &= \frac{1}{\sqrt{2}}(\mathbf{n}_1-\mathrm{i}\mathbf{n}_2)\end{aligned} \tag{8}$$

and

$$A_l(\omega) = \int_0^\infty r^2 j_l\left(\frac{\omega}{c}r\right)f_2(r)\frac{\mathrm{d}f_1(r)}{\mathrm{d}r}\mathrm{d}r, \tag{9a}$$

$$B_l(\omega) = \int_0^\infty r j_l\left(\frac{\omega}{c}r\right)f_2(r)f_1(r)\mathrm{d}r. \tag{9b}$$

The summation in equation (7) actually contains only finite terms because of the angular momentum addition rule. For the first term in the square brackets, l is restricted in the range $|l_2-l_1-1|\le l\le l_2+l_1+1$, and for the second term, in the range $|l_2-l_1+1|\le l\le l_2+l_1-1$.

The $\bar{\mathbf{G}}_\mathbf{k}$ can be obtained from equation (7) simply by the substitution

$$Y_{lm}(\theta_k\varphi_k)\to(-1)^lY_{lm}(\theta_k\varphi_k). \tag{10}$$

Substituting $\mathbf{G}_\mathbf{k}$ and the formula

$$\mathbf{n}_\mathbf{k} = \sqrt{\frac{4\pi}{3}}\sum_{\mu=-1}^{\mu=1}Y_{1\mu}(\theta_k\varphi_k)\mathbf{n}_\mu^* \tag{11}$$

into equation (4e) and carrying out the integration over θ_k and φ_k, one will obtain the first spectral function $R_1(\omega)$. The spectrum $R_2(\omega)$ can be calculated similarly.

To see explicitly these spectral functions, we consider the same example of hydrogen-like atom studied in reference [5]: $\Psi_1(\mathbf{x})$ and $\Psi_2(\mathbf{x})$ carry quantum numbers $(n_1=1,l_1=0)$ and $(n_2=2,l_2=1,m_2=1)$ respectively with the expression

$$\Psi_1(\mathbf{x}) = \frac{1}{\sqrt{4\pi}}N_1\mathrm{e}^{-r/a_1},\qquad N_1=\sqrt{\frac{4}{a_1^3}}, \tag{12}$$

$$\Psi_2(\mathbf{x}) = N_2r\mathrm{e}^{-r/a_2}Y_{11}(\theta\ \varphi),\quad N_2=\sqrt{\frac{4}{3a_2^5}}. \tag{13}$$

In this simple case, the gradient of $\Psi_1(\mathbf{x})$ may be evaluated directly. Substituting it into equation (2a) and carrying out the angular integration, one obtains [5]

$$\begin{aligned}\mathbf{G}_\mathbf{k} = \sqrt{\frac{4\pi}{3}}\frac{N_1N_2}{a_1}\Bigg[&X_0(\omega)Y_{00}(\theta_k\varphi_k)\mathbf{n}_{-1}\\ &+X_2(\omega)\left(\sqrt{\frac{6}{5}}Y_{2,-2}(\theta_k\varphi_k)\mathbf{n}_{+1}\right.\\ &-\sqrt{\frac{3}{5}}Y_{2,-1}(\theta_k\varphi_k)\mathbf{n}_0\\ &\left.+\sqrt{\frac{1}{5}}Y_{2,0}(\theta_k\varphi_k)\mathbf{n}_{-1}\right)\Bigg]\end{aligned} \tag{14}$$

where

$$X_0(\omega) = \int_0^\infty r^3 j_0\left(\frac{\omega}{c}r\right)\mathrm{e}^{-r/a}\mathrm{d}r = \frac{2a^4\left(3-\frac{\omega^2a^2}{c^2}\right)}{\left(1+\frac{\omega^2a^2}{c^2}\right)^3}, \tag{15}$$

$$X_2(\omega) = \int_0^\infty r^3 j_2\left(\frac{\omega}{c}r\right)\mathrm{e}^{-r/a}\mathrm{d}r = \frac{8a^4\frac{\omega^2a^2}{c^2}}{\left(1+\frac{\omega^2a^2}{c^2}\right)^3} \tag{16}$$

with

$$\frac{1}{a} = \frac{1}{a_1}+\frac{1}{a_2}. \tag{17}$$

In this simple example, both $A_l(\omega)$ and $B_l(\omega)$ are proportional to $X_l(\omega)$.

In equation (14) the angular momentum l only takes the value 0 and 2, hence we know from equation (10) that in this example $\bar{\mathbf{G}}_\mathbf{k}=\mathbf{G}_\mathbf{k}$, consistent with what we say below equation (2b). This is in turn implies the equality of the counter-rotating wave coupling constant $\bar{g}_{\mathbf{k}j}$ and the rotating-wave coupling constant $g_{\mathbf{k}j}$. Thus the correlation spectrum $R_2(\omega)$ is given by

$$\begin{aligned}R_2(\omega) &= \frac{V}{(2\pi)^3}\frac{\omega^2}{c^3}\int\mathrm{d}\Omega_k\sum_j g_{\mathbf{k}j}^2\\ &= \frac{e^2\hbar\omega}{4\pi^2m^2c^2}\int\mathrm{d}\Omega_k\left[\mathbf{G}_\mathbf{k}^2-(\mathbf{n}_\mathbf{k}\cdot\mathbf{G}_\mathbf{k})^2\right].\end{aligned} \tag{18}$$

It is easy to show that $\int \mathrm{d}\Omega_k \mathbf{G}_\mathbf{k}^2 = 0$. By further utilizing the coupling rule for spherical harmonics, $\mathbf{n_k} \cdot \mathbf{G_k}$ may be expressed as $\sum_{l=1}^{3} c_l Y_{l,-1}(\theta_k \varphi_k)$, hence we also have $\int \mathrm{d}\Omega_k (\mathbf{n_k} \cdot \mathbf{G_k})^2 = 0$. Consequently we obtain

$$R_2(\omega) = 0. \tag{19}$$

This may be a quite general result [10].

From equations (4e, 11, 14), one gets the result for $R_1(\omega)$ as $R(\omega)$ used in reference [5] and also in references [3,4]

$$R_1(\omega) = \frac{\gamma_A}{2\pi\omega_0} \frac{\omega}{(1+\omega^2 a^2/c^2)^4}, \tag{20}$$

in which γ_A is the Einstein A coefficient, given by $\gamma_A = 4\omega_0^3 |d_{21}|^2/3c^3\hbar$ and in our example the transition dipole moment $\mathbf{d}_{21}$ takes its absolute value as

$$|d_{21}| = \frac{64\sqrt{2}}{81} ea, \tag{21}$$

with e denoting the magnitude of electron charge.

Actually there is only one parameter in the $R_1(\omega)$, since ω_0 may be expressed by a as

$$\omega_0 = \frac{1}{\hbar}(E_2 - E_1) = \frac{\hbar}{6ma^2}, \tag{22}$$

and the two atomic radii a_1 and a_2 are related to a by multiplying constants 3/2 and 3 respectively. Since a is proportional to the atomic number $1/Z$, we see from equation (22) that ω_0 is proportional to Z^2.

The relation between $\gamma_A/\omega_0$and a is obtained from equations (21, 22), and may be expressed by

$$\frac{\gamma_A}{\omega_0} = \frac{8}{3}\left(\frac{32}{243}\right)^2 \left(\frac{e^2}{\hbar c}\right)^3 \frac{a_B^2}{a^2}, \tag{23a}$$

where a_B is the Bohr radius. The dependence of γ_A/ω_0 on the atomic number Z is given by

$$\frac{\gamma_A}{\omega_0} = \frac{1}{6}\left(\frac{64}{81}\right)^2 \left(\frac{e^2}{\hbar c}\right)^3 Z^2, \tag{23b}$$

hence the value $\gamma_A/\omega_0 = 10^{-3}$ corresponds to $Z = 157$, somewhat larger than the upper limit of the real nuclei.

A profile of $R_1(\omega)$ is shown in Figure 1 of reference [5], in which the dimensionless parameter γ_A/ω_0 (instead of a) in $R(\omega)$ is taken as 0.001.

In case the atom is taken as a pointlike particle, the factor $\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}}$ in the integrand of $\mathbf{G_k}$ is omitted, $\mathbf{G_k}$ is then independent of $\mathbf{k}$. Hence, $R_1(\omega)$ will become linear in ω as can be seen from equation (4e), and the coefficient is just $\gamma_A/2\pi\omega_0$. We will call this spectrum as pointlike dipole spectrum:

$$R_1^D(\omega) = \frac{\gamma_A}{2\pi\omega_0}\omega\,. \tag{24}$$

It also corresponds to $R_1(\omega)$ with $\omega a/c = 0$ in the denominator.

Actually in our example only electric dipole emission is allowed by the selection rule of angular momentum, thus the factor $(1+\omega_0 a/c)^{-4}$ in $R_1(\omega)$ just expresses the finite size effect on the radiative electric dipole transition.

In this example, both $u_2(t-t')$ and $\bar{u}_2(t-t')$ are equal to zero, only two correlation functions $u_1(t-t')$ and $\bar{u}_1(t-t')$ remain. The former comes from the rotating-wave interaction and the latter from the counter-rotating wave interaction. In case we make the Markovian approximation on them, namely approximate them by $C\delta(t-t')$ and $\bar{C}\delta(t-t')$ respectively to neglect the memory effect, the constants C and $\bar{C}$ will be determined by integration of equations (4a, 4b) respect to t from t' to ∞ (note that u_1 and $\bar{u}_1$ are defined only in the region $t > t'$). The results so obtained is

$$\frac{1}{2}C = \pi R_1(\omega_0) - \mathrm{i}\int_0^\infty \wp \frac{R_1(\omega)}{\omega - \omega_0}\mathrm{d}\omega\,, \tag{25a}$$

$$\frac{1}{2}\bar{C} = \mathrm{i}\int_0^\infty \frac{R_1(\omega)}{\omega + \omega_0}\mathrm{d}\omega\,, \tag{25b}$$

where $\wp$ denotes taking the principal value. The imaginary parts of C nd $\bar{C}$ contribute just an level-shift which will be canceled out in equation (3b) because of the h.c. term.

Taking the expectation value of equation (3b) and noting the upper level population $\langle \hat{N}_2(t)\rangle = (1 + \langle\hat{\sigma}_3(t)\rangle)/2$, one gets immediately

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \hat{N}_2(t)\right\rangle = \gamma \left\langle \hat{N}_2(t)\right\rangle \tag{26a}$$

with

$$\gamma = 2\pi R_1(\omega_0) = \frac{\gamma_A}{(1+\omega_0^2 a^2/c^2)^4}. \tag{26b}$$

We see that γ is different from γ_A by the finite size correction factor $(1+\omega_0^2 a^2/c^2)^{-4}$, which in our example is about 0.729.

We would like to point out that the counter-rotating wave interaction will have no effect on $\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{N}(t)\rangle$ in the case Markovian approximation is made, even if $R_2(\omega) \neq 0$.

In the next section we will study the non-Markovian approach with the counter-rotating term included.

3 Quantum stochastic trajectory approach to the spontaneous emission

We have shown by equation (20) that the two-level atom with large atomic number Z has an evident non-Markovian reservoir in its spontaneous emission. Hence we will, as described in references [7,8], introduce N additional fictitious harmonic oscillators, which interact with the atom in the same form as photons, to form an expanded system. This expanded system thus has the

Hamiltonian

$$\hat{H} = \frac{1}{2}\hbar\omega_0\hat{\sigma_3} + \sum_{j=1}^{N}\hbar\omega_j\hat{\alpha}_j^\dagger\hat{\alpha}_j + \mathrm{i}\hbar\sum_{j=1}^{N}\Big(g_j\hat{\sigma_+}\hat{\alpha_j} - g_j^*\hat{\sigma_-}\hat{\alpha_j}^\dagger + \bar{g}_j\hat{\sigma_+}\hat{\alpha_j}^\dagger - \bar{g}_j^*\hat{\sigma_-}\hat{\alpha_j}\Big) \quad (27)$$

in which the energies of the two atom-levels are taken as $\pm\frac{1}{2}\hbar\omega_0$ respectively, $\hat{\alpha}_j$ and $\hat{\alpha}_j^\dagger$ are annihilation and creation operators of the jth oscillator, $\bar{g}_j = \pm g_j$ for the relative parity of Ψ_2 and Ψ_1 equal to ∓ 1 respectively. Each of these oscillators, on the other hand, is assumed to interact with its own reservoir with no memory, hence the expanded system is Markovian. In terms of Langevin equations in Heisenberg picture the dynamics of the above system is expressed by

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\sigma}_-(t) = -\mathrm{i}\omega_0\hat{\sigma}_-(t) - \sum_{j=1}^{N}\Big[g_j\hat{\alpha_j}(t) + \bar{g}_j\hat{\alpha}_j^\dagger(t)\Big]\hat{\sigma}_3(t), \quad (28a)$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\sigma}_3(t) = 2\sum_{j=1}^{N}\Big[g_j\hat{\alpha_j}(t) + \bar{g}_j\hat{\alpha}_j^\dagger(t)\Big]\hat{\sigma}_+(t) + 2\sum_{j=1}^{N}\Big[g_j^*\hat{\alpha_j}^\dagger(t) + \bar{g}_j^*\hat{\alpha}_j(t)\Big]\hat{\sigma}_-(t), \quad (28b)$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\alpha}_j(t) = -\mathrm{i}\omega_j\hat{\alpha}_j(t) - g_j^*\hat{\sigma}_-(t) + \bar{g}_j\hat{\sigma}_+(t) - \frac{1}{2}\Gamma_j\hat{\alpha}_j(t) - \hat{F}_j(t) \quad (28c)$$

with

$$\Big\langle\hat{F}_j(t)\Big\rangle_R = 0, \qquad \Big\langle\hat{F}_i(t)\hat{F}_j(t')\Big\rangle_R = 0,$$
$$\Big\langle\hat{F}_i(t)\hat{F}_j^\dagger(t')\Big\rangle_R = \delta_{ij}\Gamma_j\delta(t-t'). \quad (28d)$$

The last two terms of equation (28c) are the usual Markovian dissipation term and fluctuation term contributed by the reservoir of jth oscillator.

When the formal solution of equation (28c) is used to eliminate the variables $\hat{\alpha}_j$ and $\hat{\alpha}_j^\dagger$ in equations (28a, 28b), the reduced equation for $\hat{\sigma}_+(t)$ and $\hat{\sigma}_3(t)$ will have non-Markovian damping terms and non-Markovian fluctuation terms, since each fictitious oscillator contributes a term with Lorentzian type spectrum. The next step is to select parameters g_j, $\bar{g}_j$, ω_j and Γ_j to simulate the original damping terms and fluctuation terms. Now there are two spectral functions, not just one spectral function as in rotating-wave approximation, the simulation task will become more complicate.

As soon as the simulation task is accomplished, one may go back to the master-equation formulation and treat it by quantum stochastic trajectory approach. The non-Hermitian Hamiltonian is now taken as

$$\hat{H}_{\mathrm{nh}} = \hat{H} - \frac{\mathrm{i}}{2}\hbar\sum_j\Gamma_j\hat{\alpha}_j^\dagger\hat{\alpha}_j, \quad (29)$$

where $\hat{H}$ is expressed by equation (27). The collapse operators acting on $|\Psi(t)\rangle$ are

$$\hat{C}_j = \sqrt{\Gamma_j\Delta t}\hat{\alpha}_j, \qquad j = 1, 2, ..., N. \quad (30)$$

To proceed with concrete analysis and compare with the result of rotating-wave approximation, we return to the example with $\Psi_2(\mathbf{x})$ and $\Psi_1(\mathbf{x})$ described by equation (12).

In reference [5] only two fictitious oscillators are introduced to simulate the spectrum $R(\omega) \equiv R_1(\omega)$ of this example, the corresponding simulation spectrum $R^{(s)}(\omega)$ fits pretty well with $R(\omega)$ in a large region $\omega/\omega_0 \geq 0.5$, which includes the important region around $\omega/\omega_0 = 1$. But the $R^{(s)}(\omega)$ drops down less slowly than $R(\omega)$ when $\omega/\omega_0 \to 0$. At the origin, $R^{(s)}(\omega)/R^{(s)}(\omega_0)$ is still about 0.36 while $R(\omega)$ drops to zero (see Fig. 1 of Ref. [5]).

Now there is an additional spectrum $R_2(\omega)$, we have to use one set of N oscillators to simulate both of them, namely to make

$$R_1(\omega) \cong R_1^{(s)}(\omega) \equiv \frac{1}{2\pi}\sum_{j=1}^{N}\frac{|g_j|^2\Gamma_j}{(\omega-\omega_j)^2 + \frac{1}{4}\Gamma_j^2}, \quad (31a)$$

$$R_2(\omega) \cong R_2^{(s)}(\omega) \equiv \frac{1}{2\pi}\sum_{j=1}^{N}\frac{g_j\bar{g}_j\Gamma_j}{(\omega-\omega_j)^2 + \frac{1}{4}\Gamma_j^2}. \quad (31b)$$

In general, the simulation is not easy to be carried out. But in the case $R_2(\omega) = 0$, we may simply take four fictitious oscillators with following parameters:

$$g_1 = \frac{1}{\sqrt{2}}0.011\omega_0, \quad \Gamma_1 = 1.3\omega_0, \quad \omega_1 = \omega_0, \quad (32a)$$

$$g_2 = \frac{1}{\sqrt{2}}0.018\omega_0, \quad \Gamma_2 = 2.4\omega_0, \quad \omega_1 = 1.85\omega_0, \quad (32b)$$

$$g_3 = \frac{\mathrm{i}}{\sqrt{2}}0.011\omega_0, \quad \Gamma_3 = 1.3\omega_0, \quad \omega_3 = \omega_0, \quad (32c)$$

$$g_4 = \frac{\mathrm{i}}{\sqrt{2}}0.018\omega_0, \quad \Gamma_4 = 2.4\omega_0, \quad \omega_4 = 1.85\omega_0. \quad (32d)$$

It is easy to check that the above set of parameters makes $R_2^{(s)}(\omega) = 0$ no matter the relative parity between Ψ_2 and Ψ_1 is positive or negative, while $R_1^{(s)}(\omega)$ remains unchanged from the $R^{(s)}(\omega)$ of reference [5].

Since the numerical evolution takes place over discrete times with a small time step Δt, the wave function $|\Psi(t)\rangle$ is represented by a sequence $|\Psi(t_n)\rangle$ with $t_n = n\Delta t$. Given the value of $|\Psi(t_n)\rangle$, the next one $|\Psi(t_{n+1})\rangle$ is determined by the following algorithm:

(1) evaluate the four kinds of collapse probabilities during interval (t_n, t_{n-1}):

$$P_j(t_n) = \Big\langle\Psi(t_n)\Big|\hat{C}_j^\dagger\hat{C}_j\Big|\Psi(t_n)\Big\rangle = \Gamma_j\Big\langle\Psi(t_n)\Big|\hat{\alpha}_j^\dagger\hat{\alpha}_j\Big|\Psi(t_n)\Big\rangle\Delta t, \ j = 1, 2, 3, 4 \quad (33)$$

in which Δt should be small enough to make $P_1(t_n)$ and $P_2(t_n)$ much small than 1;

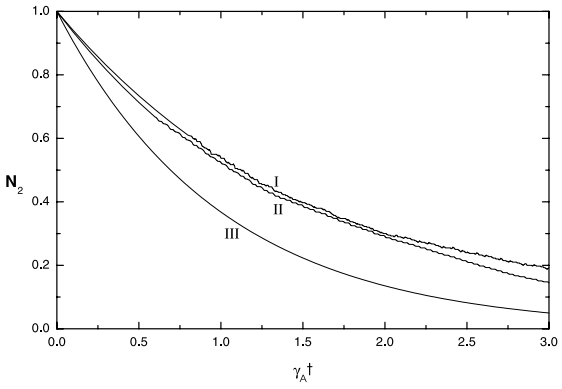

Fig. 1. The spontaneous decay of the upper level population with parameters ($\gamma_A/\omega_0 = 1\times10^{-3}$). The curve I represents the result without both rotating-wave and Markovian approximation, the curve II represents the result with rotating-wave approximation but without Markov approximation as calculated in reference [5], the curve III represents the Weisskopf-Wigner result.

(2) generate four random numbers r_j ($j = 1, 2, 3, 4$) which have uniform probability distribution among the interval $(0, 1)$;
(3) compare $P_j(t_n)$ with r_j and derive $|\Psi(t_{n+1})\rangle$ according to the following rule: if $P_j(t_n) < r_j$ and for all j,

$$|\Psi(t_{n+1})\rangle = \frac{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}_{\mathrm{nh}}\Delta t}|\Psi(t_n)\rangle}{\sqrt{\langle\Psi(t_n)|\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\hat{H}^{\dagger}_{\mathrm{nh}}-\hat{H}_{\mathrm{nh}})\Delta t}|\Psi(t_n)\rangle}}; \quad (34)$$

if $P_l(t_n) > r_l$ for some one index l and all other $P_m(t_n) \leq r_m$,

$$|\Psi(t_{n+1})\rangle = \frac{\hat{C}_l|\Psi(t_n)\rangle}{\sqrt{\langle\Psi(t_n)|\hat{C}^{\dagger}_l\hat{C}_l|\Psi(t_n)\rangle}}. \quad (35)$$

In the practical calculation, Δt should be taken sufficiently small so that the case with any two (or more) $P_j(t_n)$'s larger than the corresponding r_j in the same interval $(t_n,\ t_n + \Delta t)$ will not happen.

By carrying out the steps specified above over and over from the initial state $\begin{pmatrix}1\\0\end{pmatrix}|0,0,0,0\rangle$ where $\begin{pmatrix}1\\0\end{pmatrix}$ is the atom state in the upper level and $|0,0,0,0\rangle$ denotes the state of four oscillators with their number of quanta all being zero, we get a quantum stochastic trajectory of the Monte Carlo wave function $|\Psi(t)\rangle$. The expectation value of a given operator respect to $|\Psi(t)\rangle$ is then calculated. Finally an ensemble average of 400 trajectories is carried out to give the resultant curve.

The population on the upper level $\langle\hat{N}_2(t)\rangle$ is shown in Figure 1. We see that the correction of counter-rotating wave term to the non-Markovian result obtained in reference [5] is quite small even Z is as large as 157. Hence one may neglect this term for stable nuclei without introducing obvious error.

We note that the large difference between curve II and curve III comes from two respects as mentioned in Section 1: the first one concerns the finite size correction, corresponding to the replacement of γ_A by γ with $\gamma = 0.729\,\gamma_A$. This correction is calculated analytically and should be reliable. The second correction is the memory effect corresponding to the non-uniform of $R(\omega)$, namely the difference of $R(\omega)$ from $R(\omega_0)$. This part is evaluated numerically and has some errors from simulation and from the pseudo character of the random numbers generated by program. Both corrections make the decay slower. As shown in reference [5], the first correction is much larger than the second. As to the difference between curves I and II which comes from the effect of counter-rotating wave coupling, it is totally due to the non-Markovian contribution since in the present case $R_2(\omega) = 0$, γ remains unchanged as specified in the end of Section 2.

This work is supported by National Natural Science Foundation of China (project number 19774004), and also by the International Program of National Science Foundation of USA (ECS-9800068).

References

1. P.L. Knight, P.W. Milonni, Phys. Rev. Lett. **56**, 275 (1976)
2. P. Carrazana, G. Vetri, Nuovo Clim. B **55**, 191 (1980)
3. P.T. Robisco, Phys. Lett. A **100**, 407 (1984)
4. J. Seke, W. Herfort, Phys. Rev. A **38**, 833 (1988); Phys. Rev. A **40**, 1926 (1989)
5. C.-Q. Cao, W. Long, J. Wei, H. Cao, Phys. Rev. A **64**, 043810 (2001)
6. See for example, H.J. Carmichael, *An Open System Approach to Quantum Optics* (Springer-Verlag, Berlin, 1993), Lecture 7
7. A. Imamoglu, Phys. Rev. A **50**, 3650 (1994)
8. P. Stenius, A. Imamoglu, Quant. Semiclass. Opt. **8**, 283 (1996)
9. W.H. Louisell, *Coupled mode and parametric electronics* (Wiley, New York, 1960)
10. We may show that $R_2(\omega) = 0$, provided $m_1 \neq m_2$. First, see the integral $\int \mathrm{d}\Omega_k \mathbf{G}^2_{\mathbf{k}}$. Substituting equation (7) into it and carrying out the integration over the angular variables, we get a series over (l, m, n), and for each (l, m, n) there are four terms proportional to
$[C_{l_1+1,l_2,l;m_1-\mu,-m_2,m}C_{l_1+1,l_2,l;m_1+\mu,-m_2,-m}]$,
$[C_{l_1+1,l_2,l;m_1-\mu,-m_2,m}C_{l_1-1,l_2,l;m_1+\mu,-m_2,-m}]$,
$[C_{l_1-1,l_2,l;m_1-\mu,-m_2,m}C_{l_1+1,l_2,l;m_1+\mu,-m_2,-m}]$,
$[C_{l_1-1,l_2,l;m_1-\mu,-m_2,m}C_{l_1-1,l_2,l;m_1+\mu,-m_2,-m}]$
respectively. One may easily check that all of them will be zero unless $m_1 = m_2$. Similarly, the integral $\int(\mathbf{n_k}\cdot\mathbf{G_k})^2\mathrm{d}\Omega_k$ contains four terms proportional to
$[C_{l_1+1,l_2,l;m_1-\mu,-m_2,m}C_{l_1+1,l_2,l';m_1-\mu'-m_2,-m-\mu-\mu'}]$,
$[C_{l_1+1,l_2,l;m_1-\mu,-m_2,m}C_{l_1-1,l_2,l';m_1-\mu',-m_2,-m-\mu-\mu'}]$,
$[C_{l_1-1,l_2,l;m_1-\mu,-m_2,m}C_{l_1+1,l_2,l';m_1-\mu',-m_2,-m-\mu-\mu'}]$,
$[C_{l_1-1,l_2,l;m_1-\mu,-m_2,m}C_{l_1-1,l_2,l';m_1-\mu',-m_2,-m-\mu-\mu'}]$
for each index-set (l, m, μ, l', μ'), they also will be zero unless $m_1 = m_2$