Quantum analysis and the classical analysis of spontaneous emission in a microcavity

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Starting from a quantum Maxwell equation for the vector potential operator, we study the spontaneous emission properties of a two-level atom interacting with the electromagnetic field in a lossless and inhomogeneous dielectric structure and express the spontaneous emission rate, the external quantum efficiency, and the spontaneous emission factor in terms of the classical Green function of the dielectric structure. Comparing these results with the corresponding classical results, we show that the above quantities can be calculated from the radiation field of a classical dipole. Based on this correspondence, a numerical algorithm is developed to calculate the modification of spontaneous emission in microcavities. The line shape of the emission spectrum of the light source and the decay of the cavity resonant modes are automatically taken into account in this algorithm. The approximate expressions for the spontaneous emission rate and the spontaneous emission factor are discussed.

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I. INTRODUCTION

It is well known that the radiation process of an atom depends on its environment [1], and the study of the interaction between the atom and the electromagnetic field inside a cavity structure has come to be called cavity quantum electrodynamics (QED). The most simple, and yet fundamentally important, system of cavity QED is a single two-level atom coupled with a single cavity electromagnetic mode, which was first studied theoretically by Jaynes and Cummings [2]. An important parameter in such a system is the coupling constant between the atom and the cavity mode, which can be estimated as $\kappa=(\mu_{12}/\hbar)\sqrt{2\pi\hbar\Omega/V}$, where Ω is the atomic transition frequency, V is the cavity volume, and μ_{12} is the dipole matrix element of the atom [3]. However, to describe the radiation process of the atom, the damping of the system must be taken into account. If we assume the atom has a dipole dephasing rate γ_{12}, and the decay rate of the cavity photon is Γ_{cav}, the radiation process falls into two physically distinctive regimes: the strong coupling regime with $\kappa \gg (\gamma_{12},\Gamma_{cav})$, and the weak coupling regime with $\kappa \ll (\gamma_{12},\Gamma_{cav})$ [3]. The strong coupling regime is characterized by the double peak in the emission spectrum, and the oscillatory behavior of the excited state occupation number [4]. In this paper, we shall confine ourselves to the weak coupling regime, and study the correspondence between the quantum picture and the classical picture of spontaneous emission.

One of the most interesting aspects of the weak-coupling radiation process is the spontaneous emission enhancement or inhibition by the cavity structure [1]. The enhancement was experimentally verified by Goy *et al.* [5], and the inhibition was first demonstrated by Kleppner [6]. Such cavity-induced modification of spontaneous emission continues to be the subject of intense theoretical and experimental research. Part of the reason is that these new phenomena can deepen our understanding of the atom-field interaction and are therefore theoretically important. Another factor, however, is the practical importance of controlling the light emission by means of cavities. For example, the external quantum efficiency of a light-emitting diode is significantly improved by using a structure similar to that of a vertical cavity surface emitting laser (VCSEL) [7]. It is also demonstrated theoretically that further improvement is possible by introducing a two-dimensional photonic crystal structure [8]. Another example is the so-called ''thresholdless laser'' [9–11]. From a simple rate equation analysis, it is shown that if the spontaneous emission factor of the lasing mode is close to 1, the threshold in the light versus pumping curve disappears. Therefore, it is important to be able to theoretically calculate the spontaneous emission properties of an atom in a microcavity.

Most of the theoretical analysis of the spontaneous emission in a cavity structure concentrated on the modification of spontaneous emission rate, which can be calculated using either a classical approach or a quantum approach. In the classical picture, the modification of spontaneous emission rate is due to the radiation reaction of the reflected field on the classical dipole source [12–20]. The quantum description of spontaneous emission treat it as an emission stimulated by the vacuum field fluctuation [18,19,21–30]. The similarity between the classical approach and the quantum approach has also been noticed [12,16,31]. Using these methods, the modification of spontaneous emission rate has been calculated for various geometries, such as homogeneous absorbing media [19,26], parallel metal plates [18,22,31], metal spheres [31], dielectric slab waveguides [27,28], planar dielectric microcavities [20,25], and dielectric spheres [14]. Unfortunately, such theoretical calculations have always been quite difficult. And for complicated structures, such as the microdisk or the VCSEL, an analytical analysis of spontaneous emission is only possible under some simplifying assumptions [25,32,33]. For more complicated structures such as the two-dimensional or three-dimensional photonic crystals [34–37], an analytical solution is even more prohibitive. Therefore, to calculate the spontaneous emission properties in an arbitrary geometry, a numerical treatment can be more practical. In fact, a finite difference time domain algorithm (FDTD) [38] has been applied to compute the spontaneous emission rate [39] and the external quantum efficiency [23] in some dielectric structures. However, even though the

equivalence of the quantum approach and classical approach has been known for the case of spontaneous emission rate [12,14–16,18–20], to the authors' knowledge, such equivalence has not been established for the external quantum efficiency and the spontaneous emission factor. Furthermore, an algorithm capable of computing the spontaneous emission rate, the external quantum efficiency, and the spontaneous emission factor in the same framework is of great theoretical and practical interest. In this paper, we shall demonstrate that all these quantities can be calculated from classical electrodynamics and propose a FDTD algorithm to analyze the spontaneous emission in an arbitrary lossless, inhomogeneous medium. In the following paper [40], such an algorithm is applied to calculate the modification of spontaneous emission rate and spontaneous emission factor in a dielectric microdisk.

To fully demonstrate the equivalence of classical electrodynamics and quantum electrodynamics in the treatment of spontaneous emission, we start from the quantum Maxwell equation, which has been extensively used in the literature to quantize the electromagnetic field in a lossy medium [41–45]. In this formalism, the quantization of the radiation field is based on the classical Green's function and the quantum Langevin operators which account for the noise source necessarily associated with the lossy medium and preserve the basic equal-time commutation relation of quantum electrodynamics. In a similar way, Henry and Kazarinov [46] developed a quantum theory of lasers and amplifiers with arbitrary geometries ranging from closed cavities to traveling wave amplifiers, where both the electromagnetic vector potential and the current density are assumed to be quantum operators that satisfy the Maxwell equation. The current density operator can be split into two components: One part proportional to the external electromagnetic field, which accounts for the stimulated emission, and another part represented by a quantum Langevin operator that fluctuates randomly and acts as a source for spontaneous emission. This approach is adopted by us to analyze the spontaneous emission of a two-level atom embedded in an inhomogeneous and lossless dielectric medium, since it has a form close to that of classical electrodynamics and allows a direct comparison between the classical results and the quantum results.

An explanation of our notation is in order: Throughout this paper, all the quantum operators are denoted by an overhat. All vectorial quantum operators are represented by bold letters, such as the vector potential operator $\hat{\mathbf{A}}$. On the other hand, the classical quantities do not have an overhat. The classical vectorial quantities, such as the vector potential of the classical electromagnetic field $\vec{A}$, are indicated by an overarrow. The classical vectors are not in bold letters to differentiate them from the quantum vectorial operators. In the later sections, all the quantities in the frequency domain have a subscript or superscript ω. The subscript α or β refers to the αth or βth component of the corresponding vector quantity in Cartesian coordinates. The Gaussian units are used throughout this paper.

II. OPERATOR EQUATIONS

Let us consider the electromagnetic field in an inhomogeneous and lossless medium with dielectric constant $\epsilon(\vec{x})$. The vector potential operator $\hat{\mathbf{A}}(\vec{x},t)$ can be separated into a transverse component that satisfies the generalized Coulomb gauge condition $\nabla\cdot[\epsilon(\vec{x})\hat{\mathbf{A}}]=0$ [24], and a longitudinal component which is ignored since it does not contribute to the radiation process in a lossless medium [19]. Following Ref. [24], the transverse vector potential can be expanded into a complete set of orthonormal modes $\{\vec{A}_n(\vec{x})\}$

$$\hat{\mathbf{A}}(\vec{x},t)=\hat{\mathbf{A}}^{(-)}(\vec{x},t)+\hat{\mathbf{A}}^{(+)}(\vec{x},t), \tag{2.1a}$$

$$\hat{\mathbf{A}}^{(-)}(\vec{x},t)=\sum_n \sqrt{\frac{2\pi\hbar c^2}{\omega_n}}\hat{a}_n\vec{A}_n(\vec{x}), \tag{2.1b}$$

$$\hat{\mathbf{A}}^{(+)}(\vec{x},t)=\sum_n \sqrt{\frac{2\pi\hbar c^2}{\omega_n}}\hat{a}_n^\dagger\vec{A}_n^*(\vec{x}), \tag{2.1c}$$

where we have separated the vector potential into a positive frequency part $\hat{\mathbf{A}}^{(+)}$ and a negative frequency part $\hat{\mathbf{A}}^{(-)}$, which are the Hermitian adjoints of each other. In the above equations, $\vec{A}_n(\vec{x})$ is the nth eigenmode as defined in Appendix A, and ω_n is its eigenfrequency. $\hat{a}_n$ and $\hat{a}_n^\dagger$ are respectively the photon destruction and creation operator which fulfill the canonical commutation relations

$$[\hat{a}_n,\hat{a}_m]=[\hat{a}_n^\dagger,\hat{a}_m^\dagger]=0,\quad [\hat{a}_n,\hat{a}_m^\dagger]=\delta_{nm}. \tag{2.2}$$

If a two-level atom with a transition frequency Ω is located within this dielectric medium at position $\vec{x}_0$ and interacts with the quantized electromagnetic field, the total Hamiltonian for such system can be written as [24]

$$\hat{H}=E_2\hat{b}_2^\dagger\hat{b}_2+E_1\hat{b}_1^\dagger\hat{b}_1+\sum_n \hbar\omega_n\hat{a}_n^\dagger\hat{a}_n + \sum_n [\hbar\kappa_n\hat{b}_2^\dagger\hat{b}_1\hat{a}_n+\hbar\kappa_n^*\hat{a}_n^\dagger\hat{b}_1^\dagger\hat{b}_2], \tag{2.3}$$

where E_2 is the energy of the excited atomic state $|2\rangle$ and E_1 is the energy of the ground state $|1\rangle$. $\hat{b}_2^\dagger$ and $\hat{b}_1^\dagger$ are, respectively, the creation operators for the excited state and ground state, while $\hat{b}_2$ and $\hat{b}_1$ are the corresponding destruction operators. They satisfy the usual anticommutation rules:

$$\hat{b}_i\hat{b}_j+\hat{b}_j\hat{b}_i=\hat{b}_i^\dagger\hat{b}_j^\dagger+\hat{b}_j^\dagger\hat{b}_i^\dagger=0,\quad \hat{b}_i^\dagger\hat{b}_j+\hat{b}_j\hat{b}_i^\dagger=\delta_{ij},\quad i,j=1,2. \tag{2.4}$$

The coupling coefficient κ_n in Eq. (2.3) is defined as

$$\kappa_n=-\frac{e}{\hbar m}\sqrt{\frac{2\pi\hbar}{\omega_n}}\vec{p}_{12}\cdot\vec{A}_n(\vec{x}_0), \tag{2.5}$$

where $\vec{p}_{12}$ is the matrix element $\langle 1|\hat{\mathbf{P}}|2\rangle$ of the electron momentum operator $\hat{\mathbf{P}}$ and is assumed to be a real quantity.

Using Fermi's golden rule, the spontaneous emission rate of a atom in the excited state can be calculate in a standard way from the above Hamiltonian [24]. However, here we shall deviate from this standard procedure and assume that

the atomic source has a ''pure'' dipole dephasing rate γ_{12} which excludes the contribution from radiative decay. Associated with this nonzero dipole decay rate, a quantum Langevin operator must be introduced to preserve the commutation relation in Eq. (2.4) [47]. Using the quantum Langevin equation and the mode expansion relation Eq. (2.1), a quantum Maxwell equation can be derived for the operators $\hat{\mathbf{A}}^{(-)}(\vec{x},t)$ and $\hat{\mathbf{J}}^{(-)}_{tot}(\vec{x},t)$ which have only negative frequency components (see Appendix B for details)

$$\frac{\epsilon(\vec{x})}{c^2}\frac{\partial^2\hat{\mathbf{A}}^{(-)}(\vec{x},t)}{\partial t^2}=-\nabla\times[\nabla\times\hat{\mathbf{A}}^{(-)}(\vec{x},t)]+\frac{4\pi}{c}\hat{\mathbf{J}}^{(-)}_{tot}(\vec{x},t). \tag{2.6}$$

We can denote the Hermitian adjoints of $\hat{\mathbf{A}}^{(-)}(\vec{x},t)$ and $\hat{\mathbf{J}}^{(-)}_{tot}(\vec{x},t)$, which contain only the positive frequency components, as $\hat{\mathbf{A}}^{(+)}(\vec{x},t)$ and $\hat{\mathbf{J}}^{(+)}_{tot}(\vec{x},t)$. A similar equation for them can be obtained from the Hermitian conjugation of the above equation. The quantum current source $\hat{\mathbf{J}}^{(-)}_{tot}$, as shown in Appendix B, can be separated as $\hat{\mathbf{J}}^{(-)}_{tot}=\hat{\mathbf{J}}^{(-)}_{fluc}+\hat{\mathbf{J}}^{(-)}_{ind}$, consisting of a fluctuating component $\hat{\mathbf{J}}^{(-)}_{fluc}$ whose ensemble average satisfies

$$\begin{aligned}\langle\hat{J}^{(+)}_{fluc,\alpha}(\vec{x}',t')\hat{J}^{(-)}_{fluc,\beta}(\vec{x},t)\rangle&=\left(\frac{e}{m}\right)^2 p_{12,\alpha}p_{12,\beta}\delta(\vec{x}-\vec{x}')\,\delta(\vec{x}-\vec{x}_0)\\&\quad\times\overline{n}_2 e^{-i\Omega(t-t')}e^{-\gamma_{12}|t-t'|},\end{aligned} \tag{2.7}$$

and an induced component $\hat{\mathbf{J}}^{(-)}_{ind}$ proportional to the external vector potential

$$\hat{J}^{(-)}_{ind,\alpha}(\vec{x},t)=\int_{-\infty}^{t}d\tau\chi_{\alpha\beta}(\vec{x},t-\tau)\hat{A}^{(-)}_{\beta}(\vec{x},\tau), \tag{2.8a}$$

$$\begin{aligned}\chi_{\alpha\beta}(\vec{x},\tau)&=-\frac{i}{\hbar c}\left(\frac{e}{m}\right)^2 p_{12,\alpha}p_{12,\beta}\delta(\vec{x}-\vec{x}_0)(\overline{n}_2-\overline{n}_1)\\&\quad\times e^{-i\Omega\tau}e^{-\gamma_{12}\tau},\end{aligned} \tag{2.8b}$$

where $\overline{n}_1$ and $\overline{n}_2$ are respectively the average occupation number of the ground state and the excited state. As we have mentioned before, the subscript α or β in Eq. (2.7) and Eq. (2.8a) refers to the αth or βth component of a vectorial quantum operator in the Cartesian coordinates.

Often it is more convenient to work in the frequency domain. Hence we define the Fourier transform $\hat{O}_\omega$ of a quantum operator $\hat{O}(t)$ as

$$\hat{O}(t)=\frac{1}{\sqrt{2\pi}}\int d\omega\,\hat{O}_\omega e^{-i\omega t}, \tag{2.9a}$$

$$\hat{O}_\omega=\frac{1}{\sqrt{2\pi}}\int dt\,\hat{O}(t)e^{i\omega t}. \tag{2.9b}$$

Using these definitions, Eq. (2.7) and Eq. (2.8) can be rewritten as

$$\begin{aligned}\langle\hat{J}^{(+)}_{fluc,\omega'\alpha}(\vec{x}')\hat{J}^{(-)}_{fluc,\omega\beta}(\vec{x})\rangle&=\left(\frac{e}{m}\right)^2 p_{12,\alpha}p_{12,\beta}\delta(\omega+\omega')\,\delta(\vec{x}-\vec{x}')\\&\quad\times\delta(\vec{x}-\vec{x}_0)\overline{n}_2\frac{2\gamma_{12}}{(\Omega-\omega)^2+\gamma_{12}^2},\end{aligned} \tag{2.10a}$$

$$\hat{J}^{(-)}_{ind,\omega\alpha}(\vec{x})=\chi_{\alpha\beta}(\omega,\vec{x})\hat{A}^{(-)}_{\omega\beta}(\vec{x}), \tag{2.10b}$$

$$\begin{aligned}\chi_{\alpha\beta}(\omega,\vec{x})&=-\frac{i}{\hbar c}\left(\frac{e}{m}\right)^2 p_{12,\alpha}p_{12,\beta}\delta(\vec{x}-\vec{x}_0)\\&\quad\times(\overline{n}_2-\overline{n}_1)\frac{1}{i(\Omega-\omega)+\gamma_{12}}.\end{aligned} \tag{2.10c}$$

In laser theory [48], $\chi_{\alpha\beta}(\omega,\vec{x})$ can usually be approximated as a scalar quantity $\chi(\omega,\vec{x})$ after averaging $p_{12,\alpha}p_{12,\beta}$ over the polarizations of the gain medium . Thus in the frequency domain the quantum Maxwell equation is

$$-\nabla\times[\nabla\times\hat{\mathbf{A}}^{(-)}_\omega]+\left[\epsilon(\vec{x})\frac{\omega^2}{c^2}+\frac{4\pi}{c}\chi(\omega,\vec{x})\right]\hat{\mathbf{A}}^{(-)}_\omega=-\frac{4\pi}{c}\hat{\mathbf{J}}^{(-)}_{fluc,\omega}. \tag{2.11}$$

An operator equation for the optical transition rate of the electrons can also be derived from the Hamiltonian in Eq. (2.3) (see Appendix B)

$$\frac{d\hat{N}_2}{dt}=\frac{i}{\hbar c}\int d^3x\,[\hat{\mathbf{J}}^{(+)}_{tot}\cdot\hat{\mathbf{A}}^{(-)}-\hat{\mathbf{A}}^{(+)}\cdot\hat{\mathbf{J}}^{(-)}_{tot}], \tag{2.12}$$

where $\hat{N}_2$ is defined as $\hat{b}_2^\dagger\hat{b}_2$. This equation, together with the quantum Maxwell equation, forms the basis of our calculations in the later sections.

Having divided the current operator $\hat{\mathbf{J}}^{(-)}_{tot}$ into an induced current and a fluctuating current, we can accordingly separate the optical transition of electrons as described by Eq. (2.12) into two physically distinct processes: stimulated emission and spontaneous emission [46]. The induced current is the source of the stimulated emission, since it is proportional to the vector potential of the electromagnetic field and the resulting electron transition rate is proportional to the photon density. On the other hand, the spontaneous emission is caused by the fluctuating current [46]. At first, we might guess that the ensemble average of the product of the fluctuating current and the vector potential should be zero, since they are independent of each other. However, this is not true because a small part of the vector potential is generated by the fluctuating current according to Eq. (2.11). Therefore, the ensemble average of this product has a nonzero component and accounts for the spontaneous emission.

III. SPONTANEOUS EMISSION RATE

It is clear from Eq. (2.11) that the vector potential operator $\hat{\mathbf{A}}_{\omega}^{(-)}$ is a linear function of the current operator $\hat{\mathbf{J}}_{fluc,\omega}^{(-)}$. These two operators can be related to each other via the classical Green function defined as

$$-\nabla\times\{\nabla\times[G_{\alpha\beta}^{\omega}(\vec{x},\vec{x}')\vec{e}_{\alpha}]\}+\left[\epsilon(\vec{x})\frac{\omega^2}{c^2}+\frac{4\pi}{c}\chi(\omega,\vec{x})\right]G_{\alpha\beta}^{\omega}(\vec{x},\vec{x}')\vec{e}_{\alpha}=\vec{e}_{\beta}\delta(\vec{x}-\vec{x}'). \tag{3.1}$$

Then we can express $\hat{\mathbf{A}}_{\omega}^{(-)}$ in terms of $\hat{\mathbf{J}}_{fluc,\omega}^{(-)}$ as

$$\hat{\mathbf{A}}_{\omega}^{(-)}(\vec{x})=-\frac{4\pi}{c}\int d^3x'\,\vec{e}_{\alpha}G_{\alpha\beta}^{\omega}(\vec{x},\vec{x}')\hat{J}_{fluc,\omega\beta}^{(-)}(\vec{x}'). \tag{3.2}$$

From the discussion following Eq. (2.12), we find that the spontaneous transition rate for the electrons in the excited state is given by the beating between the fluctuating current and the vector potential radiated by this fluctuating current

$$\dot{\hat{N}}_{2spon}=\frac{i}{\hbar c}\int d^3x\,[\hat{\mathbf{J}}_{fluc}^{(+)}(\vec{x},t)\cdot\hat{\mathbf{A}}^{(-)}(\vec{x},t)-\hat{\mathbf{A}}^{(+)}(\vec{x},t)\cdot\hat{\mathbf{J}}_{fluc}^{(-)}(\vec{x},t)]. \tag{3.3}$$

Substituting Eq. (3.2) into Eq. (3.3), and taking the ensemble average using Eq. (2.10a), we obtain

$$\langle\dot{\hat{N}}_2\rangle_{spon}=\frac{4}{\hbar c^2}\frac{e^2}{m^2}p_{12,\alpha}p_{12,\beta}\overline{n}_2\times\int d\omega\,\frac{2\gamma_{12}}{(\Omega-\omega)^2+\gamma_{12}^2}\,\mathrm{Im}[G_{\alpha\beta}^{\omega}(\vec{x}_0,\vec{x}_0)]. \tag{3.4}$$

The spontaneous emission rate γ can be defined as

$$\gamma=-\frac{4}{\hbar c^2}\frac{e^2}{m^2}p_{12,\alpha}p_{12,\beta}\int d\omega\,\frac{2\gamma_{12}}{(\Omega-\omega)^2+\gamma_{12}^2}\times\mathrm{Im}[G_{\alpha\beta}^{\omega}(\vec{x}_0,\vec{x}_0)]. \tag{3.5}$$

Similar results have been found in the literature [22,26,31,46].

It has been noticed that the radiation power of a harmonic classical dipole current is proportional to the spontaneous emission rate of a two-level atom when $\gamma_{12}=0$ [15,16,18–20]. The result in Eq. (3.5), which contains a Lorentzian line-shape function, suggests that the total radiation energy of a decaying classical dipole source should give us the spontaneous emission rate when $\gamma_{12}\neq 0$. To confirm this conjecture, we split the dipole current density and the vector potential into a positive frequency part and a negative frequency part, which are each other's complex conjugate,

$$\vec{J}(\vec{x},t)=\frac{1}{2\sqrt{2\pi}}\left[\int_{-\infty}^{+\infty}d\omega\,\vec{J}_{\omega}(\vec{x})e^{-i\omega t}+\int_{-\infty}^{+\infty}d\omega\,\vec{J}_{\omega}^{*}(\vec{x})e^{i\omega t}\right], \tag{3.6a}$$

$$\vec{A}(\vec{x},t)=\frac{1}{2\sqrt{2\pi}}\left[\int_{-\infty}^{+\infty}d\omega\,\vec{A}_{\omega}(\vec{x})e^{-i\omega t}+\int_{-\infty}^{+\infty}d\omega\,\vec{A}_{\omega}^{*}(\vec{x})e^{i\omega t}\right]. \tag{3.6b}$$

The classical wave equation at a given frequency ω is

$$-\nabla\times[\nabla\times\vec{A}_{\omega}(\vec{x})]+\left[\epsilon(\vec{x})\frac{\omega^2}{c^2}+\frac{4\pi}{c}\chi(\omega,\vec{x})\right]\vec{A}_{\omega}(\vec{x})=-\frac{4\pi}{c}\vec{J}_{\omega}(\vec{x}). \tag{3.7}$$

Using the Green function defined in Eq. (3.1), the vector potential is related to the current density via

$$\vec{A}_{\omega}(\vec{x})=-\frac{4\pi}{c}\int d^3x'\,\vec{e}_{\alpha}G_{\alpha\beta}^{\omega}(\vec{x},\vec{x}')J_{\omega,\beta}(\vec{x}'). \tag{3.8}$$

In the following analysis, we assume the current density is a δ function located at $\vec{x}_0$

$$\vec{J}_{\omega}(\vec{x})=\frac{e}{m}j_{\omega}\delta(\vec{x}-\vec{x}_0)\vec{p}_{12}. \tag{3.9}$$

The radiation field of this classical dipole current is easily obtained from Eq. (3.8)

$$\vec{A}_{\omega}(\vec{x})=\vec{A}_{rad,\omega}(\vec{x})j_{\omega}, \tag{3.10a}$$

$$\vec{A}_{rad,\omega}(\vec{x})=-\frac{4\pi e}{mc}\,\vec{e}_{\alpha}G_{\alpha\beta}^{\omega}(\vec{x},\vec{x}_0)p_{12,\beta}. \tag{3.10b}$$

Using Eq. (3.8), we can also express the total energy radiated by this current source as

$$\mathcal{E}_{rad}=-\int dt\int d^3x\,\vec{J}(\vec{x},t)\cdot\vec{E}(\vec{x},t)=\frac{\pi}{c^2}\int d^3x\int d^3x'\int d\omega\,\omega[iJ_{\omega,\alpha}^{*}(\vec{x})\times J_{\omega,\beta}(\vec{x}')G_{\alpha,\beta}^{\omega}(\vec{x},\vec{x}')+\mathrm{c.c.}]. \tag{3.11}$$

Then for the current source in Eq. (3.9), the total radiation energy is

$$\mathcal{E}_{rad}=-\frac{2\pi}{c^2}\frac{e^2}{m^2}p_{12,\alpha}p_{12,\beta}\Omega\int d\omega\,|j_{\omega}|^2\mathrm{Im}\,[G_{\alpha\beta}^{\omega}(\vec{x}_0,\vec{x}_0)], \tag{3.12}$$

where we have replaced ω in Eq. (3.11) as Ω, which is equivalent to ignoring a small term of the order γ_{12}/Ω.

Notice that if we choose j_ω to be

$$j_\omega = \frac{1}{i(\Omega-\omega)+\gamma_{12}}, \tag{3.13}$$

the classical radiation energy becomes proportional to the quantum spontaneous emission rate. Therefore, we have

$$\frac{\gamma_{cavity}}{\gamma_{free}} = \frac{\mathcal{E}_{cavity}}{\mathcal{E}_{free}}, \tag{3.14}$$

where γ_{cavity} is the spontaneous emission rate of the atom inside the dielectric microcavity, and γ_{free} is that of the atom in free space, $\mathcal{E}_{cavity}$ is the total classical radiation energy of a corresponding dipole current in the same dielectric microcavity, $\mathcal{E}_{free}$ is the radiation energy of the same dipole current in free space. This proportionality allows us to calculate the spontaneous emission rate from classical electrodynamics.

To numerically calculate the total radiation energy of a classical dipole, we can use the finite difference time domain (FDTD) method [39]. In this method, we numerically solve the following two equations:

$$\frac{1}{c}\frac{\partial \vec{B}(\vec{x},t)}{\partial t} = -\nabla\times\vec{E}(\vec{x},t), \tag{3.15a}$$

$$\frac{\epsilon(\vec{x})}{c}\frac{\partial \vec{E}(\vec{x},t)}{\partial t} = \nabla\times\vec{H}(\vec{x},t) - \frac{4\pi}{c}\vec{J}(\vec{x},t). \tag{3.15b}$$

The temporal dependence of the dipole current is found through using Eq. (3.6a), Eq. (3.9) and Eq. (3.13), which gives

$$\vec{J}(\vec{x},t) = \begin{cases} 0 & t<0 \\ \dfrac{\vec{p}_{12}}{p_{12}}\delta(\vec{x}-\vec{x}_0)e^{-\gamma_{12}t}\cos(\Omega t) & t>0, \end{cases} \tag{3.16}$$

where we have normalized the current amplitude to 1. We should remember that the solutions of Eq. (3.15) contain both a longitudinal field and a transverse field, while the electromagnetic field satisfying Eq. (3.7) has a transverse component only [49]. Correspondingly, in the numerical calculations, the influence of the longitudinal field should be carefully eliminated [39].

IV. EXTERNAL QUANTUM EFFICIENCY

In Ref. [8], a classical model was used to numerically calculate the external quantum efficiency η of a two-dimensional photonic crystal structure, where η is evaluated as the ratio of the radiation power of a classical dipole source that goes through a given surface S divided by the total dipole radiation power. For a classical decaying source defined in Eq. (3.9), it is more appropriate to use the radiation energy rather than the radiation power. The radiation field of such classical source is given in Eq. (3.10), from which $\mathcal{E}_S$, the total energy emitted through surface S, can be found by integrating the Poynting vector over surface S

$$\begin{aligned}\mathcal{E}_S &= \frac{c}{4\pi}\int dt \int_S da\, \vec{n}\cdot[\vec{E}\times\vec{H}] \\ &= -\frac{1}{8\pi}\int_S da \int d\omega\, \omega\vec{n}\cdot \mathrm{Im}\,\{\vec{A}_{rad,\omega}(\vec{x}) \\ &\quad \times[\nabla\times\vec{A}^*_{rad,\omega}(\vec{x})]\}\,|j_\omega|^2. \end{aligned} \tag{4.1}$$

Dividing $\mathcal{E}_S$ by the total radiation energy $\mathcal{E}_{total}$, which is obtained from the above equation after replacing the surface S by an arbitrary surface enclosing the dipole source, we find the classical expression for the quantum efficiency η.

In the framework of quantum mechanics, the external quantum efficiency η is defined as the amount of photons go through surface S divided by the total photon emission and can be easily found by using a quantum Poynting vector, which can be derived from Eq. (2.6) and its conjugate equation for $\hat{\mathbf{A}}^{(+)}$, $\hat{\mathbf{J}}^{(+)}_{tot}$:

$$\frac{\epsilon(\vec{x})}{c^2}\frac{d\dot{\hat{\mathbf{A}}}^{(-)}}{dt} + \nabla\times[\nabla\times\hat{\mathbf{A}}^{(-)}] = \frac{4\pi}{c}\hat{\mathbf{J}}^{(-)}_{tot}, \tag{4.2a}$$

$$\frac{\epsilon(\vec{x})}{c^2}\frac{d\dot{\hat{\mathbf{A}}}^{(+)}}{dt} + \nabla\times[\nabla\times\hat{\mathbf{A}}^{(+)}] = \frac{4\pi}{c}\hat{\mathbf{J}}^{(+)}_{tot}. \tag{4.2b}$$

Multiplying $\dot{\hat{\mathbf{A}}}^{(+)}$ by Eq. (4.2a) from the left, multiplying $\dot{\hat{\mathbf{A}}}^{(-)}$ by Eq. (4.2b) from the right, and adding the two equations, we get

$$\begin{aligned}&\frac{d}{dt}\left\{\frac{\epsilon(\vec{x})}{c^2}\dot{\hat{\mathbf{A}}}^{(+)}\cdot\dot{\hat{\mathbf{A}}}^{(-)} + [\nabla\times\hat{\mathbf{A}}^{(+)}]\cdot[\nabla\times\hat{\mathbf{A}}^{(-)}]\right\} \\ &\quad + \nabla\cdot\{-\dot{\hat{\mathbf{A}}}^{(+)}\times[\nabla\times\hat{\mathbf{A}}^{(-)}] + [\nabla\times\hat{\mathbf{A}}^{(+)}]\times\dot{\hat{\mathbf{A}}}^{(-)}\} \\ &\quad = \frac{4\pi}{c}(\dot{\hat{\mathbf{A}}}^{(+)}\cdot\hat{\mathbf{J}}^{(-)}_{tot} + \hat{\mathbf{J}}^{(+)}_{tot}\cdot\dot{\hat{\mathbf{A}}}^{(-)}), \end{aligned} \tag{4.3}$$

which has the right form for energy conservation. However, we still need a constant factor to fully determine the energy density and the Poynting vector. Notice that the last term of the above equation should represent the spatial density of the energy emission rate. Thus, apart from a constant factor C, the spatial integration of this quantity should equal to the atomic transition rate multiplied by the amount of energy emission from each atomic transition. Consequently, from Eq. (2.12) we have

$$\begin{aligned}-\hbar\Omega\frac{d\hat{N}_2}{dt} &= -\hbar\Omega\frac{i}{\hbar c}\int d^3x\,[\hat{\mathbf{J}}^{(+)}_{tot}\cdot\hat{\mathbf{A}}^{(-)} - \hat{\mathbf{A}}^{(+)}\cdot\hat{\mathbf{J}}^{(-)}_{tot}] \\ &= C\frac{4\pi}{c}(\dot{\hat{\mathbf{A}}}^{(+)}\cdot\hat{\mathbf{J}}^{(-)}_{tot} + \hat{\mathbf{J}}^{(+)}_{tot}\cdot\dot{\hat{\mathbf{A}}}^{(-)}). \end{aligned} \tag{4.4}$$

Approximate the time dependence of $\hat{\mathbf{A}}^{(-)}(t)$ and $\hat{\mathbf{A}}^{(+)}(t)$ as $e^{-i\Omega t}$ and $e^{i\Omega t}$, respectively, we find the constant factor to be

$1/4\pi$. Putting this constant factor into Eq. (4.3), we get the following equations for energy conservation

$$\frac{d\hat{\mathcal{E}}}{dt}+\nabla\cdot\hat{\mathcal{S}}=\hat{\mathcal{P}}, \tag{4.5a}$$

$$\hat{\mathcal{E}}=\frac{1}{4\pi}\left\{\frac{\epsilon(\vec{x})}{c^2}\dot{\hat{\mathbf{A}}}^{(+)}\cdot\dot{\hat{\mathbf{A}}}^{(-)}+[\nabla\times\hat{\mathbf{A}}^{(+)}]\cdot[\nabla\times\hat{\mathbf{A}}^{(-)}]\right\}, \tag{4.5b}$$

$$\hat{\mathcal{S}}=\frac{1}{4\pi}\{-\dot{\hat{\mathbf{A}}}^{(+)}\times[\nabla\times\hat{\mathbf{A}}^{(-)}]+[\nabla\times\hat{\mathbf{A}}^{(+)}]\times\dot{\hat{\mathbf{A}}}^{(-)}\}, \tag{4.5c}$$

$$\hat{\mathcal{P}}=\frac{1}{c}\{\dot{\hat{\mathbf{A}}}^{(+)}\cdot\hat{\mathbf{J}}_{tot}^{(-)}+\hat{\mathbf{J}}_{tot}^{(+)}\cdot\dot{\hat{\mathbf{A}}}^{(-)}\}, \tag{4.5d}$$

where $\hat{\mathcal{E}}$ is the energy density operator, $\hat{\mathcal{S}}$ is the quantum Poynting operator, and they closely resemble the results in classical electrodynamics [49]. Similar forms for the Poynting vector $\hat{\mathcal{S}}$ have been used in the literature [46,50]. With this result, the amount of power emitted through surface S can be found by using Eq. (3.2), integrating the quantum Poynting vector $\hat{\mathcal{S}}$ over surface S, and taking ensemble average by applying Eq. (2.10a). The result is

$$\langle\hat{\mathcal{S}}_S\rangle=-\frac{1}{4\pi^2}\overline{n}_2\int_S da\int d\omega\,\omega\vec{n}\cdot\mathrm{Im}\{\vec{A}_{rad,\omega}(\vec{x})\times[\nabla\times\vec{A}^{*}_{rad,\omega}(\vec{x})]\}\frac{2\gamma_{12}}{(\Omega-\omega)^2+\gamma_{12}^2}. \tag{4.6}$$

Once again, choosing $j_\omega=1/[i(\Omega-\omega)+\gamma_{12}]$ and comparing Eq. (4.6) with Eq. (4.1), we find the external quantum efficiency η satisfies

$$\eta=\frac{\langle\hat{\mathcal{S}}_S\rangle}{\langle\hat{\mathcal{S}}_{total}\rangle}=\frac{\mathcal{E}_S}{\mathcal{E}_{total}}, \tag{4.7}$$

where $\langle\hat{\mathcal{S}}_{total}\rangle$ is calculated using Eq. (4.6) with the integration surface S replaced by a closed surface that contains the atomic source. From this relation, we conclude that the external quantum efficiency can also be evaluated using a classical algorithm.

V. SPONTANEOUS EMISSION FACTOR

The spontaneous emission factor β of a given optical mode is defined as the rate of spontaneous emission into that mode divided by the total spontaneous emission rate and can be derived from the photon rate equation in the following way.

We assume that $\chi(\omega,\vec{x})$ in Eq. (2.11) is purely imaginary with no frequency dependence, and contains two parts $\chi(\omega,\vec{x})=-i\chi_a(\vec{x})+i\chi_e(\vec{x})$, where $\chi_a(\vec{x})$ gives the atomic gain and $\chi_e(\vec{x})$ represents the mode loss. With this approximation, Eq. (2.6) becomes

$$\frac{\epsilon(\vec{x})}{c^2}\frac{\partial^2\hat{\mathbf{A}}^{(-)}}{\partial t^2}=-\nabla\times[\nabla\times\hat{\mathbf{A}}^{(-)}]+\frac{4\pi}{c}[-i\chi_a(\vec{x})+i\chi_e(\vec{x})]\hat{\mathbf{A}}^{(-)}+\frac{4\pi}{c}\hat{\mathbf{J}}_{fluc}^{(-)}. \tag{5.1}$$

From Sec. II, we know that the vector potential operator $\hat{\mathbf{A}}^{(-)}(\vec{x},t)$ in the above equation can be expanded as

$$\hat{\mathbf{A}}^{(-)}(\vec{x},t)=\sum_n\sqrt{\frac{2\pi\hbar c^2}{\omega_n}}\hat{\mathcal{A}}_n(t)e^{-i\omega_n t}\vec{A}_n(\vec{x}), \tag{5.2}$$

where $\hat{a}_n(t)$ in Eq. (2.1b) is replaced by $\hat{a}_n(t)=\hat{\mathcal{A}}_n(t)e^{-i\omega_n t}$ and the operator $\hat{\mathcal{A}}_n(t)$ represents the slow changing envelope of $\hat{a}_n(t)$. If we are interested in an optical mode $\vec{A}_0(\vec{x})$, we can substitute Eq. (5.2) into Eq. (5.1) and multiply both sides by $\vec{A}_0^{*}(\vec{x})$. After spatial integration, we obtain

$$\frac{d\hat{\mathcal{A}}_0}{dt}=-\frac{\Gamma_0}{2}\hat{\mathcal{A}}_0+i\sqrt{\frac{2\pi}{\hbar\omega_0}}\int d^3x\vec{A}_0^{*}(\vec{x})\cdot\hat{\mathbf{J}}_{fluc}^{(-)}(\vec{x},t)e^{i\omega_0 t}, \tag{5.3a}$$

$$\Gamma_0=-\frac{4\pi c}{\omega_0}\int d^3x(\chi_a(\vec{x})-\chi_e(\vec{x}))\vec{A}_0^{*}(\vec{x})\cdot\vec{A}_0(\vec{x}), \tag{5.3b}$$

where the small term $d^2\hat{\mathcal{A}}_0/dt^2$ is ignored. Taking the ensemble average using Eq. (2.7), from the above equation we can derive the rate equation for the average photon number in the 0th mode

$$\frac{d}{dt}\langle\hat{\mathcal{A}}_0^{\dagger}\hat{\mathcal{A}}_0\rangle=-\Gamma_0\langle\hat{\mathcal{A}}_0^{\dagger}\hat{\mathcal{A}}_0\rangle+\gamma_0\overline{n}_2, \tag{5.4a}$$

$$\gamma_0=\frac{4\pi}{\hbar\omega_o}\frac{e^2}{m^2}|\vec{p}_{12}\cdot\vec{A}_0(\vec{x}_0)|^2\frac{\gamma_{12}+\frac{\Gamma_0}{2}}{(\omega_0-\Omega)^2+\left(\gamma_{12}+\frac{\Gamma_0}{2}\right)^2}, \tag{5.4b}$$

where γ_0 is the rate of spontaneous emission into the 0th mode. The spontaneous emission factor β for the this mode can then be written as

$$\beta=\frac{\gamma_0}{\gamma}$$

$$=-\frac{\pi c^2}{2\omega_0}\frac{|\vec{p}_{12}\cdot\vec{A}_0(\vec{x}_0)|^2\dfrac{\gamma_{12}+\dfrac{\Gamma_0}{2}}{(\omega_0-\Omega)^2+\left(\gamma_{12}+\dfrac{\Gamma_0}{2}\right)^2}}{p_{12,\alpha}p_{12,\beta}\displaystyle\int d\omega\,\frac{\gamma_{12}}{(\omega-\Omega)^2+\gamma_{12}^2}\,\mathrm{Im}[G^{\omega}_{\alpha\beta}(\vec{x}_0,\vec{x}_0)]}, \tag{5.5}$$

where γ, the spontaneous emission rate of the two-level atom in the microcavity, has been found in Eq. (3.5).

It is also interesting to calculate the spontaneous emission factor from another perspective. First we notice that the spontaneous emission rate is proportional to the imaginary part of the Green function

$$\gamma\sim\int d\omega\,\frac{1}{(\omega-\Omega)^2+\gamma_{12}^2}\,\mathrm{Im}\,[G^{\omega}_{\alpha\beta}(\vec{x}_0,\vec{x}_0)]. \tag{5.6}$$

In Appendix C, we have expanded the Green function in terms of the optical modes $\{\vec{A}_n\}$. For each resonance mode, it has a frequency dependence of the form $1/(\omega-\omega_n+i\Gamma_n/2)$, a function with a sharp peak for a high Q optical mode. Therefore, it is natural to define γ_0 as the rate of the spontaneous emission as it goes into the frequency range of $|\omega-\omega_0|\sim\Gamma_0$. More specifically, from Eq. (3.5) and Eq. (C5), γ_0 is

$$\gamma_0=\frac{4}{\hbar\omega_0}\frac{e^2}{m^2}|\vec{p}_{12}\cdot\vec{A}_0(\vec{x}_0)|^2 \times\int d\omega\,\frac{\gamma_{12}}{(\Omega-\omega)^2+\gamma_{12}^2}\,\frac{\dfrac{\Gamma_0}{2}}{(\omega-\omega_0)^2+\left(\dfrac{\Gamma_0}{2}\right)^2}. \tag{5.7}$$

Since the convolution of two Lorentzian functions is still a Lorentzian function, we have the following result for γ_0:

$$\gamma_0=\frac{4\pi}{\hbar\omega_0}\frac{e^2}{m^2}|\vec{p}_{12}\cdot\vec{A}_0(\vec{x}_0)|^2\frac{\gamma_{12}+\dfrac{\Gamma_0}{2}}{(\omega_0-\Omega)^2+\left(\gamma_{12}+\dfrac{\Gamma_0}{2}\right)^2}, \tag{5.8}$$

which is the same as Eq. (5.4b) derived from the photon rate equation analysis.

In our previous analysis, we have shown that both the spontaneous emission rate and the external quantum efficiency can be calculated from the radiation field of a classical decaying dipole. For the spontaneous emission factor, a classical analogy would be the ratio of the energy emitted into a given optical mode by a classical dipole. However, we need to specify what the ''energy emitted into an optical mode'' is and how to calculate it.

For any classical electromagnetic field, we can expand it as

$$\vec{A}(\vec{x},t)=\frac{1}{2}\sum_n\,[\alpha_n(t)\vec{A}_n(\vec{x})+\alpha_n^*(t)\vec{A}_n^*(\vec{x})], \tag{5.9a}$$

$$\vec{E}(\vec{x},t)=\sum_n\,\left\{-\frac{1}{2c}[\dot{\alpha}_n(t)\vec{A}_n(\vec{x})+\dot{\alpha}_n^*(t)\vec{A}_n^*(\vec{x})]\right\}, \tag{5.9b}$$

where $\alpha_n(t)$ represents the negative frequency part and $\alpha_n^*(t)$, its complex conjugate, is the positive frequency part. The Fourier transform $\alpha_{n,\omega}$ of the expansion coefficient $\alpha_n(t)$ is defined as

$$\alpha_n(t)=\frac{1}{\sqrt{2\pi}}\int d\omega\;\alpha_{n,\omega}e^{-i\omega t}. \tag{5.10}$$

Using the above definitions and the mode orthogonality condition, we have

$$\alpha_{n,\omega}=\int d^3x\;\epsilon(\vec{x})\vec{A}_n^*(\vec{x})\cdot\vec{A}_\omega(\vec{x}), \tag{5.11}$$

where $\vec{A}_\omega(\vec{x})$ is given in Eq. (3.6). For a classical current in Eq. (3.9), the radiation field is given by Eq. (3.10) and can be expanded according to Eq. (5.9a). The expansion coefficient $\alpha_{0,\omega}$ of the 0th mode is found from Eq. (5.11)

$$\alpha_{0,\omega}=-\frac{2\pi ec}{m\omega_0}\,\vec{p}_{12}\cdot\vec{A}_0^*(\vec{x}_0)\frac{j_\omega}{\omega-\omega_0+i\dfrac{\Gamma_0}{2}}, \tag{5.12}$$

where we have used Eqs. (C5), (3.9), (3.10), and the mode orthogonality condition.

The energy emitted into the 0th mode $\vec{A}_0$ is naturally defined as

$$\mathcal{E}_0=-\int dt\int d^3x\,\vec{J}(\vec{x},t)\cdot\left\{-\frac{1}{2c}[\dot{\alpha}_0(t)\vec{A}_0(\vec{x}) +\dot{\alpha}_0^*(t)\vec{A}_0^*(\vec{x})]\right\}. \tag{5.13}$$

After using Eq. (5.12), $\mathcal{E}_0$ becomes

$$\mathcal{E}_0=\frac{e}{8\pi mc}\int dt\left[\int d\omega\, j_\omega e^{-i\omega t}+\text{c.c.}\right]\cdot\left[\int d\omega'(-i\omega')\times\alpha_{0,\omega'}e^{-i\omega' t}\vec{p}_{12}\cdot\vec{A}_0(\vec{x}_0)+\text{c.c.}\right]$$

$$=\frac{\pi\Omega}{\omega_0}\frac{e^2}{m^2}|\vec{p}_{12}\cdot\vec{A}_0(\vec{x}_0)|^2\int d\omega\,|j_\omega|^2\frac{\frac{\Gamma_0}{2}}{(\omega-\omega_0)^2+\left(\frac{\Gamma_0}{2}\right)^2}. \tag{5.14}$$

Once again, we choose j_ω to be $j_\omega=1/[i(\Omega-\omega)+\gamma_{12}]$ and carry out the frequency integration in Eq. (5.14) to get

$$\mathcal{E}_0=\frac{\pi^2\Omega}{\omega_0\gamma_{12}}\frac{e^2}{m^2}|\vec{p}_{12}\cdot\vec{A}_0(\vec{x}_0)|^2\frac{\gamma_{12}+\frac{\Gamma_0}{2}}{(\Omega-\omega_0)^2+\left(\gamma_{12}+\frac{\Gamma_0}{2}\right)^2}. \tag{5.15}$$

Finally, in the classical framework, we define the spontaneous emission factor for the mode $\vec{A}_0$ as

$$\beta=\frac{\mathcal{E}_0}{\mathcal{E}}$$

$$=-\frac{\pi c^2}{2\omega_0}\frac{|\vec{p}_{12}\cdot\vec{A}_0(\vec{x}_0)|^2\frac{\gamma_{12}+\frac{\Gamma_0}{2}}{(\omega_0-\Omega)^2+\left(\gamma_{12}+\frac{\Gamma_0}{2}\right)^2}}{p_{12,\alpha}p_{12,\beta}\int d\omega\frac{\gamma_{12}}{(\omega-\Omega)^2+\gamma_{12}^2}\text{Im}[G^\omega_{\alpha\beta}(\vec{x}_0,\vec{x}_0)]}, \tag{5.16}$$

where $\mathcal{E}$, the total energy emitted by this current source, is given by Eq. (3.12). This equation shows that the spontaneous emission factor obtained from classical electrodynamics is the same as our quantum result given in Eq. (5.5).

This classical analysis can also be implemented numerically to obtain the spontaneous emission factor. As before, we can solve Eq. (3.15) to get the radiation field of the classical dipole current source given in Eq. (3.16). However, we would like to find a simpler expansion scheme than Eq. (5.9a) and it is more convenient to work with real number instead of complex number. We recall that if the dielectric constant $\epsilon(\vec{x})$ is real, the eigenmode function $\vec{A}_n(\vec{x})$ can be chosen to be a real function. In this case, the electric field can be expanded as

$$\vec{E}(\vec{x},t)=\sum_n\tilde{\alpha}_n(t)\vec{A}_n(\vec{x}), \tag{5.17a}$$

$$\tilde{\alpha}_n(t)=\int d^3x\,\epsilon(\vec{x})\vec{A}_n(\vec{x})\cdot\vec{E}(\vec{x},t), \tag{5.17b}$$

$$\mathcal{E}_0=-\int dt\int d^3x\,\tilde{\alpha}_0(t)\vec{J}(\vec{x},t)\cdot\vec{A}_0(\vec{x}). \tag{5.17c}$$

Thus to calculate the spontaneous emission factor, first we find a properly normalized mode function $\vec{A}_0(\vec{x})$, either numerically or analytically. Then we can use the above expansion relations to evaluate $\tilde{\alpha}_0$ from the dipole radiation field, which in turn gives $\mathcal{E}_0$. Finally, dividing $\mathcal{E}_0$ by $\mathcal{E}$, the total dipole radiation energy, we obtain the spontaneous emission factor β.

VI. DISCUSSION

As a simple exercise in using the previous theoretical results, we calculate the spontaneous emission rate in a bulk medium with dielectric constant ϵ_{bulk}. Assuming the dielectric medium is placed in a big box of volume V, the appropriate normalized modes are simply

$$\vec{A}_{n,\sigma}(\vec{x})=\frac{1}{\sqrt{\epsilon_{bulk}V}}\vec{e}_\sigma e^{-i\vec{k}_n\cdot\vec{x}}, \tag{6.1}$$

where $\vec{e}_\sigma$ represents the polarization of the electromagnetic mode. Applying Eq. (5.8) and averaging over the mode polarization, the spontaneous emission rate into each individual mode becomes

$$\gamma_n=\frac{4\pi\Omega}{3\hbar\epsilon_{bulk}V}|\vec{\mu}_{12}|^2\frac{\gamma_{12}}{(\omega_n-\Omega)^2+\gamma_{12}^2}, \tag{6.2}$$

where we have used $\vec{p}_{12}=-im\Omega\vec{\mu}_{12}/e$ and set the cavity mode decay rate to 0. The total spontaneous emission rate is then obtained from multiplying Eq. (6.2) by the density of modes, $V\epsilon_{bulk}^{3/2}\omega^2/\pi^2c^3$, and integrating over the frequency domain

$$\gamma=\frac{4\Omega\sqrt{\epsilon_{bulk}}}{3\pi\hbar c^3}|\vec{\mu}_{12}|^2\int d\omega\,\omega^2\frac{\gamma_{12}}{(\omega-\Omega)^2+\gamma_{12}^2}$$

$$=\frac{4\Omega^3\sqrt{\epsilon_{bulk}}|\vec{\mu}_{12}|^2}{3\hbar c^3}, \tag{6.3}$$

which is identical to the quantum mechanical result [48].

The previous theoretical analysis can also be directly applied to estimate the spontaneous emission factor in two types of microcavities: the dielectric microcavity, such as the defect cavity in a photonic crystal [51] or a microdisk cavity [36], and the concentric or confocal cavities [52,53] (see also Fig. 1). Since an analytical solution is very difficult for such complicated structures, the spontaneous emission rate and the spontaneous emission factor are usually estimated by making various approximations. These estimations have been discussed, and their range of validity has been generalized in Ref. [52]. As we shall show here, these results can be directly derived from Eq. (5.8).

The first type of microcavity can be designed such that it supports a high Q mode. Usually we can define an effective

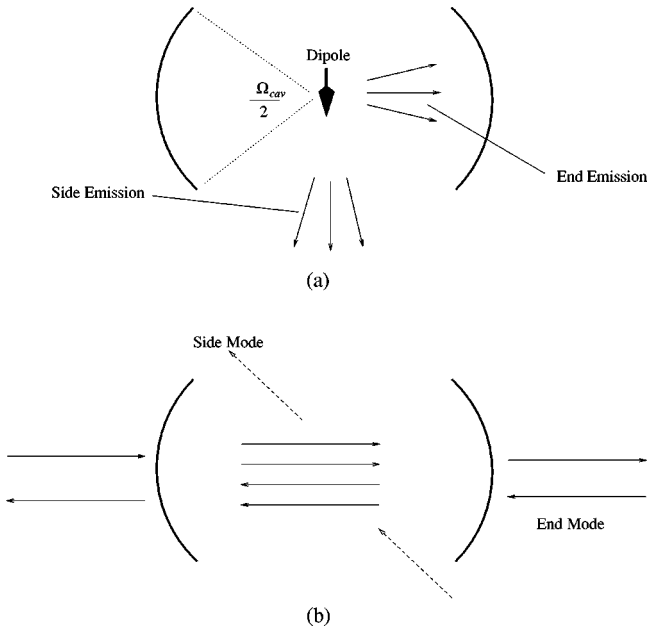

FIG. 1. Spontaneous emission in an optical resonator: (a) The end emission and the side emission; (b) the side mode and the end mode.

cavity volume V_e such that $\vec{A}_{0,\sigma}(\vec{x}_0)$, the mode function at $\vec{x}_0$, can be approximated as $\vec{e}_\sigma/\sqrt{\epsilon V_e}$, where $\vec{e}_\sigma$ is a unit vector and ϵ is the dielectric constant of the cavity medium. With this approximation, the spontaneous emission rate into the cavity mode, γ_{cav}, is directly obtained from Eq. (5.8)

$$\gamma_{cav}=\frac{4\pi\Omega}{\hbar\epsilon V_e}|\vec{\mu}_{12}\cdot\vec{e}_\sigma|^2\frac{\gamma_{12}+\frac{\Gamma_{cav}}{2}}{(\omega_{cav}-\Omega)^2+\left(\gamma_{12}+\frac{\Gamma_{cav}}{2}\right)^2}, \tag{6.4}$$

where ω_{cav} is the cavity frequency and Γ_{cav} is the cavity photon decay rate. If we assume the total spontaneous emission rate is essentially the same as the bulk value given in Eq. (6.3), the spontaneous emission factor is

$$\beta=\frac{3}{8\pi^2}\frac{\lambda_e^3}{V_e}\frac{|\vec{\mu}_{12}\cdot\vec{e}_\sigma|^2}{|\vec{\mu}_{12}|^2}\frac{\Omega\left(\gamma_{12}+\frac{\Gamma_{cav}}{2}\right)}{(\omega_{cav}-\Omega)^2+\left(\gamma_{12}+\frac{\Gamma_{cav}}{2}\right)^2}, \tag{6.5}$$

where λ_e is the light wavelength in dielectric medium. This estimation is quite close to the ''one photon per mode'' approach in Ref. [52]. However, we should stress that in many cases, this estimation is only qualitatively correct, since the spontaneous emission rate can be greatly modified by the high Q cavity modes, such as the whispering gallery modes in a dielectric sphere [14]. If an exact result is needed, we can always use the algorithm described in Sec. V.

The second type of cavities, the concentric or the confocal cavities, which consist of two mirrors in free space with high reflectivity, are widely used in atomic beam experiments [3,53]. The spontaneous emission process in such cavities can usually be classified into two types: the side emission and the end emission [3] [see Fig. 1(a)]. In the side emission process, the photons are radiated to the side of the cavity and enter into free space without passing through the end mirrors. Assuming that the end mirror of the cavity spans a solid angle of $\Delta\Omega_{cav}$ to the emission atom, the side spontaneous emission rate is just proportional to $(1-\Delta\Omega_{cav}/4\pi)\gamma_f$, where γ_f is the free space spontaneous emission rate. In the end emission process, the photons are first radiated into the cavity mode, and then coupled to the outside free space mode through the decay of the cavity mode. Therefore, the end emission rate can be estimated from Eq. (6.4). The total spontaneous emission rate, as a result of the two emission processes, becomes

$$\gamma=\gamma_f\left(1-\frac{\Delta\Omega_{cav}}{4\pi}\right)+\gamma_f\frac{3}{8\pi^2}\frac{\lambda^3}{V_e}\frac{\Omega\left(\gamma_{12}+\frac{\Gamma_{cav}}{2}\right)}{(\omega_{cav}-\Omega)^2+\left(\gamma_{12}+\frac{\Gamma_{cav}}{2}\right)^2}, \tag{6.6}$$

as has been shown in Ref. [52].

The spontaneous rate can also be estimated in another way similar to the Fano-type approach in Ref. [52]. Instead of using the cavity mode, we assume that the cavity is inside a big box of volume V and use the electromagnetic modes within the whole box to calculate the spontaneous emission rate. Corresponding to the two emission processes in the previous analysis, these electromagnetic modes can also be classified into two types: the side modes and the end modes [see Fig. 1(b)]. The side modes are defined as the modes whose wave vector $\vec{k}_n$ is mostly outside the solid angle $\Delta\Omega_{cav}$ spanned by the end mirrors, and the rest modes are called the end modes. Assuming that the box is big enough so that the mode density is not changed by the presence of the cavity, the density of states for the side modes and the end modes are, respectively, $(1-\Delta\Omega_{cav}/4\pi)V\omega^2/\pi^2c^3$, and $(\Delta\Omega_{cav}/4\pi)V\omega^2/\pi^2c^3$.

For the end modes, the field intensity inside the cavity is enhanced due to the interference of the two mirrors. The enhancement factor is [52,54]

$$A(\omega)=\frac{2\omega_{fsr}}{\pi\Gamma_{cav}}\frac{\left(\frac{\Gamma_{cav}}{2}\right)^2}{(\omega-\omega_{cav})^2+\left(\frac{\Gamma_{cav}}{2}\right)^2}, \tag{6.7}$$

where the ω_{cav} is the cavity resonant frequency, Γ_{cav} is the cavity mode decay rate, ω_{fsr} is the free spectral range. The Γ_{cav} and ω_{fsr} are defined as follows:

$$\Gamma_{cav}=\frac{1-R}{\pi}\omega_{fsr}, \tag{6.8a}$$

$$\omega_{fsr}=\frac{\pi c}{L}, \tag{6.8b}$$

where R is the intensity reflectivity of the end mirror, and L is the cavity length. To find the spontaneous emission rate of the end modes, we multiply Eq. (6.2) by this enhancement factor $A(\omega)$, and the density of end modes, which is $(1-\Delta\Omega_{cav}/4\pi)V\omega^2/\pi^2c^3$, then integrate the product, with the result

$$\gamma_{end}=\frac{\Delta\Omega_{cav}}{4\pi}\frac{4\Omega}{3\pi\hbar c^3}|\vec{\mu}_{12}|^2\int d\omega\,\omega^2 A(\omega)\frac{\gamma_{12}}{(\omega-\Omega)^2+\gamma_{12}^2}$$

$$=\frac{\Delta\Omega_{cav}}{4\pi}\gamma_f\frac{\Gamma_{cav}}{1-R}\frac{\gamma_{12}+\dfrac{\Gamma_{cav}}{2}}{(\omega_{cav}-\Omega)^2+\left(\gamma_{12}+\dfrac{\Gamma_{cav}}{2}\right)^2}. \tag{6.9}$$

For the side modes, such interference enhancement is absent since the electromagnetic field of the modes does not propagate through the two mirrors. So the mode amplitude of $\vec{A}_n(\vec{x}_0)$ is still $1/\sqrt{V}$. We can use the density of modes given before to include the spontaneous emission rate of every side modes. The result is

$$\gamma_{side}=\left(1-\frac{\Delta\Omega_{cav}}{4\pi}\right)\frac{4\Omega}{3\pi\hbar c^3}|\vec{\mu}_{12}|^2\int d\omega\,\omega^2\frac{\gamma_{12}}{(\omega-\Omega)^2+\gamma_{12}^2}$$

$$=\left(1-\frac{\Delta\Omega_{cav}}{4\pi}\right)\gamma_f. \tag{6.10}$$

The total spontaneous emission rate is the sum of γ_{end} and γ_{side}

$$\gamma=\gamma_f\left(1-\frac{\Delta\Omega_{cav}}{4\pi}\right)$$

$$+\gamma_f\frac{\Delta\Omega_{cav}}{4\pi}\frac{\Gamma_{cav}}{1-R}\frac{\gamma_{12}+\dfrac{\Gamma_{cav}}{2}}{(\omega_{cav}-\Omega)^2+\left(\gamma_{12}+\dfrac{\Gamma_{cav}}{2}\right)^2}. \tag{6.11}$$

From diffraction considerations, V_e can be estimated as [52]

$$V_e\sim\frac{\lambda^2 L}{\Delta\Omega_{cav}}. \tag{6.12}$$

Using this result, Eqs. (6.6) and (6.11), which give the spontaneous emission rate using a different approach, agree with each other, as in Ref. [52]. The spontaneous emission factor can also be estimated using either Eq. (6.6) or Eq. (6.11), and naturally the two results are essentially the same.

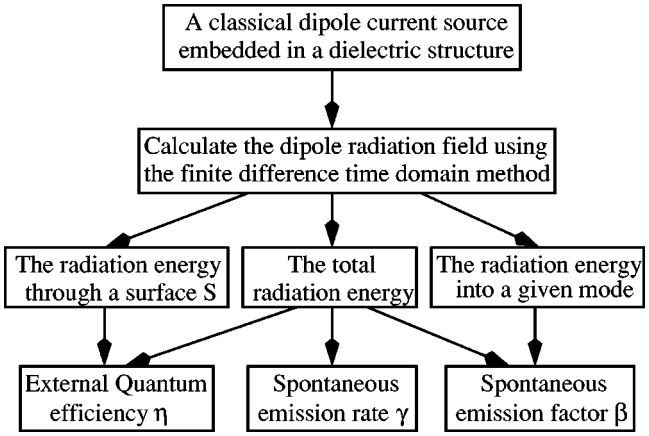

FIG. 2. Schematic of the classical algorithm for the calculation of the spontaneous emission rate, external quantum efficiency, and spontaneous emission factor.

VII. SUMMARY

Starting from the quantum Maxwell equation, we analyze the spontaneous emission process of a two-level atom in a lossless and inhomogeneous dielectric cavity. We find that a decaying current source is the classical analogy of a two-level atom with finite dipole dephasing rate. By establishing the equivalence between the classical approach and quantum approach, we show that a classical numerical algorithm can be used to simulate the spontaneous emission process in a microcavity, as illustrated in Fig. 2. First we use the finite difference time domain method to calculate the radiation field of a classical current given by Eq. (3.16). The modification of the spontaneous emission rate can be found by calculating the total radiation energy of this classical dipole current source in the microcavity. The external quantum efficiency is found from the energy emission by this current source through a given surface S divided by the total radiation energy. The spontaneous emission factor of a given mode can also be obtained by calculating the energy emission into that particular mode and dividing the result by the total radiation energy.

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APPENDIX A

We summarize some important properties of the eigenmodes $\{\vec{A}_n(\vec{x})\}$ that were used by Glauber and Lewenstein to quantize the electromagnetic field in a linear, lossless dielectric medium [24]. First, they satisfy the following eigenmode equations:

$$\nabla\times[\nabla\times\vec{A}_n(\vec{x})]=\frac{\omega_n^2\epsilon(\vec{x})}{c^2}\vec{A}_n(\vec{x}), \tag{A1}$$

where ω_n is the eigenvalue for the nth eigenmode. Also, the eigenmodes are orthonormal and complete

$$\int d^3x\, \epsilon(\vec{x})\vec{A}_m^*(\vec{x})\cdot\vec{A}_n(\vec{x})=\delta_{mn}, \tag{A2a}$$

$$\delta^{\epsilon}_{\alpha\beta}(\vec{x},\vec{x}')=\epsilon(\vec{x})\sum_n A_{n\alpha}(\vec{x})A^*_{n\beta}(\vec{x}'), \tag{A2b}$$

where $A_{n\alpha}(\vec{x})$ is the αth components of the vector eigenmode $\vec{A}_n(\vec{x})$. This $\delta^{\epsilon}_{\alpha\beta}(\vec{x},\vec{x}')$ is analogous to the standard transverse δ function and was discussed in Ref. [24]. In this paper, we approximate it as

$$\delta^{\epsilon}_{\alpha\beta}(\vec{x},\vec{x}')=\delta_{\alpha\beta}\delta(\vec{x}-\vec{x}'). \tag{A3}$$

APPENDIX B

From the Hamiltonian in Eq. (2.3) and the Heisenberg equation of motion, we can derive the following operator equations:

$$\frac{d\hat{a}_n}{dt}=-i\omega_n\hat{a}_n-i\kappa_n^*\hat{b}_1^\dagger\hat{b}_2, \tag{B1a}$$

$$\frac{d\hat{b}_1^\dagger\hat{b}_2}{dt}=-i\Omega\hat{b}_1^\dagger\hat{b}_2+i\sum_n \kappa_n(\hat{b}_2^\dagger\hat{b}_2-\hat{b}_1^\dagger\hat{b}_1)\hat{a}_n, \tag{B1b}$$

$$\frac{d\hat{b}_2^\dagger\hat{b}_2}{dt}=-\frac{d\hat{b}_1^\dagger\hat{b}_1}{dt}=-i\sum_n \kappa_n\hat{b}_2^\dagger\hat{b}_1\hat{a}_n+i\sum_n \kappa_n^*\hat{a}_n^\dagger\hat{b}_1^\dagger\hat{b}_2. \tag{B1c}$$

To account for a finite dipole dephasing rate γ_{12}, Eq. (B1b) should also include a quantum Langevin operator $\Gamma_{12}(t)$ [47]

$$\frac{d\hat{b}_1^\dagger\hat{b}_2}{dt}=(-i\Omega-\gamma_{12})\hat{b}_1^\dagger\hat{b}_2+i\sum_n \kappa_n(\hat{b}_2^\dagger\hat{b}_2-\hat{b}_1^\dagger\hat{b}_1)\hat{a}_n+\hat{\Gamma}_{12}(t). \tag{B2}$$

If we ignore the dipole dephasing due to radiative decay, the ensemble average of the Langevin operator Γ_{12} is [47]

$$\langle\hat{\Gamma}_{12}^\dagger(t)\hat{\Gamma}_{12}(t')\rangle=2\gamma_{12}\overline{n_2}\,\delta(t-t'), \tag{B3a}$$

$$\langle\hat{\Gamma}_{12}(t)\hat{\Gamma}_{12}^\dagger(t')\rangle=2\gamma_{12}\overline{n_1}\,\delta(t-t'), \tag{B3b}$$

where $\overline{n_1}$ and $\overline{n_2}$ are the average occupation number of the ground state and the excited state. If we define a dipole polarization operator $\hat{p}_{tot}$ as $\hat{p}_{tot}=\hat{b}_1^\dagger\hat{b}_2$ and integrate Eq. (B2), we find that the operator $\hat{p}_{tot}$ can be separated into an induced part $\hat{p}_{ind}$ proportional to the external electromagnetic field and a randomly fluctuating part $\hat{p}_{fluc}$

$$\hat{p}_{tot}(t)=\hat{p}_{ind}(t)+\hat{p}_{fluc}(t), \tag{B4a}$$

$$\hat{p}_{ind}(t)=(\hat{b}_2^\dagger\hat{b}_2-\hat{b}_1^\dagger\hat{b}_1)\int_{-\infty}^{t}d\tau\, i\sum_n \kappa_n\hat{a}_n(\tau)e^{-(i\Omega+\gamma_{12})(t-\tau)}, \tag{B4b}$$

$$\langle\hat{p}^\dagger_{fluc}(t)\hat{p}_{fluc}(t')\rangle=\overline{n_2}e^{i\Omega(t-t')}e^{-\gamma_{12}|t-t'|}, \tag{B4c}$$

$$\langle\hat{p}_{fluc}(t)\hat{p}^\dagger_{fluc}(t')\rangle=\overline{n_1}e^{i\Omega(t'-t)}e^{-\gamma_{12}|t-t'|}, \tag{B4d}$$

where in the derivation of Eqs. (B4c) and (B4d), we have used Eq. (B3). Generally the term $\hat{b}_2^\dagger\hat{b}_2-\hat{b}_1^\dagger\hat{b}_1$ can be replaced by its ensemble average $\overline{n_2}-\overline{n_1}$ [46].

Taking the time derivative of Eq. (B1a), we find

$$\frac{d^2\hat{a}_n}{dt^2}=-\omega_n^2\hat{a}_n-2\omega_n\kappa_n^*\hat{p}_{tot}, \tag{B5}$$

where the time derivative $d\hat{p}_{tot}/dt$ is approximated by $-i\omega_n\hat{p}_{tot}$. This approximation is legitimate in the weak coupling regime, since $d\hat{p}_{tot}/dt$ is roughly $-i\Omega\hat{p}_{tot}$ and the difference between ω_n and Ω is a small quantity of the order of γ_{12}. Using the mode expansion given in Eq. (2.1), we find the quantum Maxwell equation which takes the form of Eq. (2.6), where the quantum current operator $\hat{\mathbf{J}}^{(-)}_{tot}$ is simply

$$\hat{\mathbf{J}}^{(-)}_{tot}=\hat{\mathbf{J}}^{(-)}_{fluc}+\hat{\mathbf{J}}^{(-)}_{ind}, \tag{B6a}$$

$$\hat{\mathbf{J}}^{(-)}_{fluc}=\frac{e}{m}\vec{p}_{12}\delta(\vec{x}-\vec{x}_0)\hat{p}_{fluc}, \tag{B6b}$$

$$\hat{\mathbf{J}}^{(-)}_{ind}=\frac{e}{m}\vec{p}_{12}\delta(\vec{x}-\vec{x}_0)\hat{p}_{ind}. \tag{B6c}$$

According to this relation, Eqs. (2.7) and (2.8) can also be derived from Eqs. (2.1) and (B4).

Similarly, from Eqs. (2.1) and (B1c), we find the quantum operator equation for the electron transition rate Eq. (2.12).

APPENDIX C

The expansion of the classical Green function is derived in this section. Take the loss and the gain of the optical mode into account, the eigenmode equation becomes

$$-\boldsymbol{\nabla}\times[\boldsymbol{\nabla}\times\vec{A}_n(\vec{x})]+\frac{4\pi i}{c}[-\chi_a(\vec{x})+\chi_e(\vec{x})]\vec{A}_n(\vec{x})=-\frac{\epsilon(\vec{x})}{c^2}\,\overline{\omega}_n^2\vec{A}_n(\vec{x}), \tag{C1a}$$

$$\overline{\omega}_n=\omega_n-i\frac{\Gamma_n}{2}, \tag{C1b}$$

$$\Gamma_n = -\frac{4\pi c}{\omega_n}\int d^3x[\chi_a(\vec{x})-\chi_e(\vec{x})]\vec{A}_n^*(\vec{x})\cdot\vec{A}_n(\vec{x}), \tag{C1c}$$

where $\chi_a(\vec{x})$ and $\chi_e(\vec{x})$ are defined in Eq. (5.1). Correspondingly, the Green function satisfies

$$-\nabla\times\{\nabla\times[G^{\omega}_{\alpha\beta}(\vec{x},\vec{x}')\vec{e}_\alpha]\}+\left[\frac{\epsilon(\vec{x})\omega^2}{c^2}+\frac{4\pi i}{c}[-\chi_a(\vec{x})+\chi_e(\vec{x})]\right]G^{\omega}_{\alpha\beta}(\vec{x},\vec{x}')\vec{e}_\alpha=\delta(\vec{x}-\vec{x}')\vec{e}_\beta, \tag{C2}$$

and can be expanded as

$$G^{\omega}_{\alpha\beta}(\vec{x},\vec{x}')=\sum_n g_n A_{n,\alpha}(\vec{x}). \tag{C3}$$

Using Eqs. (C1), (C2), and (A2a), we solve for g_n and find

$$g_n=\frac{c^2}{2\omega_n}\frac{A^*_{n,\beta}(\vec{x}')}{\omega-\omega_n+i\dfrac{\Gamma_n}{2}}, \tag{C4}$$

where we have replaced $\omega^2-\omega_n^2$ by $2\omega_n(\omega-\omega_n)$. Finally, we have

$$G^{\omega}_{\alpha\beta}(\vec{x},\vec{x}')=\sum_n \frac{c^2}{2\omega_n}\frac{A_{n,\alpha}(\vec{x})A^*_{n,\beta}(\vec{x}')}{\omega-\omega_n+i\Gamma_n/2}. \tag{C5}$$

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