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Temporal coupled mode theory for thermal emission from a single thermal emitter supporting either a single mode or an orthogonal set of modes

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We propose a temporal coupled mode theory for thermal emission from a single emitter supporting either a single mode or an orthogonal set of modes. This temporal coupled mode theory provides analytic insights into the general behaviors of resonant thermal emitters. We validate the coupled mode theory formalism by a direct numerical simulation of the emission properties of single emitters. © *2013 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4794981]

The ability of nanophotonic structures to tailor thermal emission is of great importance for a number of applications including thermophotovoltaics,[1–5] thermal imaging,[6,7] thermal circuits,[8–10] local heating,[11] and cooling.[12] Among all nanophotonic structures, the use of resonant thermal emitters, such as nanowires or thermal antennas, are of particular interest. These resonant thermal emitters generate narrow-band thermal emission that is attractive for thermophotovoltaic applications.[1,13] In addition, it is known that the absorption cross-section of a single antenna can significantly exceed its geometric cross-section,[14] resulting in significant enhancement of thermal emission.

Direct calculations of the emission properties of resonant thermal emitters can be carried out using the formalism of fluctuational electrodynamics.[15] For complex structures, such calculations are typically quite involved. For a single emitter with complex geometries in three dimensions, such direct emission calculations in fact have not been reported, most of the existing calculations instead focus on array structures.[13,16,17]

In this Letter, we introduce a theoretical formalism, combining the fluctuation-dissipation theorem,[15] with temporal coupled mode theory (CMT), to arrive at simple formulas for the emission properties of resonant thermal emitters. These formulas provide analytic insights into the general behaviors of resonant thermal emitters. We validate the theory by numerical calculations of thermal emission from single emitters using direct numerical approach.

We consider a resonant mode with a resonance frequency ω_0. We start by assuming that the resonance does not couple to external radiation. Instead, it only has an intrinsic decay rate $1/\tau_o$, resulting from the material loss inside the resonator. The coupled mode equation for the resonant mode amplitude a can be written as

$$\frac{d}{dt}a = i\omega_0 a - \frac{1}{\tau_o}a + \sqrt{\frac{2}{\tau_o}}n. \quad (1)$$

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We normalize the amplitude so that the mode energy is given by $|a|^2$. At thermal equilibrium, one should have

$$\langle |a|^2 \rangle = \langle a^*(t)a(t) \rangle = \Theta(\omega_0, T), \quad (2)$$

where $\Theta(\omega, T) = \frac{\hbar\omega}{e^{\hbar\omega/k_BT}-1}$. Notice that we have introduced a noise source n in Eq. (1), to compensate for the intrinsic resonator loss and maintain thermal equilibrium.[18] This noise source must have a correlation function

$$\langle n^*(\omega)n(\omega') \rangle = \frac{1}{2\pi}\Theta(\omega, T)\delta(\omega - \omega'), \quad (3)$$

which can be proved as follows:

We assume the noise source is stationary (i.e., $|n(t)|^2$ is time-independent), and, therefore, $\langle n^*(\omega)n(\omega') \rangle = S(\omega)\delta(\omega - \omega')$. It follows that

$$\begin{aligned}\langle a^*(t)a(t) \rangle &= \int_0^\infty d\omega \int_0^\infty d\omega' \, e^{-i(\omega-\omega')t} \langle a^*(\omega)a(\omega') \rangle \\ &= \int_0^\infty d\omega \int_0^\infty d\omega' \frac{\frac{2}{\tau_o}}{(\omega-\omega_0)^2 + \left(\frac{1}{\tau_o}\right)^2} \\ &\quad \times S(\omega)\delta(\omega - \omega') \\ &= \int_0^\infty d\omega \frac{\frac{2}{\tau_o}}{(\omega-\omega_0)^2 + \left(\frac{1}{\tau_o}\right)^2} S(\omega). \end{aligned} \quad (4)$$

We further assume that the noise source is broadband. $S(\omega)$ in the integrand of Eq. (4) can then be replaced by $S(\omega_0)$, and accordingly Eq. (4) simplifies to

$$\langle a^*(t)a(t) \rangle = 2\pi S(\omega_0). \quad (5)$$

Comparing Eqs. (2) and (5), we have $S(\omega_0) = \frac{1}{2\pi}\Theta(\omega_0, T)$. Since this derivation can be carried out for resonances at any resonant frequency ω_0, we have $S(\omega) = \frac{1}{2\pi}\Theta(\omega, T)$, thus proving Eq. (3). This result is consistent with standard literature[18] and is quite general. Equation (1), on the other hand, is applicable only for a single-mode resonance having relatively high quality factor.

Now we assume that the resonator additionally couples to external radiation as described by an external decay rate $1/\tau_e$. With consideration of the external decay rate, the coupled mode equation for the resonant mode amplitude a can be written as

$$\frac{d}{dt}a = i\omega_0 a - \left(\frac{1}{\tau_o}+\frac{1}{\tau_e}\right)a + \sqrt{\frac{2}{\tau_o}}n. \tag{6}$$

The thermal emission power $\langle P\rangle$ can then be calculated as

$$\begin{aligned}\langle P(t)\rangle &= \frac{2}{\tau_e}\langle a^*(t)a(t)\rangle = \frac{2}{\tau_e}\int_0^\infty d\omega\int_0^\infty d\omega' e^{-i(\omega-\omega')t}\langle a^*(\omega)a(\omega')\rangle \\ &= \frac{2}{\tau_e}\int_0^\infty d\omega\int_0^\infty d\omega' \frac{\frac{2}{\tau_o}\langle n^*(\omega)n(\omega')\rangle}{\left[i(\omega-\omega_0)+\left(\frac{1}{\tau_o}+\frac{1}{\tau_e}\right)\right]\left[-i(\omega'-\omega_0)+\left(\frac{1}{\tau_o}+\frac{1}{\tau_e}\right)\right]} \\ &= \int_0^\infty d\omega\frac{\Theta(\omega,T)}{2\pi}\frac{4\frac{1}{\tau_o}\frac{1}{\tau_e}}{(\omega-\omega_0)^2+\left(\frac{1}{\tau_o}+\frac{1}{\tau_e}\right)^2},\end{aligned} \tag{7}$$

where we have used Eq. (3). Therefore, the power spectral density of thermal emission (which we note is not the Fourier transform of $P(t)$) is

$$P(\omega) = \frac{\Theta(\omega,T)}{2\pi}\frac{4\frac{1}{\tau_o}\frac{1}{\tau_e}}{(\omega-\omega_0)^2+\left(\frac{1}{\tau_o}+\frac{1}{\tau_e}\right)^2}. \tag{8}$$

The derivation above assumes a single mode resonator. For a multimode resonator, if these modes are orthogonal,[19]

$$P(\omega) = \sum_i \frac{\Theta(\omega,T)}{2\pi}\frac{4\frac{1}{\tau_o^i}\frac{1}{\tau_e^i}}{(\omega-\omega_i)^2+\left(\frac{1}{\tau_o^i}+\frac{1}{\tau_e^i}\right)^2}. \tag{9}$$

Therefore, if the resonator supports modes that are degenerate due to symmetry, the power spectral density of thermal emission will be

$$P(\omega) = N_d\frac{\Theta(\omega,T)}{2\pi}\frac{4\frac{1}{\tau_o}\frac{1}{\tau_e}}{(\omega-\omega_0)^2+\left(\frac{1}{\tau_o}+\frac{1}{\tau_e}\right)^2}, \tag{10}$$

where N_d is the mode degeneracy.

Equations (8)–(10) are the main results of the paper. They enable us to predict the power spectral density of thermal emission from a single resonant emitter, no matter how complicated the shape is. For a resonator supporting either a single or a degenerate set of resonances, the maximum power spectral density of thermal emission is $N_d\frac{\Theta(\omega,T)}{2\pi}$. Such a maximum is reached when the intrinsic decay time τ_o matches the external decay time τ_e.

To validate the coupled mode theory described above, we perform direct calculations for a variety of geometries using either analytic calculations for simple geometries, or the finite-difference time-domain (FDTD) method for complex geometries. In the FDTD method, one places a collection of random sources, with their amplitudes determined from fluctuation dissipation theorem,[15] and calculates the resulting thermal emission. More details can be found in Refs. 16, 17, 20, and 21. This approach was previously used for periodic arrays of emitters,[16,17,20] but can be straightforwardly applied to single emitter calculation, which is what we do here.

As a first example, we study analytically the case of a single emitter made of a homogeneous dielectric sphere.[22] The dielectric constant is described by a Lorentz model $\epsilon = \epsilon_\infty - \sigma/(\omega^2 - i\omega\gamma - \omega_0^2)$, with $\epsilon_\infty = 7$, $\sigma = 0.16(2\pi c/a)^2$, $\gamma = 0.01(2\pi c/a)$, and $\omega_0 = 0.1(2\pi c/a)$, where c is the velocity of light and $a = 1\,\mu$m. The radius of the sphere is 500 nm. Figure 1 shows that both the coupled mode theory prediction (red line) and finite-difference time-domain simulation result (blue crosses) accurately match the analytic solution (green squares). Note, as the mode investigated here is a triply degenerate dipole mode, we use Eq. (10) with $N_d = 3$ for our theory.

Next, we consider a more complicated structure as shown in Fig. 2(a), for which no closed-form analytic solution exists. Thermal emission from a periodic array of such emitters was studied in Ref. 23. Here, we instead examine a single emitter. The structure has 90° rotational symmetry and consists of three layers. The parameters of the structure are provided in the caption of Fig. 2. The top and bottom layers are modeled as gold using a Drude model.[24] We use alumina as the central layer, and describe its dielectric function in the wavelength region of interest with a Lorentz model $\epsilon = \epsilon_\infty - \sigma/(\omega^2 - i\omega\gamma - \omega_0^2)$, with $\epsilon_\infty = 2.228$, $\sigma = 0.008385(2\pi c/a)^2$, $\gamma = 0.04(2\pi c/a)$, and

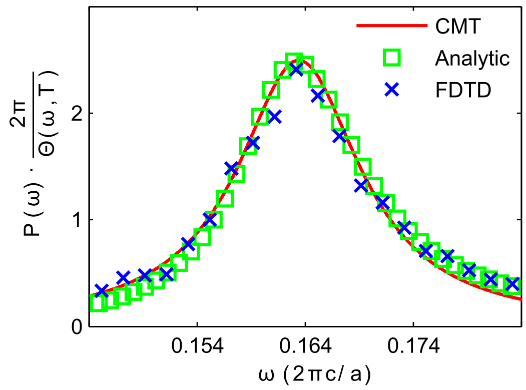

FIG. 1. Thermal emission power spectrum comparison among coupled mode theory prediction (red line), exact analytic equation result (green squares), and finite-difference time-domain simulation result averaged over 60 runs (blue crosses), for a spherical single emitter of radius 500 nm.

$\omega_0 = 0.08(2\pi c/a)$, where c is the velocity of light and $a = 1\,\mu$m.

Due to its symmetry, the structure supports a doubly degenerate mode at $\omega = 0.195(2\pi c/a)$. One of these modes has the modal pattern shown in Fig. 2(b). We notice that the intensity does not have 90° rotational symmetry, as expected for a doubly degenerate state. Accordingly, we use Eq. (10) with $N_d = 2$ for our theory. In Fig. 2(c), the coupled mode theory prediction (red line) agrees with finite-difference time-domain simulation result (blue crosses).

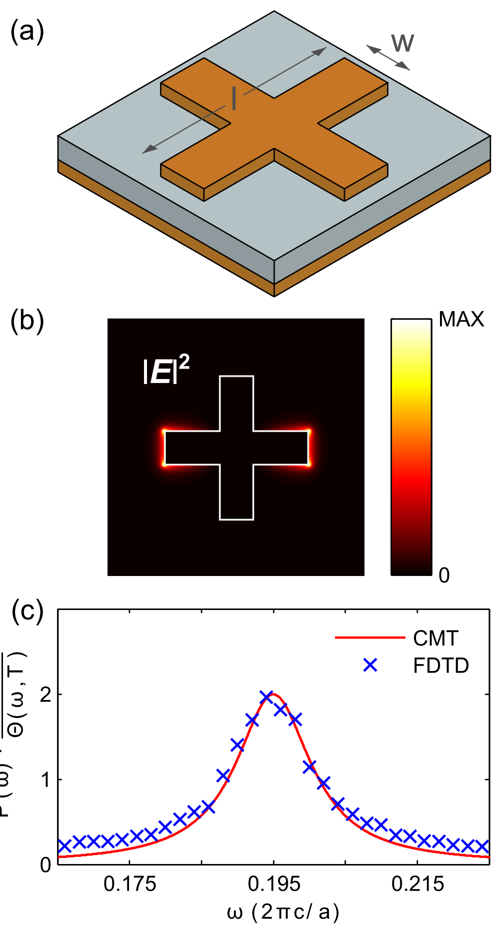

FIG. 2. (a) Geometry for a single emitter. The top cross-shaped layer has dimensions $l = 1.7\,\mu$m and $w = 0.4\,\mu$m, with $0.1\,\mu$m in thickness. The sizes of the central and bottom layers are $2\,\mu m \times 2\,\mu m \times 0.19\,\mu m$ and $2\,\mu m \times 2\,\mu m \times 0.1\,\mu m$, respectively. (b) Electric field intensity distribution ($|E|^2$) for the mode at $\omega = 0.195(2\pi c/a)$. (c) Thermal emission power spectrum comparison between coupled mode theory prediction (red line) and finite-difference time-domain simulation result averaged over 100 runs (blue crosses).

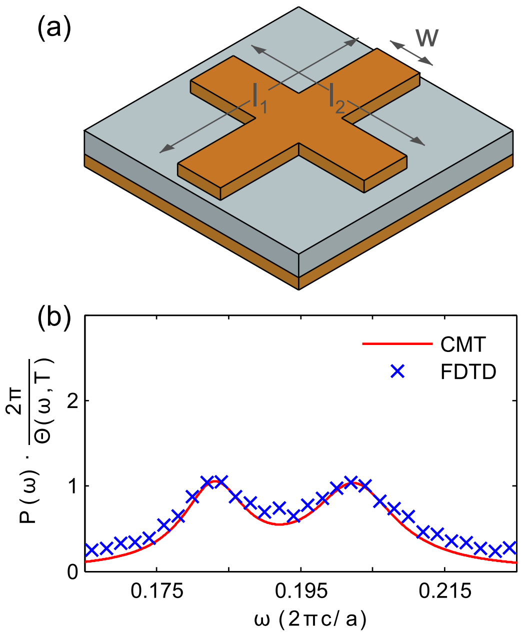

FIG. 3. (a) Modified geometry for an emitter. The top cross-shaped layer has dimensions $l_1 = 1.86\,\mu$m, $l_2 = 1.62\,\mu$m, and $w = 0.4\,\mu$m, with $0.1\,\mu$m in thickness. The sizes of the central and bottom layers are $2\,\mu m \times 2\,\mu m \times 0.19\,\mu m$ and $2\,\mu m \times 2\,\mu m \times 0.1\,\mu m$, respectively. (b) Thermal emission power spectrum comparison between coupled mode theory prediction (red line) and finite-difference time-domain simulation result averaged over 100 runs (blue crosses).

We can remove the modal degeneracy by breaking the spatial symmetry. For this purpose, we modify the geometry in Figs. 2(a) to 3(a), by making the two arms of the cross have different lengths. The structure now supports two non-degenerate modes at $\omega_1 = 0.183(2\pi c/a)$ and $\omega_2 = 0.2025$ $(2\pi c/a)$, respectively. As a result, in Fig. 3(b), we see two peaks in the emission spectrum. The height of either peak is much smaller than that of the single peak obtained in the degenerate case of Fig. 2(c). Again, the coupled mode theory result, now with Eq. (9), agrees very well with direct numerical simulation.

When using coupled mode theory formalism, the parameters, such as the resonant frequency and various linewidths, are also determined from separate FDTD simulations. The FDTD simulations that determine these parameters, however, are far less involved compared with direct calculations of thermal emission. Therefore, the use of coupled mode theory formalism greatly simplifies the theoretical study of complex emitter structures.

In conclusion, we have developed a coupled mode theory that describes the thermal emission from a single resonant emitter with complex shapes and validated the model with direct numerical calculations. The coupled mode theory provides accurate predictions while takes far less time than the direct numerical calculations. We have also used this model to highlight analytically the importance of modal degeneracy in thermal emission. Such a model should prove useful in the quest to tailor thermal emission for a variety of applications.

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