

Green's-function expansion for multiple coupled optical resonators with finite retardation using quasinormal modes

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(Received 17 October 2025; accepted 17 March 2026; published 13 April 2026)

The electromagnetic Green's function is a crucial ingredient for the theoretical study of modern photonic quantum devices, but is often difficult or even impossible to calculate directly. We present a numerically efficient framework for calculating the scattered electromagnetic Green's function of a multicavity system with spatially separated open cavities (with arbitrary shape, dispersion, and loss) and finite retardation times. The framework is based on a Dyson scattering equation that enables the construction of the Green's function from the quasinormal modes of the individual resonators within a few-mode approximation and a finite number of iteration steps without requiring nested integrals. The approach shows excellent agreement with the full numerical Green's function for the example of two coupled dipoles located in the gaps of two metal dimers serving as quasinormal mode cavities, and is easily extended to arbitrarily large separations and multiple cavities.

DOI: [10.1103/bbk5-l3tt](https://doi.org/10.1103/bbk5-l3tt)

Introduction. Open optical cavity resonators coupled to quantum emitters (such as atoms, molecules, and quantum dots) are a fundamental building block for many modern quantum technologies such as nanolasers [1–3], quantum sensors [4,5], quantum computers [6–9], and quantum networks [10–13]. For a theoretical treatment of such systems, knowledge of the full electromagnetic Green's function is of great importance and a requirement to many quantum optics formalisms. For example, it is used to calculate the Purcell enhancement of optical cavities [14–17], in the quantization of the electromagnetic field [16,18–22], and in the derivation of coupling elements between photons and quantum emitters [23,24]. Therefore, an efficient scheme for obtaining a good approximation of the full Green's function is central to many theoretical treatments of light-matter coupling in such systems.

One approach to open cavity systems is through quasinormal modes (QNMs), which are solutions to the source-free Helmholtz equation under open boundary conditions [15,25–27]. The QNMs have complex eigenfrequencies with a negative imaginary part, so that the temporal decay is inherent to the mode, making the QNMs the natural modes of open cavity systems with material losses. Quasinormal mode theories have been used to study a variety of setups in recent works

[15,28–32], and play a crucial role in rigorous open cavity quantum optics [16,18,22].

For positions within (or close to) the resonator, an expansion in terms of a few dominant QNMs yields a very good approximation of the full Green's function [16,25,26,33,34]. For positions far away from the resonator, however, the QNMs diverge due to their complex eigenfrequencies. Even for properly normalized modes, a large number of QNMs is usually necessary for a good approximation of the Green's function [35,36]. This makes the approach impractical for many quantum optics or quantum dynamics applications, where the Hilbert space scales exponentially with the number of modes.

For single resonators, the QNMs outside the cavity region can be replaced with regularized frequency-dependent fields [23,33,37], which can be calculated efficiently using a near-field-to-far-field transformation together with a pole approximation [37]. For many applications, this approach makes a few-QNM expansion sufficient, even for positions far away from the resonator.

However, many modern quantum devices consist of multiple, spatially separated and interacting cavities. A calculation of the exact QNMs of such coupled structures is often not feasible. It is instead desirable to express the multicavity Green's function in terms of the single-cavity QNMs. For example, in the coupled quasinormal mode theory (CQT) [17,38,39], symmetrized eigenfrequencies and hybridized QNMs are derived from single-cavity properties. However, CQT relies on QNMs that diverge spatially, and is therefore not accurate for large separations.

In this Letter, we introduce a powerful and accurate Dyson equation approach to obtain the multicavity scattered Green's function for systems with large spatial separations and non-negligible retardation from only single-cavity QNMs, within a few-mode approximation. We use regularized QNM fields

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outside the individual resonators to characterize the inter-cavity scattering, so that retardation effects are included. Multicavity scattering naturally decomposes into products of two-cavity scattering processes within the QNM expansion, avoiding nested integrals. This approach allows for a few-mode expansion of the multicavity Green's function, and thus the implementation in quantum optics applications. We calculate the coupling between two dipole emitters located in the gaps of metal dimers serving as QNM cavities, and compare the QNM expansion with the full numerical Green's function, showing excellent agreement.

Coupled-cavity system. We consider a system of N spatially separated cavities or plasmonic nanoparticles. The full permittivity, satisfying causality, reads

$$\epsilon(\mathbf{r}, \omega) = \epsilon_{\text{back}}(\mathbf{r}, \omega) + \sum_{i=1}^N V_i(\mathbf{r}, \omega), \quad (1)$$

where $\epsilon_{\text{back}}(\mathbf{r}, \omega)$ is the permittivity of the background medium, and $V_i(\mathbf{r}, \omega) = \chi_{V_i}(\mathbf{r})[\epsilon(\mathbf{r}, \omega) - \epsilon_{\text{back}}(\mathbf{r}, \omega)]$ is the perturbation of the permittivity due to the presence of the cavity, with V_i the cavity volume, and the function $\chi_{V_i}(\mathbf{r})$ is unity for $\mathbf{r} \in V_i$ and zero elsewhere. We make no assumption about the background permittivity ϵ_{back} except those necessary to define QNMs, i.e., that there is a discontinuity between the permittivity of the cavity medium and ϵ_{back} , and that there is no backscattering of waves from the far field [40].

The full electromagnetic Green's tensor (or dyad) is the solution to the Helmholtz equation

$$\left[\nabla \times \nabla \times - \frac{\omega^2}{c^2} \epsilon(\mathbf{r}, \omega) \right] \mathbf{G}(\mathbf{r}, \mathbf{r}', \omega) = \frac{\omega^2}{c^2} \mathbb{1} \delta(\mathbf{r} - \mathbf{r}'), \quad (2)$$

under appropriate boundary conditions, which is sufficient for defining the Green's function mathematically. For cavities in vacuum, as considered in this Letter, this is the Silver-Müller radiation condition [41,42].

Single-cavity QNMs. We define the single-cavity permittivity $\epsilon_i(\mathbf{r}, \omega) = \epsilon_{\text{back}}(\mathbf{r}, \omega) + V_i(\mathbf{r}, \omega)$, where the permittivity is set to the background value everywhere except at the i th cavity. The QNMs $\tilde{\mathbf{f}}_{i\mu}(\mathbf{r})$ of the i th cavity solve the source-free Helmholtz equation for this (single-cavity) permittivity [15,25–27,32],

$$\nabla \times \nabla \times \tilde{\mathbf{f}}_{i\mu}(\mathbf{r}) - \frac{\tilde{\omega}_{i\mu}^2}{c^2} \epsilon_i(\mathbf{r}, \tilde{\omega}_{i\mu}) \tilde{\mathbf{f}}_{i\mu}(\mathbf{r}) = \mathbf{0}, \quad (3)$$

under open boundary conditions, such as the Silver-Müller radiation condition for cavities in a homogeneous background medium [16,34], or waveguide radiation conditions for waveguide-coupled cavities [43]. Due to the outgoing boundary conditions and complex permittivity, QNMs have complex eigenfrequencies with negative imaginary part: $\tilde{\omega}_{i\mu} = \omega_{i\mu} - i\gamma_{i\mu}$, $\gamma_{i\mu} > 0$.

We assume that, near the resonator, the single-cavity Green's function can be expanded as usual in terms of the QNMs $\tilde{\mathbf{f}}_{i\mu}(\mathbf{r})$, so that [16,25,26,33,34]

$$\mathbf{G}_i(\mathbf{r}, \mathbf{r}', \omega)|_{\mathbf{r}, \mathbf{r}' \in V_i} = \sum_{\mu} A_{i\mu}(\omega) \tilde{\mathbf{f}}_{i\mu}(\mathbf{r}) \tilde{\mathbf{f}}_{i\mu}(\mathbf{r}'), \quad (4)$$

where $A_{i\mu}(\omega) = \omega/[2(\tilde{\omega}_{i\mu} - \omega)]$.

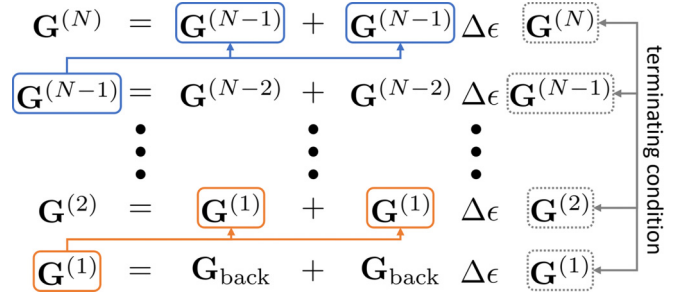


FIG. 1. Sketch of the framework for obtaining the N -cavity Green's function via a set of N scattering equations. Starting from the single-cavity Green's function $\mathbf{G}^{(1)}$, we iteratively add more cavities with $\mathbf{G}^{(n-1)}$ from the previous step serving as an input for the scattering equation for the Green's function $\mathbf{G}^{(n)}$ [cf. Eq. (7)]. In each step, the recursive Dyson equation is terminated using the condition from Eq. (8).

For positions far away from the resonator, the QNMs spatially diverge due to the complex eigenfrequencies [15,26,44]. Even if properly normalized, a large number of QNMs is generally required for an accurate expansion of the Green's function [35,36]. A common alternative replaces the QNMs outside the cavity volume with nondivergent frequency-dependent regularized QNM fields $\tilde{\mathbf{F}}_{i\mu}(\mathbf{r}, \omega)$, which are obtained from a Dyson equation [33],

$$\tilde{\mathbf{F}}_{i\mu}(\mathbf{r}, \omega) = \int_{V_i} d^3 r' \Delta\epsilon(\mathbf{r}', \omega) \mathbf{G}_{\text{back}}(\mathbf{r}, \mathbf{r}', \omega) \cdot \tilde{\mathbf{f}}_{i\mu}(\mathbf{r}'), \quad (5)$$

where $\Delta\epsilon(\mathbf{r}, \omega) = \epsilon(\mathbf{r}, \omega) - \epsilon_{\text{back}}(\mathbf{r}, \omega)$, and $\mathbf{G}_{\text{back}}(\mathbf{r}, \mathbf{r}', \omega)$ is the Green's function of the background medium, which solves the Helmholtz equation (2) with the background permittivity $\epsilon_{\text{back}}(\mathbf{r}, \omega)$. For a more efficient calculation, regularized QNMs can be obtained from integrals over the cavity surface only, using the field-equivalence principle [45] or a near-field-to-far-field transformation [37].

Multicavity Green's-function expansion. We wish to construct the Green's function for N cavities from the single-cavity QNMs. We do this via a set of scattering equations where, starting from the single-cavity Green's function, we iteratively add more cavities until all N cavities are included. We sketch this framework in Fig. 1.

Let $\mathbf{G}^{(n)}(\mathbf{r}, \mathbf{r}', \omega)$ be the Green's function for n cavities which solves the Helmholtz equation (2) for

$$\epsilon^{(n)}(\mathbf{r}, \omega) = \epsilon_{\text{back}}(\mathbf{r}, \omega) + \sum_{i=1}^n V_i(\mathbf{r}, \omega). \quad (6)$$

Now, $\mathbf{G}^{(n)}(\mathbf{r}, \mathbf{r}', \omega)$ can be obtained from the Green's function $\mathbf{G}^{(n-1)}(\mathbf{r}, \mathbf{r}', \omega)$ for $n-1$ cavities via the scattering equation [see Sec. S2 A in Supplemental Material (SM) [46] for the derivation]

$$\mathbf{G}^{(n)}(\mathbf{r}, \mathbf{r}', \omega) = \mathbf{G}^{(n-1)}(\mathbf{r}, \mathbf{r}', \omega) + \int_{V_n} d^3 s \Delta\epsilon(\mathbf{s}, \omega) \mathbf{G}^{(n-1)}(\mathbf{r}, \mathbf{s}, \omega) \cdot \mathbf{G}^{(n)}(\mathbf{s}, \mathbf{r}', \omega), \quad (7)$$

where V_n is the volume of the n th cavity. For $n=1$ and using $\mathbf{G}^{(0)} \equiv \mathbf{G}_{\text{back}}$, we recover the Dyson equation for the single-cavity case from Ref. [33].

For any fixed $n = k$, Eq. (7) is recursive, since $\mathbf{G}^{(k)}$ appears also on the right-hand side (RHS) of Eq. (7). While a perturbative treatment of Eq. (7) is generally possible (cf. Sec. S2 C in SM [46]), this $\mathbf{G}^{(k)}$ on the RHS *only* depends on positions within the same cavity [47]. Consequently, we can terminate the Dyson equation at low order for any k by replacing $\mathbf{G}^{(k)}$ at the RHS with the single-cavity QNM Green's function ($1 \leq i \leq k$)

$$\mathbf{G}^{(k)}(\mathbf{r}, \mathbf{r}', \omega)|_{\mathbf{r}, \mathbf{r}' \in \mathcal{V}_i} \approx \mathbf{G}_i(\mathbf{r}, \mathbf{r}', \omega), \quad (8)$$

i.e., we assume that the Green's function for positions inside the cavity can be approximated by the single-cavity Green's function of that cavity [cf. Eq. (4)]. This assumption holds well for many applications, such as three-dimensional (3D) cavities in homogeneous media (where the influence of other cavities scales as $1/R$ with separations on the order of the QNM wavelength or more (see Fig. 4 as well as Figs. S2 and S3 in SM [46])). For cases where the assumption breaks down, the perturbative approach (see Sec. S2 C in SM [46]) or the established CQT are employed.

As a consequence, the full Green's function for N cavities, $\mathbf{G}(\mathbf{r}, \mathbf{r}', \omega) = \mathbf{G}^{(N)}(\mathbf{r}, \mathbf{r}', \omega)$, is obtained iteratively from a set of N scattering equations (7) for $n = 1, \dots, N$ (cf. Fig. 1).

As we show for three coupled cavities in Sec. S2 D of SM [46] the ordering of the cavities $1, \dots, N$ should be performed such that the Dyson equation (7) terminates [i.e., the case from Eq. (8) is obtained on the RHS] at low order for each step in the iteration.

This formalism yields the scattered Green's function for an arbitrary number of cavities within a finite number of iterations. In addition, the QNM expansion factorizes the Green's function [cf. Eq. (4)], so that multicavity scattering processes naturally decompose into products of two-cavity scattering processes (see Sec. S2 D in SM [46] for an example of three-cavity scattering), thus avoiding numerically demanding nested integrals.

For a practical and efficient numerical calculation, the volume integral representation from Eq. (7) can be converted into surface integrals. Towards this, we note that from Eq. (6), it follows that $\Delta\epsilon(\mathbf{s}, \omega)|_{\mathbf{s} \in \mathcal{V}_n} = \epsilon^{(n)}(\mathbf{s}, \omega) - \epsilon^{(n-1)}(\mathbf{s}, \omega)$ in Eq. (7). Thus, we employ the Helmholtz equation (2) with $\epsilon^{(n)}$ for $\mathbf{G}^{(n)}$ and with $\epsilon^{(n-1)}$ for $\mathbf{G}^{(n-1)}$ in Eq. (7), to find via the second Green's theorem (omitting the ω dependence in the Green's functions for a brief notation, see Sec. S2 B in SM [46] for details),

$$\begin{aligned} & \frac{\omega^2}{c^2} \mathbf{G}^{(n)}(\mathbf{r}, \mathbf{r}')|_{\mathbf{r} \notin \mathcal{V}_n} \\ &= \chi_{\bar{\mathcal{V}}_n}(\mathbf{r}') \frac{\omega^2}{c^2} \mathbf{G}^{(n-1)}(\mathbf{r}, \mathbf{r}') \\ &+ \oint_{S_n} dA_s \{ [\nabla_s \times \mathbf{G}^{(n-1)}(\mathbf{s}, \mathbf{r})]^T \cdot [\hat{\mathbf{n}}_s \times \mathbf{G}^{(n)}(\mathbf{s}, \mathbf{r}')] \\ &\quad - [\hat{\mathbf{n}}_s \times \mathbf{G}^{(n-1)}(\mathbf{s}, \mathbf{r})]^T \cdot [\nabla_s \times \mathbf{G}^{(n)}(\mathbf{s}, \mathbf{r}')] \}, \end{aligned} \quad (9)$$

where $\bar{\mathcal{V}}_n$ is the complement of the cavity volume $\mathcal{V}_n$, and S_n is a closed surface around $\mathcal{V}_n$ with the outward-pointing surface normal vector $\hat{\mathbf{n}}_s$.

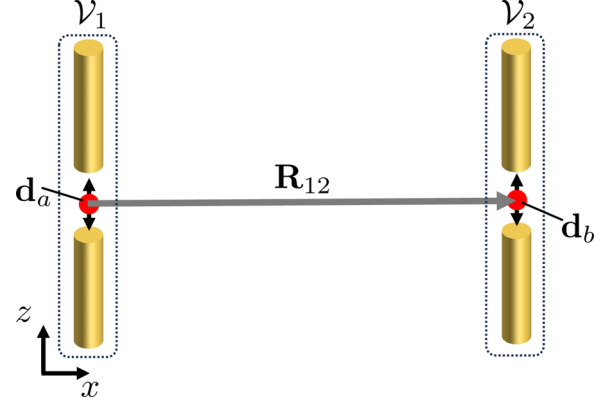


FIG. 2. Sketch of two metal dimers serving as QNM cavities. The dimers are described by a Drude permittivity [cf. Eq. (10)], and separated by the center-to-center distance R_{12} . Two dipole emitters $\mathbf{r}_a \in \mathcal{V}_1$ and $\mathbf{r}_b \in \mathcal{V}_2$ are placed in the dimer gaps.

In principle, the volume integral in Eq. (7) and the surface integral in Eq. (9) should yield the same result for the Green's function. However, since different parts of the QNMs dominate inside the cavity volume and on the surface, the two representations only fully agree when all QNMs are included [45]. Hence, one representation should be used consistently, e.g., if the regularized QNM fields $\tilde{\mathbf{F}}_{i\mu}(\mathbf{r}, \omega)$ are calculated using surface integrals (as we do below), the representation from Eq. (9) should be used. We note that the use of surface integrals can also help circumvent problems arising in the context of perturbation theories with volume integrals due to the discontinuity of the electric field at the boundary between media [29,48–50].

Coupled metal dimers. For an illustrative practical example, we consider two metal dimers with volumes $\mathcal{V}_1$ and $\mathcal{V}_2$ in vacuum as QNM cavities [46]. We assume that each dimer is dominated by a single QNM and described by the Drude model

$$\epsilon_j(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + i\omega\gamma_{pj}}, \quad (10)$$

where $j = 1, 2$, and $\hbar\omega_p = 8.2934$ eV, $\hbar\gamma_{p1} = 0.0928$ eV are the plasma frequency and damping rate for gold, while dimer 2 has a reduced damping rate of $\hbar\gamma_{p2} = 0.3\hbar\gamma_{p1}$ to obtain a higher-quality plasmon mode. The QNM of dimer 1 has the eigenfrequency $\hbar\tilde{\omega}_1 = (1.6904 - i0.0652)$ eV, corresponding to a wavelength of $\lambda_1 \approx 733.46$ nm. For the QNM of dimer 2, we obtain $\hbar\tilde{\omega}_2 = (1.6482 - i0.0388)$ eV and $\lambda_2 \approx 752.24$ nm.

As shown in Fig. 2, we place two identical z -polarized dipoles $\mathbf{d}_a = \mathbf{d}_b = d\hat{\mathbf{e}}_z$ in the dimer gaps ($\mathbf{r}_a \in \mathcal{V}_1, \mathbf{r}_b \in \mathcal{V}_2$). We use the coupling between the dipoles,

$$g_{ba}(\omega) = \frac{1}{\epsilon_0} \mathbf{d}_b \cdot \mathbf{G}(\mathbf{r}_b, \mathbf{r}_a, \omega) \cdot \mathbf{d}_a, \quad (11)$$

as an indicator to compare the QNM expansion from Eq. (9) to the full Green's function, which is obtained numerically from the scattered electric field of a point dipole source (see Sec. S1 in SM [46]).

To obtain $\mathbf{G}(\mathbf{r}_b, \mathbf{r}_a, \omega)$ from Eq. (9), we use $\mathcal{S}_n \rightarrow \mathcal{S}_1$ so that $\mathbf{s}, \mathbf{r}_a \in \mathcal{V}_1$, allowing us to apply the termination condition from Eq. (8). We also employ the single-cavity QNM expansion [23]

$$\begin{aligned} \mathbf{G}^{(n-1)}(\mathbf{s}, \mathbf{r}_b, \omega) &\rightarrow \mathbf{G}_2(\mathbf{s}, \mathbf{r}_b, \omega)|_{\mathbf{s} \notin \mathcal{V}_2, \mathbf{r}_b \in \mathcal{V}_2} \\ &= A_2(\omega) \tilde{\mathbf{F}}_2(\mathbf{s}, \omega) \tilde{\mathbf{f}}_2(\mathbf{r}_b). \end{aligned} \quad (12)$$

Thus, we arrive at

$$\mathbf{G}(\mathbf{r}_b, \mathbf{r}_a, \omega)|_{\mathbf{r}_b \in \mathcal{V}_2, \mathbf{r}_a \in \mathcal{V}_1} = B_{21}(\omega) \tilde{\mathbf{f}}_2(\mathbf{r}_b) \tilde{\mathbf{f}}_1(\mathbf{r}_a), \quad (13)$$

where

$$\begin{aligned} B_{21}(\omega) &= \frac{c^2}{\omega^2} A_2(\omega) A_1(\omega) \\ &\times \oint_{\mathcal{S}_1} dA_s \{ [\nabla_s \times \tilde{\mathbf{F}}_2(\mathbf{s}, \omega)] \cdot [\hat{\mathbf{n}}_s \times \tilde{\mathbf{f}}_1(\mathbf{s})] \\ &- [\hat{\mathbf{n}}_s \times \tilde{\mathbf{F}}_2(\mathbf{s}, \omega)] \cdot [\nabla_s \times \tilde{\mathbf{f}}_1(\mathbf{s})] \}. \end{aligned} \quad (14)$$

Note that $B_{21}(\omega) = B_{12}(\omega)$ holds, preserving $\mathbf{G}(\mathbf{r}_a, \mathbf{r}_b, \omega) = [\mathbf{G}(\mathbf{r}_b, \mathbf{r}_a, \omega)]^T$ for reciprocal media.

For an efficient calculation of the expansion from Eq. (13), we rewrite the regularized QNM field $\tilde{\mathbf{F}}_2(\mathbf{s}, \omega)|_{\mathbf{s} \in \mathcal{V}_1} = \tilde{\mathbf{F}}'_2(\mathbf{s}, \omega) e^{i\omega R_{21}/c}$, where $\tilde{\mathbf{F}}'_2(\mathbf{s}, \omega)$ is a slow-rotating envelope function, and $R_{21} = R_{12} = 2020$ nm is the center-to-center distance between the dimers [22]. The envelope function $\tilde{\mathbf{F}}'_2(\mathbf{s}, \omega)$ is treated in a pole approximation $\omega \rightarrow \omega_2$ near the poles contained in $A_2(\omega), A_1(\omega)$, and we arrive at

$$B_{21}(\omega) \approx N_{21} \frac{c^2}{\omega^2} A_2(\omega) A_1(\omega) e^{i\omega R_{21}/c}, \quad (15)$$

with

$$\begin{aligned} N_{21} &= \oint_{\mathcal{S}_1} dA_s \{ [\nabla_s \times \tilde{\mathbf{F}}'_2(\mathbf{s}, \omega_2)] \cdot [\hat{\mathbf{n}}_s \times \tilde{\mathbf{f}}_1(\mathbf{s})] \\ &- [\hat{\mathbf{n}}_s \times \tilde{\mathbf{F}}'_2(\mathbf{s}, \omega_2)] \cdot [\nabla_s \times \tilde{\mathbf{f}}_1(\mathbf{s})] \}. \end{aligned} \quad (16)$$

In Fig. 3, we show the imaginary and real parts of $g_{ba}(\omega)$, calculated using the full numerical Green's function and the QNM approximation from Eq. (13) together with Eq. (15) [$N_{21} = (2.0773 - i0.0657) \times 10^{-7} \text{ nm}^{-2}$], and observe excellent agreement. We stress that we do not use any fitting parameters in the calculations. The frequency-dependent phase $e^{i\omega R_{12}/c}$ from Eq. (15) is crucial for cases with significant separation. We show in Fig. 3 the case where the exponential is included in the pole approximation ($G_{\text{pole}}^{\text{QNM}}$),

$$B_{21}(\omega)|^{\text{pole}} \approx N_{21} \frac{c^2}{\omega^2} A_2(\omega) A_1(\omega) e^{i\omega_2 R_{21}/c}, \quad (17)$$

which does not match the full numerical results, since it does not fully account for retardation effects.

For comparison, we also show in Fig. 3 a single-cavity expansion of the Green's function [cf. Eq. (12), $1 \leftrightarrow 2$]

$$g_{ba}(\omega)|^{\text{single}} \approx \frac{1}{\epsilon_0} \mathbf{d}_b \cdot \mathbf{G}_1(\mathbf{r}_b, \mathbf{r}_a, \omega) \cdot \mathbf{d}_a, \quad (18)$$

where we assume that the electric field of dipole a (located in cavity $\mathcal{V}_1$) can be approximated in terms of the QNMs of cavity 1 only. Evidently, this expansion significantly underestimates the strength of the dipole coupling and fails to capture

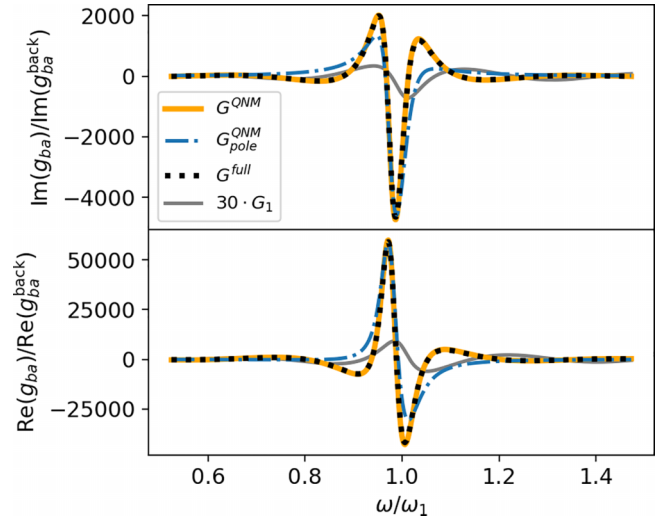


FIG. 3. Normalized coupling $g_{ba}(\omega)$ [cf. Eq. (11)] between the two dipoles in Fig. 2 for $R_{12} = 2020$ nm $\approx 2.75\lambda_1$. The QNM expansion from Eq. (13) together with Eq. (15) (G^{QNM}) yields excellent agreement with the full numerical Green's-function calculation (G^{full}). Using Eq. (17) instead of Eq. (15) ($G_{\text{pole}}^{\text{QNM}}$) does not fully include retardation effects. The single-cavity QNM expansion (G_1) [Eq. (18)] does not match the full numerical results, confirming the coupling of the QNMs. The coupling is normalized to $g_{ba}^{\text{back}}(\omega_1)$ (i.e., without the dimers).

the specific shape which is dominated by the intercavity QNM coupling, which is contained in the expansion from Eq. (13) but not in Eq. (18).

In Fig. 4, we show the coupling $g_{ba}(\omega)$ for a shorter dimer separation of $R_{21} = 760$ nm, which is close to the QNM resonance wavelengths. The QNM

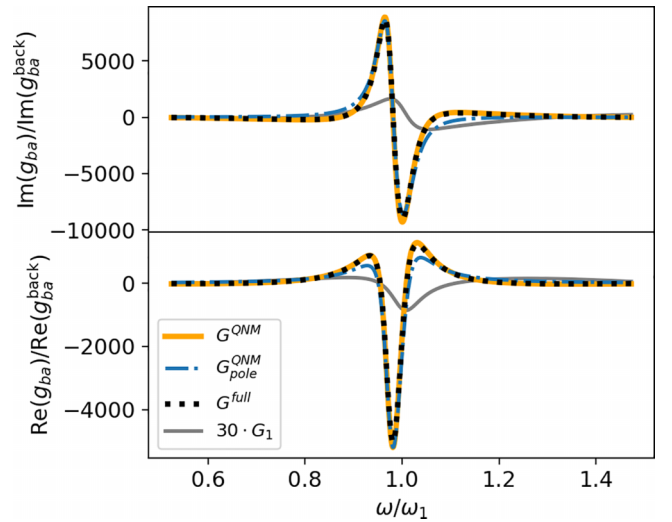


FIG. 4. Same as in Fig. 3, but with $R_{12} = 760$ nm $\approx 1.04\lambda_1$. Equation (13) together with Eq. (15) (G^{QNM}) agrees excellently with the full numerical solution (G^{full}). Equation (17) ($G_{\text{pole}}^{\text{QNM}}$) yields better agreement than for larger separations, while the single-cavity QNM expansion (G_1) from Eq. (18) fails to capture the shape and magnitude of the coupling.

expansion from Eq. (13) together with Eq. (15) [where $N_{21} = (5.3797 + i0.4523) \times 10^{-7} \text{ nm}^{-2}$] again shows excellent agreement with full numerical calculations. Including the phase in the pole approximation [Eq. (17)] yields better agreement with the full solution than for $R_{21} = 2020 \text{ nm}$, since retardation effects are weaker for shorter separations. The single-cavity expansion [Eq. (18)] again fails to capture the full coupling, both quantitatively and qualitatively.

Conclusions and discussion. We have presented a multicavity expansion of the electromagnetic Green's function using single-cavity QNMs. Starting from the single-cavity QNM Green's function, the scheme iteratively adds more cavities via a set of scattering equations where the Green's function obtained from each step serves as input in the next step. Thus, the full scattered Green's function for an arbitrary number of cavities is easily obtained from a finite number of iterations.

Fixing a well-known problem for coupled QNMs over large distances, our framework permits an accurate few-mode approximation by using regularization and including retardation effects, making it suitable for quantum dynamics applications where the Hilbert space scales exponentially with the number of modes. Multicavity scattering terms naturally decompose into products of two-cavity scattering processes, avoiding nested integrals.

Comparing rigorous numerical solutions of the full 3D Maxwell equations to the QNM expansion, we demonstrated the quantitative accuracy of the approach for two coupled metal dimers serving as QNM cavities at two different distances between the dimers.

The scheme presented here can help in the study and design of novel quantum devices by simplifying their numerical simulation and providing an intuitive framework for scattering between open resonators with finite retardation delays.

Acknowledgments. R.M.F. and M.R. acknowledge support from the Deutsche Forschungsgemeinschaft (Project No. 525575745). J.R. and S.H. acknowledge funding from Queen's University, Canada, the Canadian Foundation for Innovation (CFI), the Natural Sciences and Engineering Research Council of Canada (NSERC), and CMC Microsystems for the provision of COMSOL Multiphysics; S.H. also thanks the Alexander von Humboldt Foundation for support through a Humboldt Award.

Data availability. The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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