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Resonant-state expansion for open optical systems: generalization to magnetic, chiral, and bi-anisotropic materials

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The resonant-state expansion, a recently developed powerful method in electrodynamics, is generalized here for open optical systems containing magnetic, chiral, or bi-anisotropic materials. It is shown that the key matrix eigenvalue equation of the method remains the same, but the matrix elements of the perturbation now contain variations of the permittivity, permeability, and bi-anisotropy tensors. A general normalization of resonant states in terms of the electric and magnetic fields is presented.

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The resonant state expansion (RSE) is a novel powerful theoretical method that has been recently developed in electrodynamics [1]. The RSE is a rigorous perturbation theory that is not limited to small perturbations and warrants an efficient calculation of all resonant states (RSs) of an open optical system in an arbitrarily selected spectral range. This calculation is based on knowing the RSs of another, so-called basis system, which is usually (but not necessarily) simpler than the system of interest, ideally having an exact analytic solution. The RSE was verified and tested on optical systems of different shape and dimensionality [2–5], demonstrating its superior computational efficiency [3,5] compared to available numerical methods, such as finite-difference time-domain [6,7], finite element [8], and the aperiodic Fourier modal method [9,10].

Being originally introduced in nuclear physics almost a century ago [11,12], RSs in electrodynamics present eigensolutions of Maxwell's equations satisfying outgoing boundary conditions, which correspond to electromagnetic excitations decaying in time, with the electromagnetic energy leaking out of the system. This leakage, however, causes an exponential growth of the RS wave function with distance, so that the standard normalization used, for example, for bound states in quantum mechanics or for waveguide modes in optics, diverges. While the correct normalization for scalar fields was known [13], expressions for the normalization of the electromagnetic vector fields of the RSs, intensively used in the literature [14,15], are only approximate, as has been recently clarified [16,17]. The correct normalization of RSs in finite optical systems, which is a cornerstone of the RSE, was presented in the very first paper on the method [1] and was later generalized to arbitrary systems with frequency dispersion of the permittivity [18]. Recently, it has been used to formulate an exact theory of the Purcell effect [16]. Furthermore, the exact normalization was extended to photonic crystal structures [19,20] and applied to resonantly enhanced refractive index sensing using the RSE with only one and two RSs in the basis.

The RSE has also been generalized to optical systems with frequency dispersion of the permittivity [18] without affecting the computational complexity, which is a very important step towards describing realistic materials and specifically plasmonic effects. This was achieved by treating the dispersion as an analytical function with a finite number of simple poles in the lower half-plane of the complex frequency, known in the literature as the generalized Drude–Lorentz model [21].

So far, the RSE was applied to non-magnetic optical systems ($\mu = 1$), which are fully described by the wave equation containing solely the electric field, the permittivity tensor, and an electric current. Naturally, the RS normalization and the RSE itself dealing with perturbations of the permittivity were formulated in terms of the electric field only. However, the most general materials with local responses are bi-anistropic and have non-zero magnetic susceptibility and coupling tensors between the electric and magnetic fields, including the chiral optical activity and circular dichroism [22]. Describing such systems, which include but are not limited to metamaterials [23], chiral plasmonics [24,25], and chiral sensors, is of growing interest. Therefore, it is crucial to have a general formulation of the RSE and the RS normalization, in which the electric and magnetic fields contribute as equal partners, and the local linear response of an optical system is taken in the most general form. This is done in the this Letter below by using a novel approach for deriving the RSE that is based on Maxwell's equations.

Maxwell's equations and Green's dyadic: An arbitrary linear optical system is described by Maxwell's equations in a medium:

$$\nabla\times\mathbf{E}=ik\mathbf{B},\quad \nabla\times\mathbf{H}=-ik\mathbf{D}+\frac{4\pi}{c}\mathbf{j},\tag{1}$$

where $k=\omega/c$ is the wave number in vacuum, and ω is the frequency of the electromagnetic field. Generally, for systems with a spatially local linear response, one can write

$$\mathbf{D}=\hat{\boldsymbol{\varepsilon}}\mathbf{E}+\hat{\boldsymbol{\xi}}\mathbf{H},\quad \mathbf{B}=\hat{\boldsymbol{\mu}}\mathbf{H}+\hat{\boldsymbol{\zeta}}\mathbf{E},\tag{2}$$

with frequency dependent tensors of permittivity $\hat{\boldsymbol{\varepsilon}}(k,\mathbf{r})$ and permeability $\hat{\boldsymbol{\mu}}(k,\mathbf{r})$, and bi-anisotropy tensors $\hat{\boldsymbol{\xi}}(k,\mathbf{r})$ and $\hat{\boldsymbol{\zeta}}(k,\mathbf{r})$. In the following, we concentrate on systems satisfying the reciprocity relation, leading additionally to $\hat{\boldsymbol{\varepsilon}}^T=\hat{\boldsymbol{\varepsilon}}$, $\hat{\boldsymbol{\mu}}^T=\hat{\boldsymbol{\mu}}$, and $\hat{\boldsymbol{\xi}}^T=-\hat{\boldsymbol{\zeta}}$. Equations (1) and (2) can be written in the following compact symmetric way:

$$\hat{\mathbb{M}}(k,\mathbf{r})\vec{\mathbb{F}}(\mathbf{r})=\vec{\mathbb{J}}(\mathbf{r})\tag{3}$$

with 6×6 matrix operator $\hat{\mathbb{M}}(k,\mathbf{r})=k\hat{\mathbb{P}}(k,\mathbf{r})-\hat{\mathbb{D}}(\mathbf{r})$, where

$$\hat{\mathbb{P}}(k,\mathbf{r})=\begin{pmatrix}\hat{\boldsymbol{\varepsilon}} & \hat{\boldsymbol{\eta}}\\ \hat{\boldsymbol{\eta}}^T & \hat{\boldsymbol{\mu}}\end{pmatrix},\quad \hat{\mathbb{D}}(\mathbf{r})=\begin{pmatrix}0 & \nabla\times\\ \nabla\times & 0\end{pmatrix},\tag{4}$$

and $\hat{\boldsymbol{\eta}}=-i\hat{\boldsymbol{\xi}}$. The electric and magnetic fields, as well as the currents, are now represented by six-dimensional vectors:

$$\vec{\mathbb{F}}(\mathbf{r})=\begin{pmatrix}\mathbf{E}\\ i\mathbf{H}\end{pmatrix}\quad\text{and}\quad \vec{\mathbb{J}}(\mathbf{r})=\begin{pmatrix}\mathbf{J}_E\\ i\mathbf{J}_H\end{pmatrix},\tag{5}$$

respectively, where $\mathbf{J}_E=-4\pi i\mathbf{j}/c$, and the magnetic current $\mathbf{J}_H$ is introduced artificially for symmetry purposes.

We now introduce a generalized dyadic Green's function (GF) $\hat{\mathbb{G}}_k(\mathbf{r},\mathbf{r}')$ with outgoing boundary conditions in the regions outside the optical system, satisfying the equation

$$\hat{\mathbb{M}}(k,\mathbf{r})\hat{\mathbb{G}}_k(\mathbf{r},\mathbf{r}')=\hat{\mathbb{I}}\delta(\mathbf{r}-\mathbf{r}'),\tag{6}$$

in which $\hat{\mathbb{I}}$ is the 6×6 identity matrix. The GF has simple poles [2,3] at $k=k_n$, which are the wave numbers of the RSs of the system. The RSs, in turn, are the eigensolutions of the homogeneous Maxwell's equations:

$$\hat{\mathbb{M}}(k_n,\mathbf{r})\vec{\mathbb{F}}_n(\mathbf{r})=0,\tag{7}$$

satisfying outgoing boundary conditions, where the index n is used to label the RSs. Owing to the reciprocity principle and the Mittag-Leffler (ML) theorem, the GF is represented as a series [2]:

$$\hat{\mathbb{G}}_k(\mathbf{r},\mathbf{r}')=\sum_n\frac{\vec{\mathbb{F}}_n(\mathbf{r})\otimes\vec{\mathbb{F}}_n(\mathbf{r}')}{k-k_n},\tag{8}$$

determining the normalization of RSs that is considered below. Note that Eq. (8) is valid within the system, or rather within a minimal convex volume including it.

Closure relation and sum rules: Substituting the ML expansion Eq. (8) into Eq. (6) for the GF and using Eq. (7), we obtain

$$\sum_n\frac{k\hat{\mathbb{P}}(k,\mathbf{r})-k_n\hat{\mathbb{P}}(k_n,\mathbf{r})}{k-k_n}\vec{\mathbb{F}}_n(\mathbf{r})\otimes\vec{\mathbb{F}}_n(\mathbf{r}')=\hat{\mathbb{I}}\delta(\mathbf{r}-\mathbf{r}').\tag{9}$$

In the absence of dispersion, Eq. (9) immediately results in the following closure relation:

$$\hat{\mathbb{P}}(\mathbf{r})\sum_n\vec{\mathbb{F}}_n(\mathbf{r})\otimes\vec{\mathbb{F}}_n(\mathbf{r}')=\hat{\mathbb{I}}\delta(\mathbf{r}-\mathbf{r}').\tag{10}$$

In the case of a frequency dispersion described by a generalized Drude–Lorentz model [18,21], the matrix $\hat{\mathbb{P}}$ becomes

$$\hat{\mathbb{P}}(k,\mathbf{r})=\hat{\mathbb{P}}_\infty(\mathbf{r})+\sum_j\frac{\hat{\mathbb{Q}}_j(\mathbf{r})}{k-\Omega_j},\tag{11}$$

having complex poles at $k=\Omega_j$ with generalized conductivities $\hat{\mathbb{Q}}_j(\mathbf{r})$ playing the role of the residues in the ML expansion of the permittivity, permeability, and bi-anisotropy tensors. Examples of such an expansion for plasmonic and chiral materials are given in Refs. [18] and [24], respectively. Substituting Eq. (11) into Eq. (9) and using the algebraic identity

$$\frac{1}{k-k_n}\left(\frac{k}{k-\Omega_j}-\frac{k_n}{k_n-\Omega_j}\right)=\frac{-\Omega_j}{(k-\Omega_j)(k_n-\Omega_j)},\tag{12}$$

yields

$$\sum_n\left[\hat{\mathbb{P}}_\infty(\mathbf{r})-\sum_j\frac{\Omega_j\hat{\mathbb{Q}}_j(\mathbf{r})}{(k-\Omega_j)(k_n-\Omega_j)}\right]\vec{\mathbb{F}}_n(\mathbf{r})\otimes\vec{\mathbb{F}}_n(\mathbf{r}')$$
$$=\hat{\mathbb{I}}\delta(\mathbf{r}-\mathbf{r}').\tag{13}$$

Since the Lorentzian functions are linearly independent, Eq. (13) splits into sum rules

$$\hat{\mathbb{Q}}_j(\mathbf{r})\sum_n\frac{\vec{\mathbb{F}}_n(\mathbf{r})\otimes\vec{\mathbb{F}}_n(\mathbf{r}')}{k_n-\Omega_j}=0\tag{14}$$

and a closure relation

$$\hat{\mathbb{P}}_\infty(\mathbf{r})\sum_n\vec{\mathbb{F}}_n(\mathbf{r})\otimes\vec{\mathbb{F}}_n(\mathbf{r}')=\hat{\mathbb{I}}\delta(\mathbf{r}-\mathbf{r}'),\tag{15}$$

similar to the non-dispersive one, Eq. (10). Summing Eq. (14) over all j and adding it to Eq. (15), we can reformulate the closure relation as

$$\sum_n\hat{\mathbb{P}}(k_n,\mathbf{r})\vec{\mathbb{F}}_n(\mathbf{r})\otimes\vec{\mathbb{F}}_n(\mathbf{r}')=\hat{\mathbb{I}}\delta(\mathbf{r}-\mathbf{r}').\tag{16}$$

Normalization of resonant states: As already mentioned, the form of the GF Eq. (8) determines the normalization of the RS wave functions $\vec{\mathbb{F}}_n(\mathbf{r})$. To derive this normalization, we introduce an analytic continuation $\vec{\mathbb{F}}(k,\mathbf{r})$ of RS field $\vec{\mathbb{F}}_n(\mathbf{r})$ in the complex k-plane around the $k=k_n$ point. $\vec{\mathbb{F}}(k,\mathbf{r})$ satisfies Eq. (3), which can be solved with the help of the GF. Using Eq. (8), we obtain

$$\vec{\mathbb{F}}(k,\mathbf{r})=\sum_n\frac{\vec{\mathbb{F}}_n(\mathbf{r})}{k-k_n}\int\vec{\mathbb{F}}_n(\mathbf{r}')\cdot\vec{\mathbb{J}}(\mathbf{r}')d\mathbf{r}'.\tag{17}$$

The requirement that $\vec{\mathbb{F}}(k,\mathbf{r})\to\vec{\mathbb{F}}_n(\mathbf{r})$ in the limit $k\to k_n$ results in the following k dependence of the current: $\vec{\mathbb{J}}(\mathbf{r})=(k-k_n)\vec{\mathbb{S}}(\mathbf{r})$, where $\vec{\mathbb{S}}(\mathbf{r})$ is normalized such that

$$\int\vec{\mathbb{F}}_n(\mathbf{r})\cdot\vec{\mathbb{S}}(\mathbf{r})d\mathbf{r}=1.\tag{18}$$

While $\vec{\mathbb{S}}(\mathbf{r})$ is an arbitrary function of k and $\mathbf{r}$, vanishing outside the system, it can be chosen to be independent of k. Equation (18) then provides the normalization of the RSs. Indeed, multiplying Eq. (3) with $\vec{\mathbb{F}}_n(\mathbf{r})$, Eq. (7) with $\vec{\mathbb{F}}(k,\mathbf{r})$, and taking the difference between the two, yields

$$k\vec{\mathbb{F}}_n\cdot\hat{\mathbb{P}}(k)\vec{\mathbb{F}}-k_n\vec{\mathbb{F}}\cdot\hat{\mathbb{P}}(k_n)\vec{\mathbb{F}}_n-\vec{\mathbb{F}}_n\cdot\hat{\mathbb{D}}\vec{\mathbb{F}}+\vec{\mathbb{F}}\cdot\hat{\mathbb{D}}\vec{\mathbb{F}}_n$$
$$=(k-k_n)\vec{\mathbb{F}}_n\cdot\vec{\mathbb{S}}, \tag{19}$$

where the k and $\mathbf{r}$ dependencies are dropped for brevity of notations. The third and the fourth terms in the left-hand side of Eq. (19) can be written as

$$-\vec{\mathbb{F}}_n\cdot\hat{\mathbb{D}}\vec{\mathbb{F}}+\vec{\mathbb{F}}\cdot\hat{\mathbb{D}}\vec{\mathbb{F}}_n=i\nabla\cdot(\mathbf{E}_n\times\mathbf{H}-\mathbf{E}\times\mathbf{H}_n).$$

Integrating Eq. (19) over an arbitrary volume V containing the system, using the divergence theorem, and taking the limit $k\to k_n$, we obtain a general formula for the RS normalization:

$$1=\int_V\vec{\mathbb{F}}_n\cdot[k\hat{\mathbb{P}}(k)]'\vec{\mathbb{F}}_n\mathrm{d}\mathbf{r}+i\oint_{S_V}(\mathbf{E}_n\times\mathbf{H}_n'-\mathbf{E}_n'\times\mathbf{H}_n)\cdot\mathrm{d}\mathbf{S}, \tag{20}$$

where S_V is the boundary of V, and the prime means the derivative with respect to k taken at $k=k_n$. The differentiation of the matrix $k\hat{\mathbb{P}}(k)$ is straightforward, whereas the derivatives of the analytic continuation of the fields outside the system can be expressed as [1,16]

$$\mathbf{F}_n'=\frac{1}{k_n}(\mathbf{r}\cdot\nabla)\mathbf{F}_n, \tag{21}$$

in which $\mathbf{F}_n$ is either $\mathbf{E}_n$ or $\mathbf{H}_n$. The normalization Eq. (20) then takes an explicit form in terms of the electric and magnetic fields of a given RS:

$$1=\int_V[\mathbf{E}_n\cdot(k\hat{\varepsilon})'\mathbf{E}_n+\mathbf{E}_n\cdot(k\hat{\xi})'\mathbf{H}_n]\mathrm{d}\mathbf{r}$$
$$-\int_V[\mathbf{H}_n\cdot(k\hat{\zeta})'\mathbf{E}_n+\mathbf{H}_n\cdot(k\hat{\mu})'\mathbf{H}_n]\mathrm{d}\mathbf{r}$$
$$+\frac{i}{k_n}\oint_{S_V}[\mathbf{E}_n\times(\mathbf{r}\cdot\nabla)\mathbf{H}_n+\mathbf{H}_n\times(\mathbf{r}\cdot\nabla)\mathbf{E}_n]\cdot\mathrm{d}\mathbf{S}. \tag{22}$$

This general normalization is fully consistent with the analytic normalizations we have previously used in terms of the electric field [1,3,16,18,19], for systems described by the permittivity, as we demonstrate below. We note, however, that writing the GF as in Eq. (8), the electric field of the normalized RS is a factor of $\sqrt{2}$ smaller than the one used in our previous works. Furthermore, as we also show below, the general normalization Eq. (22) is suited for both static and non-static RSs, which is consistent with two different expressions used previously for these cases [3].

Let us show that for non-magnetic materials, described by only the permittivity, the general normalization Eq. (22) reduces to the one previously used in terms of the electric field only [1,3,16,18,19]. In this case, $\hat{\boldsymbol{\xi}}=\hat{\boldsymbol{\zeta}}=0$ and $\hat{\boldsymbol{\mu}}=\hat{\mathbf{1}}$, where $\hat{\mathbf{1}}$ is a 3×3 identity matrix, and Eq. (22) becomes

$$1=\int_V\mathbf{E}_n\cdot(k\hat{\boldsymbol{\varepsilon}})'\mathbf{E}_n\mathrm{d}\mathbf{r}-\int_V\mathbf{H}_n\cdot\mathbf{H}_n\mathrm{d}\mathbf{r}+i\oint_{S_V}(\mathbf{E}_n\times\mathbf{H}_n'-\mathbf{E}_n'\times\mathbf{H}_n)\cdot\mathrm{d}\mathbf{S}, \tag{23}$$

where we have taken the surface term again in the form of the field derivatives, as in Eq. (20). Using the Poynting theorem for the RS wave function, we can transform the second volume integral in Eq. (23) into

$$-\int_V\mathbf{H}_n\cdot\mathbf{H}_n\mathrm{d}\mathbf{r}=\frac{i}{k_n}\oint_{S_V}\mathbf{E}_n\times\mathbf{H}_n\cdot\mathrm{d}\mathbf{S}+\int_V\mathbf{E}_n\cdot\hat{\boldsymbol{\varepsilon}}\mathbf{E}_n\mathrm{d}\mathbf{r}. \tag{24}$$

For the surface integral in Eq. (23), we obtain

$$i\oint_{S_V}(\mathbf{E}_n\times\mathbf{H}_n'-\mathbf{E}_n'\times\mathbf{H}_n)\cdot\mathrm{d}\mathbf{S}=-\frac{i}{k_n}\oint_{S_V}\mathbf{E}_n\times\mathbf{H}_n\cdot\mathrm{d}\mathbf{S}$$
$$+\frac{1}{k_n}\oint_{S_V}\left(\frac{\partial\mathbf{E}_n'}{\partial s}\cdot\mathbf{E}_n-\frac{\partial\mathbf{E}_n}{\partial s}\cdot\mathbf{E}_n'\right)\mathrm{d}S, \tag{25}$$

using vector identities, as well as $\nabla\times\mathbf{E}_n'=i\mathbf{H}_n+ik_n\mathbf{H}_n'$ and the fact that $\nabla\cdot\mathbf{E}_n=\nabla\cdot\mathbf{E}_n'=0$ outside the system. Collecting all terms, we obtain the normalization condition for RSs with $k_n\neq0$:

$$1=2\int_V\mathbf{E}_n\cdot\frac{\partial(k^2\hat{\boldsymbol{\varepsilon}})}{\partial(k^2)}\bigg|_{k_n}\mathbf{E}_n\mathrm{d}\mathbf{r}+\frac{1}{k_n}\oint_{S_V}\left(\frac{\partial\mathbf{E}_n'}{\partial s}\cdot\mathbf{E}_n-\frac{\partial\mathbf{E}_n}{\partial s}\cdot\mathbf{E}_n'\right)\mathrm{d}S, \tag{26}$$

where $\partial/\partial s$ means the spatial derivative along the surface normal, and $\mathbf{E}_n'=(\mathbf{r}\cdot\nabla)\mathbf{E}_n/k_n$, according to Eq. (21).

For static electric modes with $k_n=0$, the condition $\mathbf{H}_n=0$ leads to the volume term in Eq. (23) with the magnetic field vanishing. Since the electric field of a static mode $\mathbf{E}_n\to0$ far away from the system [3] and the surface of integration can be chosen as any closed surface including the system, one can get rid of the surface integral, ending up with the volume integral of the electric field over the entire space:

$$1=\int\mathbf{E}_n\cdot\frac{\partial(k^2\hat{\boldsymbol{\varepsilon}})}{\partial(k^2)}\bigg|_{k_n}\mathbf{E}_n\mathrm{d}\mathbf{r}. \tag{27}$$

Both results Eq. (26) and Eq. (27) are identical to the normalization of RSs in non-magnetic materials obtained in [1,3,16,18], with the already noted factor of 2 introduced in this Letter.

Resonant-state expansion: Let us now consider a perturbed system described by a general frequency dependent perturbation $\Delta\hat{\mathbb{P}}(k,\mathbf{r})$ of the permittivity, permeability, and bi-anisotropy tensors. The Maxwell equation for a perturbed RS $\vec{\mathbb{F}}(\mathbf{r})$ then takes the form

$$\hat{\mathbb{M}}(k,\mathbf{r})\vec{\mathbb{F}}(\mathbf{r})=-k\Delta\hat{\mathbb{P}}(k,\mathbf{r})\vec{\mathbb{F}}(\mathbf{r}), \tag{28}$$

where k is the perturbed eigenvalue. Note that the unperturbed system and the perturbation are chosen in such a way that the perturbation is included in the minimal convex volume containing the unperturbed system. Solving Eq. (28) with the help of the GF, we obtain

$$\vec{\mathbb{F}}(\mathbf{r})=-k\int\hat{\mathbb{G}}_k(\mathbf{r},\mathbf{r}')\Delta\hat{\mathbb{P}}(k,\mathbf{r}')\vec{\mathbb{F}}(\mathbf{r}')\mathrm{d}\mathbf{r}'. \tag{29}$$

Let us first assume a non-dispersive perturbation $\Delta\hat{\mathbb{P}}(\mathbf{r})$. Substituting the ML expansion Eq. (8) into Eq. (29) and expanding the perturbed field inside the system into the unperturbed RSs as

$$\vec{\mathbb{F}}(\mathbf{r})=\sum_n c_n\vec{\mathbb{F}}_n(\mathbf{r}), \tag{30}$$

we obtain

$$\sum_n c_n\vec{\mathbb{F}}_n(\mathbf{r})=-k\sum_n\frac{\vec{\mathbb{F}}_n(\mathbf{r})}{k-k_n}\sum_m V_{nm}c_m, \tag{31}$$

where the matrix elements of the perturbation are given by

$$V_{nm}=\int\vec{\mathbb{F}}_n(\mathbf{r})\cdot\Delta\hat{\mathbb{P}}(\mathbf{r})\vec{\mathbb{F}}_m(\mathbf{r})\mathrm{d}\mathbf{r}. \tag{32}$$

Equating coefficients at the basis functions $\vec{\mathbb{F}}_n(\mathbf{r})$, Eq. (31) reduces to

$$(k - k_n)c_n = -k\sum_m V_{nm}c_m, \quad (33)$$

which is the standard non-dispersive RSE equation [1,3].

Taking into account the dispersion of the perturbation in a generalized Drude–Lorentz form,

$$\Delta\hat{\mathbb{P}}(k, \mathbf{r}) = \Delta\hat{\mathbb{P}}_\infty(\mathbf{r}) + \sum_j \frac{\Delta\hat{\mathbb{Q}}_j(\mathbf{r})}{k - \Omega_j}, \quad (34)$$

Eq. (29) becomes

$$\vec{\mathbb{F}}(\mathbf{r}) = -k\int \hat{\mathbb{G}}_k(\mathbf{r}, \mathbf{r}')\Delta\hat{\mathbb{P}}_\infty(\mathbf{r}')\vec{\mathbb{F}}(\mathbf{r}')d\mathbf{r}' - k\sum_j \int \hat{\mathbb{G}}_k^j(\mathbf{r}, \mathbf{r}')\frac{\Delta\hat{\mathbb{Q}}_j(\mathbf{r}')}{k - \Omega_j}\vec{\mathbb{F}}(\mathbf{r}')d\mathbf{r}', \quad (35)$$

where we have added in the second line zeros in the form of the sum rules defined by Eq. (14):

$$\hat{\mathbb{G}}_k^j(\mathbf{r}, \mathbf{r}') = \hat{\mathbb{G}}_k(\mathbf{r}, \mathbf{r}') + \frac{\Omega_j}{k}\sum_n \frac{\vec{\mathbb{F}}_n(\mathbf{r}) \otimes \vec{\mathbb{F}}_n(\mathbf{r}')}{k_n - \Omega_j}. \quad (36)$$

Using again the ML expansion Eq. (8) of the GF $\hat{\mathbb{G}}_k(\mathbf{r}, \mathbf{r}')$ and the algebraic identity Eq. (12), we arrive, after equating coefficients at the basis functions $\vec{\mathbb{F}}_n(\mathbf{r})$, at the linear eigenvalue equation of the dispersive RSE:

$$(k - k_n)c_n = -k\sum_m V_{nm}(\infty)c_m + k_n\sum_m [V_{nm}(\infty) - V_{nm}(k_n)]c_m, \quad (37)$$

with the matrix elements of the dispersive perturbation given by

$$V_{nm}(k) = \int \vec{\mathbb{F}}_n(\mathbf{r}) \cdot \Delta\hat{\mathbb{P}}(k, \mathbf{r})\vec{\mathbb{F}}_m(\mathbf{r})d\mathbf{r}. \quad (38)$$

Note that Eq. (37) has the same form as that developed in Ref. [18] and, in the case of no frequency dispersion, it reduces back to Eq. (33). However, the matrix elements Eq. (38) now have the most general form, which can be written explicitly as

$$V_{nm}(k) = \int_V [\mathbf{E}_n \cdot \Delta\hat{\boldsymbol{\varepsilon}}(k)\mathbf{E}_m + \mathbf{E}_n \cdot \Delta\hat{\boldsymbol{\xi}}(k)\mathbf{H}_m]d\mathbf{r} - \int_V [\mathbf{H}_n \cdot \Delta\hat{\boldsymbol{\zeta}}(k)\mathbf{E}_m + \mathbf{H}_n \cdot \Delta\hat{\boldsymbol{\mu}}(k)\mathbf{H}_m]d\mathbf{r}. \quad (39)$$

The matrix elements Eq. (39) are expressed in terms of the electric and magnetic fields of basis RSs n and m and generally dispersive changes of the tensors of the permittivity $\Delta\hat{\boldsymbol{\varepsilon}}(k, \mathbf{r})$, permeability $\Delta\hat{\boldsymbol{\mu}}(k, \mathbf{r})$, and bi-anisotropy couplings $\Delta\hat{\boldsymbol{\xi}}(k, \mathbf{r})$ and $\Delta\hat{\boldsymbol{\zeta}}(k, \mathbf{r})$ between the electric and magnetic fields. Solving the matrix eigenvalue problem Eq. (37) of the RSE determines the wave numbers k of the perturbed RSs and the coefficients c_n of the expansion of the perturbed wave functions into the known RSs of a basis system. Presently, this is the most efficient and intuitive computational approach for finding the RSs of open optical systems, as demonstrated in numerous publications [1–5,18–20]. This approach is now generalized to bi-anisotropic systems.

In conclusion, we have generalized the resonant-state expansion for open optical systems containing arbitrary reciprocal bi-anisotropic materials or metamaterials, including those having magnetic and chiral optical activity, as well as circular dichroism. We have presented the theory in the most general, compact, and symmetrized way, with the electric and magnetic field vectors contributing on equal footing. We have addressed both cases of non-dispersive systems and systems having frequency dispersion described by a generalized Drude-Lorentz model. We have derived a general compact formula for the normalization of resonant states, expressed in terms of the electric and magnetic fields, and shown its equivalence to the one used previously for systems fully described by their permittivity and expressed in terms of the electric field only. The presented theory has the widest spectrum of applications, ranging from the modeling and optimization of chirality sensors to the accurate description of the optics of magnetic and metamaterial systems.

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