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

E. A. Muljarov\textsuperscript{1,*} and T. Weiss\textsuperscript{2}

\textsuperscript{1}School of Physics and Astronomy, Cardiff University, Cardiff CF24 3AA, United Kingdom
\textsuperscript{2}4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, D-70550 Stuttgart, Germany
\textsuperscript{*}Corresponding author: Egor.Muljarov@astro.cf.ac.uk

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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. © 2018 Optical Society of America

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

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

where \( k = \omega / c \) is the wave number in vacuum, and \( \omega \) is the

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frequency of the electromagnetic field. Quite generally, for systems with a spatially local linear response, one can write

\[
D = \varepsilon E + \hat{\varepsilon}_H, \quad B = \mu H + \hat{\mu}_E,
\]

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

\[
\hat{M}(k, r)\hat{F}(r) = \hat{J}(r),
\]

where \(\hat{M}(k, r) = k\hat{P}(k, r) - \hat{D}(r)\) is a 6x6 matrix operator, with

\[
\hat{P}(k, r) = \begin{pmatrix} \varepsilon & \eta \\ \eta^T & \text{identity} \end{pmatrix}, \quad \hat{D}(r) = \begin{pmatrix} 0 & \nabla \times \\ \nabla \times & 0 \end{pmatrix},
\]

and \(\eta = -i\hat{\varepsilon}\). The electric and magnetic fields as well as the currents are now represented by 6-dimensional vectors,

\[
\hat{F}(r) = \begin{pmatrix} E \\ iH \end{pmatrix} \quad \text{and} \quad \hat{J}(r) = \begin{pmatrix} J_E \\ iJ_H \end{pmatrix},
\]

respectively, where \(J_E = -4\pi i j / c\), and the magnetic current \(J_H\) is introduced for symmetry purposes (although this is not necessary).

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

\[
\hat{M}(k, r)\hat{G}_k(r, r') = \hat{\delta}(r - r'),
\]

in which \(\hat{\delta}\) is the 6x6 identity matrix. The GF has simple poles [3, 4] at \(k = k_n\), which are the wave numbers of the RSs of the system. The RSs are in turn the eigen solutions of the homogeneous Maxwell’s equations,

\[
\hat{M}(k_n, r)\hat{F}_n(r) = 0,
\]

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 [3]

\[
\hat{G}_k(r, r') = \sum_n \hat{F}_n(r) \otimes \hat{F}_n(r') / (k - k_n),
\]

determinining 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

\[
\sum_n k\hat{P}(k, r) - k_n\hat{P}(k_n, r) / (k - k_n)\hat{F}_n(r) \otimes \hat{F}_n(r') = \hat{\delta}(r - r').
\]

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

\[
\hat{P}(r) \sum_n \hat{F}_n(r) \otimes \hat{F}_n(r') = \hat{\delta}(r - r').
\]

In the case of a frequency dispersion described by a generalized Drude-Lorentz model [19, 22], the matrix \(\hat{P}\) becomes

\[
\hat{P}(k, r) = \hat{P}_\infty(r) + \sum_j Q_j(r) / (k - \Omega_j),
\]

having complex poles at \(k = \Omega_j\) with generalized conductivities \(Q_j(r)\). Substituting Eq. (11) into Eq. (9) and using the algebraic identity

\[
1 / (k - k_n) = 1 / (k - \Omega_j) / (k_n - \Omega_j)
\]

yields

\[
\sum_n \left[ \hat{P}_\infty(r) - \sum_j \Omega_j Q_j(r) / (k_n - \Omega_j) \right] \hat{F}_n(r) \otimes \hat{F}_n(r') = \hat{\delta}(r - r'),
\]

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

\[
Q_j(r) \sum_n \hat{F}_n(r) \otimes \hat{F}_n(r') = 0
\]

and a closure relation

\[
\hat{P}_\infty(r) \sum_n \hat{F}_n(r) \otimes \hat{F}_n(r') = \hat{\delta}(r - r'),
\]

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

\[
\sum_n \hat{P}(k_n, r) \hat{F}_n(r) \otimes \hat{F}_n(r') = \hat{\delta}(r - r').
\]

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

\[
\hat{F}(k, r) = \int \hat{G}_k(r, r')\hat{F}(r')dr' = \sum_n \hat{F}_n(r) / k - k_n \int \hat{F}_n(r') \cdot \hat{F}(r')dr'.
\]

The requirement that \(\hat{F}(k, r) \to \hat{F}_n(r)\) in the limit \(k \to k_n\) results in the following \(k\) dependence of the current: \(\hat{J}(r) = (k - k_n)\hat{S}(r)\), where \(\hat{S}(r)\) can be chosen as a \(k\)-independent function, normalized in such a way that

\[
\int \hat{F}_n(r) \cdot \hat{S}(r)dr = 1.
\]

Equation (18) then provides the normalization of the RSs. Indeed, multiplying Eq. (3) with \(\hat{F}_n(r)\), Eq. (7) with \(\hat{F}(k, r)\), and taking the difference between the two, yields

\[
k\hat{F}_n \cdot \hat{P}(k)\hat{F}_n - k_n\hat{F}_n \cdot \hat{P}(k_n)\hat{F}_n = (k - k_n)\hat{F}_n \cdot \hat{S},
\]

where the \(k\) and \(r\) 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

\[
-k\hat{F}_n \cdot \hat{D}(k)\hat{F}_n + \hat{F}_n \cdot \hat{D}(k_n)\hat{F}_n = i\nabla \cdot (E_n \times H - E \times H_n).
\]
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:

\[
1 = \int_V \hat{\mathbf{F}}_n \cdot [\hat{k} \hat{\mathbf{P}}(\hat{k})] \hat{F}_n \, d\mathbf{r} + \int_{S_V} \mathbf{E}_n \times \mathbf{H}'_n - \mathbf{E}'_n \times \mathbf{H}_n \, dS,
\]

(20)

where \( S_V \) is the boundary of \( V \), and the prime means the derivative with respect to \( k \) taken at \( k = k_n \). Differentiation of the matrix \( k \hat{\mathbf{P}}(\hat{k}) \) is straightforward, whereas the derivatives of the analytic continuation of the fields outside the system can be expressed as \[1, 17\]

\[
\mathbf{F}'_n = \frac{1}{k_n}(\mathbf{r} \cdot \nabla) \mathbf{F}_n,
\]

(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:

\[
1 = \int_V \left[ \mathbf{E}_n \cdot (\hat{k} \hat{\mathbf{P}}) \mathbf{E}_n + \mathbf{E}_n \cdot (\hat{\mathbf{k}} \hat{\mathbf{P}}) \mathbf{H}_n \right] \, d\mathbf{r} \\
- \int_V \left[ \mathbf{H}_n \cdot (\hat{k} \hat{\mathbf{P}}) \mathbf{E}_n + \mathbf{H}_n \cdot (\hat{\mathbf{k}} \hat{\mathbf{P}}) \mathbf{H}_n \right] \, d\mathbf{r} \\
+ \frac{i}{k_n} \int_{S_V} \left[ \mathbf{E}_n \times (\mathbf{r} \cdot \nabla) \mathbf{H}_n + \mathbf{H}_n \times (\mathbf{r} \cdot \nabla) \mathbf{E}_n \right] \, dS.
\]

(22)

This general normalization is fully consistent with the analytic normalizations we have previously used in terms of the electric field [1, 4, 17, 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 expression used previously for these cases [4].

**Normalization of RSs in terms of the electric field.** 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, 4, 17, 19]. In this case \( \hat{\xi} = \xi = 0 \) and \( \hat{\mu} = \hat{1} \), where \( \hat{1} \) is a 3x3 identity matrix, and Eq. (22) becomes

\[
1 = \int_V \mathbf{E}_n \cdot (k \hat{\mathbf{P}}) \mathbf{E}_n \, d\mathbf{r} - \int_V \mathbf{H}_n \cdot \mathbf{H}_n \, d\mathbf{r} \\
+ \frac{i}{k_n} \int_{S_V} \left[ \mathbf{E}_n \times \mathbf{H}'_n - \mathbf{E}'_n \times \mathbf{H}_n \right] \, dS,
\]

(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 wavefunction, we can transform the second volume integral in Eq. (23) into

\[
- \int_V \mathbf{H}_n \cdot \mathbf{H}_n \, d\mathbf{r} = \frac{i}{k_n} \int_{S_V} \mathbf{E}_n \times \mathbf{H}_n \, dS + \int_V \mathbf{E}_n \cdot \mathbf{E}_n \, d\mathbf{r}.
\]

(24)

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

\[
i \int_{S_V} \left( \mathbf{E}_n \times \mathbf{H}'_n - \mathbf{E}'_n \times \mathbf{H}_n \right) \, dS = \frac{i}{k_n} \int_{S_V} \mathbf{E}_n \times \mathbf{H}_n \, dS
\]

\[
+ \frac{1}{k_n} \int_{S_V} \left( \frac{\partial \mathbf{E}'_n}{\partial s} \cdot \mathbf{E}_n - \frac{\partial \mathbf{E}_n}{\partial s} \cdot \mathbf{E}'_n \right) \, dS,
\]

(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 \( k_n \neq 0 \):

\[
1 = 2 \int_V \mathbf{E}_n \cdot \frac{\partial (k^2 \hat{\mathbf{P}})}{\partial (k^2)} \mathbf{E}_n \, d\mathbf{r} + \frac{1}{k_n} \int_{S_V} \left( \frac{\partial \mathbf{E}'_n}{\partial s} \cdot \mathbf{E}_n - \frac{\partial \mathbf{E}_n}{\partial s} \cdot \mathbf{E}'_n \right) \, dS,
\]

(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 \( \mathbf{E}_n \to 0 \) far away from the system [4] 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:

\[
1 = \int_V \mathbf{E}_n \cdot \frac{\partial (k^2 \hat{\mathbf{P}})}{\partial (k^2)} \mathbf{E}_n \, d\mathbf{r}.
\]

(27)

Both results Eq. (26) and Eq. (27) are identical to the normalization of resonant states in non-magnetic materials obtained in [1, 4, 17, 19], with the already noted factor of 2 introduced in the present work.

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

\[
\hat{\mathbf{M}}(\mathbf{k}, \mathbf{r}) \hat{\mathbf{F}}(\mathbf{r}) = -k \Delta \hat{\mathbf{P}}(\mathbf{k}, \mathbf{r}) \hat{\mathbf{F}}(\mathbf{r}),
\]

(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

\[
\hat{\mathbf{F}}(\mathbf{r}) = -k \int \hat{\mathbf{G}}(\mathbf{r}, \mathbf{r}') \Delta \hat{\mathbf{P}}(\mathbf{k}, \mathbf{r}') \hat{\mathbf{F}}(\mathbf{r}') \, d\mathbf{r}'.
\]

(29)

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

\[
\hat{\mathbf{F}}(\mathbf{r}) = \sum_n c_n \hat{\mathbf{F}}_n(\mathbf{r}),
\]

(30)

we obtain

\[
\sum_n c_n \hat{\mathbf{F}}_n(\mathbf{r}) = -k \sum_n \frac{\hat{\mathbf{F}}_n(\mathbf{r})}{k - k_n} \sum_m V_{nm} c_m,
\]

(31)

where the matrix elements of the perturbation are given by

\[
V_{nm} = \int \hat{\mathbf{F}}_n(\mathbf{r}) \cdot \Delta \hat{\mathbf{F}}(\mathbf{r}) \hat{\mathbf{F}}_m(\mathbf{r}) \, d\mathbf{r}.
\]

(32)

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

\[
(k - k_n)c_n = -k \sum_m V_{nm} c_m,
\]

(33)

which is the standard non-dispersive RSE equation [1, 4].

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

\[
\Delta \hat{\mathbf{P}}(\mathbf{k}, \mathbf{r}) = \Delta \hat{\mathbf{P}}_0(\mathbf{r}) + \sum_j \frac{\Delta Q_j(\mathbf{r})}{k - \Omega_j},
\]

(34)
We have derived a general compact expression for the normal-
permeability \( \Delta k \) wave numbers \( \Omega_k \) where we have added in the second line zeros in the form of the
matrix eigenvalue problem Eq. (12), we arrive, after equating coefficients
at the basis functions \( \vec{F}_n \), at the linear eigenvalue equation of the
dispersive RSE:

\[
(k - k_n) c_n = -k \sum_m v_{nm}(\infty)c_m + k_n \sum_m [v_{nm}(\infty) - v_{nm}(k_n)]c_m
\]

with the matrix elements of the dispersive perturbation given by

\[
V_{nm}(k) = \int \vec{F}_n(r) \cdot \Delta \vec{P}(k, \vec{r}) \vec{F}_m(\vec{r}) d\vec{r}.
\]

Note that Eq. (37) has exactly the same form as that developed in [19], and in 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

\[
V_{nm}(k) = \int [E_n \cdot \Delta \vec{H}(k) E_m + E_n \cdot \Delta \vec{E}(k) H_m] d\vec{r}.
\]

The matrix elements Eq. (39) are expressed in terms of the elec-
tric and magnetic fields of basis RSs \( n \) and \( m \) and generally
dispersive changes of the tensors of the permittivity \( \Delta \vec{E}(k, \vec{r}) \),
permeability \( \Delta \vec{H}(k, \vec{r}) \), and bi-anisotropy couplings \( \Delta \vec{E}(k, \vec{r}) \) and
\( \Delta \vec{H}(k, \vec{r}) \) between the electric and magnetic fields.

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–
6, 19–21]. 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 dichro-
isism. We have presented the theory in the most general, com-
 pact 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 expression for the normal-
extension of resonant states, expressed in terms of the electric and
magnetic fields and shown its equivalence to the one used previ-
ously for systems fully described by their permittivity and ex-
pressed in terms of the electric field only. The presented theory
has the widest spectrum of applications, ranging from model-
ing and optimization of chirality sensors to accurate description
of the optics of magnetic and metamaterial systems.