Non-Hermitian Hamiltonian of optical cavity based on perfectly matched layer

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The optical resonance problem is similar to but different from time-steady Schrödinger equation. One big challenge is that the eigenfunctions in resonance problem is exponentially growing. We give physical explanation to this boundary condition and introduce perfectly matched layer (PML) method to transform eigenfunctions from exponential-growth to exponential-decay. Based on the complex stretching technique, we construct a non-Hermitian Hamiltonian for the optical resonance problem. We successfully validate the effectiveness of the Hamiltonian by calculate its eigenvalues in the circular cavity and compare with the analytical results. We also use the proposed Hamiltonian to investigate the mode evolution around exceptional points in the quad-cosine cavity.

With the well-developed fabrication process, the optical resonance phenomena in dielectric microcavities [1] have been applied in varieties of emerging photonic technologies, such as microlasers [2, 3], optical filters [4], photonic circuits [5, 6], nanoparticle sensors [7, 8], and optical gyroscopes [9] etc. The resonance states formed in cavities are intrinsically lossy because optical cavities are open systems with electromagnetic energy radiating to infinity. The openness makes the effective Hamiltonian of optical resonance systems being non-Hermitian [10, 11], and therefore novel phenomena happen, such as wave chaos [12–14] and exceptional points [15, 16].

The optical resonance problem can be analytically solved for cavities with regular shapes including circular shapes [17, 18], square shapes [19], and rectangular shapes [20]. For deformed cavity shapes, analytical approximations are obtained by means of perturbation theories. One perturbation approach is based on a perturbation ansatz for only symmetric cavities [21], and later the ansatz is modified for asymmetric cavities [22]. This approach is applied to calculate optical modes in cavity shapes of cut-disk [21], Limaçon [23], spiral [22] and polar-cosine [24]. Another perturbation approach is based on rigorous perturbation theory without presumed ansatz and the method is justified as successfully applied to Limaçon and spiral cavity [25]. For largely deformed and more general cavity shapes, numerical solutions are necessary. A boundary-element based numerical method has been developed, but spurious solutions exist in this method and has been discussed [26].

Perfectly matched layer (PML) is an artificial absorbing layer at far field region for solving acoustic and electromagnetic wave equations. The PML method is first proposed by Bérenger for wave scattering problems [27, 28], and the original formulation involves field splitting in the absorbing layer. Then Chew and Weedon [29], avoiding this splitting, realize that Bérenger’s formulation is equivalent to a complex-coordinate stretching. Based on the complex stretching, PML equations for curvilinear coordinates [30–32] and for convex geometries [33] are developed, with analysis on the existence and uniqueness of PML solutions proved [34, 35]. The PML methods has also been adopted in solving resonance problems in open systems for fluid dynamics [36], aero acoustics [37] and electromagnetics [38].

In this letter, based on the PML technique, we construct a non-Hermitian Hamiltonian for a real physical system—optical resonance cavity; then we develop a finite-element method to calculate eigen solutions of the Hamiltonian operator. To validate the effectiveness of the proposed Hamiltonian, we study its spectrum for circular cavity and also investigate mode transition near exceptional points in quad-cosine cavity.

Because optical devices are fabricated in layered materials, we only consider 2-dimensional (2D) optical resonance problem in this letter. The method could be easily extended to 3-dimensional (3D) resonance problems.

The resonance states are time-steady solutions of Maxwell’s equation, in which field components could be decomposed into transverse magnetic (TM) modes and transverse electric (TE) modes. We take TM modes as illustration in the letter, and the formulation could be extended to TE modes. For TM modes, the stationary field components satisfy the Helmholtz-type eigen equation

$$\nabla^2 \psi(r) + k^2 n^2(r) \psi(r) = 0, \tag{1}$$

where $k^2$ is the eigenvalue, $\psi(r)$ is the eigenfunction, and refractive index function $n(r)$ is regarded as the weight function in the eigen-problem. The wave number $k$ (also stands for resonance frequency $\omega = ck$ where $c$ is the speed of light) is a complex number with real part denoting mode frequency and imaginary part denoting decay rate. The field components could be expressed as

$$E_r = 0, \quad E_\theta = 0, \quad E_z = \psi; \tag{2a}$$

$$B_r = -\frac{i}{\omega r} \frac{\partial \psi}{\partial \theta}, \quad B_\theta = \frac{i}{\omega} \frac{\partial \psi}{\partial r}, \quad B_z = 0. \tag{2b}$$

All field components are associated with the time-dependent factor $e^{-i\omega t} = e^{-iRe(k)ct} e^{Im(k)ct}$. The optical systems considered in the resonance problem are passive cavities, meaning that there is no energy supply once modes are excited. Therefore, the energy keeps radiating to infinity and field components are exponentially decaying in time, i.e. $Im(k) < 0$. Thus we denote $k = k_r - ik_i$ for some $k_r, k_i > 0$. In fact, when reaching time-steady state, field components are only relatively invariant.
The exponential-decay in time would result in the field components exponential-growth in space. This is the retardation effect [39]: the wavefront propagating farther away is originated from the cavity at an earlier time when the field amplitude in the cavity is exponentially larger than that of the current moment. Therefore, in the view of spatial domain at a fixed time, the field component is exponentially growing at far field region. Based on this observation, the radiation boundary condition for the resonance problem is given: as \( r \to \infty, \)

\[
\psi(r, \theta) \sim \frac{F(\theta)}{\sqrt{r}} e^{inkr} = \frac{F(\theta)}{\sqrt{r}} e^{i\omega k_0 r} \cdot e^{inkr},
\]  

(3)

where we assume the refractive index being constant \( n_0 \) as \( r \to \infty \). In the radiation boundary condition, \( F(\theta) \) represents far field pattern; \( e^{inkr} \) is the spatial phase term; and the exponential growth term \( e^{i\omega k_0 r} \) reflects the retardation effect as explain above. The denominator \( \sqrt{r} \) is to account for the fact that the 2D cylindrical wavefront propagates in normal direction of the circle with perimeter \( 2\pi r \), i.e. radial component of Poynting vector is proportional to \( 1/r \):

\[
S \cdot e_r = -(E_z e^{-i\omega t})^* \cdot B_\theta e^{-i\omega t} \sim \frac{n_0}{c} \frac{|F(\theta)|^2}{r}.
\]

(4)

For 3D problem, \( \sqrt{r} \) in the boundary condition should be replaced by \( r \), because it is spherical wavefront propagating in normal direction of the spherical surface with area \( 4\pi r^2 \).

The radiation boundary condition Eq. (3) is similar to but yet different from Sommerfeld radiation condition [40], which is stated as: for some \( k > 0, \)

\[
\lim_{r \to \infty} \sqrt{r} \left( \frac{\partial \psi}{\partial r} - i k \psi \right) = 0
\]

(5)

holds uniformly in all directions. Sommerfeld radiation condition is often applied to ensure there exists a unique solution being physically meaningful for inhomogeneous Helmholtz equation [40], and it describes constant power radiation while Eq. (3) describes the radiation from a source which is exponential-decaying in time. Certainly, the optical resonance problem is an energy-dissipating process and it subject to the boundary condition Eq. (3).

Researchers assimilate the resonance eigen Eq. (1) with time-independent Schrödinger equation to flourish the study on optical cavities from fruitful results in quantum mechanics [41]. The major difference is that standard quantum mechanics requires wavefunction being square-integrable while eigenfunctions in the resonance problem are exponentially growing at infinity. This makes the resonance problem difficult to formulate under the framework of quantum mechanics and even more difficult to solve. The perfectly matched layer (PML) method is an ideal technique to transform eigenfunctions from exponential-growth into exponential-decay, and hence square-integrable. Accordingly, a non-Hermitian Hamiltonian for the optical resonance system can be constructed.

As schematically illustrated in Figure 1, the PML technique is to introduce from the far field region (\( r > R_0 \)) an absorbing layer which is totally free of reflection. Because no reflections interfere with inner waves, the eigenfunctions \( \psi(r) \) inside PML (\( r < R_0 \)) would preserve as if PML does not exist. Once penetrating into PML, waves are absorbed when propagating forward, and field amplitude goes exponential-decay.

The absorption is introduced by building up a dimensionless damping function \( \tilde{\sigma} \in C^2(\mathbb{R}^+) \) as

\[
\tilde{\sigma}(r) = \begin{cases} 
0 & 0 \leq r < R_0, \\
\sigma_0 & R_0 \leq r < R_0 + d, \\
r & r \geq R_0 + d,
\end{cases}
\]

(6)

for some real constant \( \sigma_0 > 0 \). In order to be reflectionless, the 2nd order derivative of \( \tilde{\sigma} \) must be continuous, i.e. \( \tilde{\sigma} \in C^2(\mathbb{R}^+) \), however its exact form does not matter.

We then introduce \( \tilde{\sigma}(r) \) to build up a complex coordinate \( (r, \phi) \) based on current real-valued polar coordinate \( (r, \theta) \) through relations:

\[
\rho(r, \theta) = r [1 + i \tilde{\sigma}(r)], \quad \phi(r, \theta) = \theta.
\]

(7)

The complex stretching is expressed by derivative relations of the two coordinate systems:

\[
\frac{\partial}{\partial \rho} = \frac{1}{1 + i \sigma(r)} \frac{\partial}{\partial r}, \quad \frac{\partial}{\partial \phi} = \frac{\partial}{\partial \theta},
\]

(8)

in which, we simplified the expression by the notation:

\[
\sigma(r) := \frac{d(\tilde{\sigma})}{dr} = \tilde{\sigma}(r) + r \frac{d\tilde{\sigma}(r)}{dr}.
\]

(9)

Replacing the Laplace operator \( \nabla^2_{(r, \theta)} \) in Eq. (1) with the complex stretching operator \( \nabla^2_{(\rho, \phi)} \) leads to a damping eigen-equation. To simplify expressions, we also introduce dimensionless variables

\[
\alpha(r) := 1 + i \sigma(r), \quad \beta(r) := 1 + i \sigma(r).
\]

(10)
With the relations in Eq. (8) and Eq. (10), the damping eigen-equation is expressed in polar coordinates as
\[
\frac{1}{\alpha \beta} \frac{\partial}{\partial r} \left( \frac{\alpha r \partial \psi}{\beta} \right) + \frac{1}{\alpha^2 \beta^2} \frac{\partial^2 \psi}{\partial \theta^2} + k^2 n^2(r, \theta) \psi = 0, \tag{11}
\]
or expressed in Cartesian coordinates as
\[
\frac{\partial}{\partial x} \left( \frac{x^2 + y^2}{\alpha^2} \frac{1}{r^2} \frac{\partial \psi}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{1}{\beta^2} - \frac{1}{\alpha^2} \right) \frac{xy}{r^2} \frac{\partial \psi}{\partial y} + \frac{1}{\alpha^2} \frac{d}{dr} \left( \frac{r x \partial \psi}{\partial x} + \frac{y \partial \psi}{\partial y} \right) + k^2 n^2(x, y) \psi = 0. \tag{12}
\]
By defining a 2-by-2 matrix \(A(r)\)
\[
A(r) := \frac{1}{r^2} \begin{pmatrix} x^2 & \frac{xy}{\alpha^2} - \frac{xy}{\beta^2} \\ \frac{xy}{\beta^2} & \frac{x^2}{\alpha^2} + \frac{y^2}{\beta^2} \end{pmatrix},
\]
the damping eigen-equation becomes
\[
\nabla \cdot (A \nabla \psi) + \frac{1}{\alpha^2 \beta^2} \nabla (\alpha \beta) \cdot \nabla \psi + k^2 n^2(r) \psi = 0. \tag{14}
\]

Then we consider complex stretching in boundary condition. Replacing \((r, \theta)\) with \((\rho, \phi)\) in Eq. (3), the boundary condition becomes: as \(r \to \infty\)
\[
\psi \sim F(\theta) e^{i \sigma_0 \rho} = \frac{F(\theta)}{\sqrt{1 + i \sigma_0 r}} e^{i \sigma_0 (k_r r, \sigma_0 \phi)} e^{-n_0 (k_r r, \sigma_0 \phi)}.
\]
This shows that complex stretching technique transforms exponential-growth eigenfunctions into exponential-decay (hence, square-integrable) if \(\sigma_0\) is preset large enough.

Therefore, with the damping eigen-Eq. (14), the optical resonance system is assimilated to a quantum system:
\[
\mathcal{H}_0 \psi = k^2 n^2(r) \psi, \tag{15}
\]
in which, the Hamiltonian \(\mathcal{H}_0\) is defined:
\[
\mathcal{H}_0 \psi := -\nabla \cdot (A \nabla \psi) - \frac{1}{\alpha \beta} \nabla (\alpha \beta) \cdot \nabla \psi, \tag{17}
\]
and the eigenfunctions are subject to the exponential-growth boundary condition Eq. (15). The adjoint \(\mathcal{H}^\dagger\) of the Hamiltonian also can be derived:
\[
\mathcal{H}^\dagger \psi = -\nabla \cdot (A^\dagger \nabla \psi) + \nabla \cdot \left( \frac{1}{\alpha \beta} \nabla (\alpha \beta)^\dagger \psi \right), \tag{18}
\]
where asterisk denotes complex conjugate. It’s clear to see \(\mathcal{H} \neq \mathcal{H}^\dagger\), therefore the optical resonance system is non-Hermitian.

Next, we derive the weak form of the damping eigen-equation in a cutoff region. Although PML is built up from far field region and extend to infinity, it is sufficient to cut off PML where field component decays almost to vanished [35]. Here we cut off PML at a finite width \(d\), see Figure 1, and restrict the problem in a circular domain \(\Omega\) with radius \(R_0 + d\). We apply Dirichlet boundary condition to the outer edge of PML:
\[
\psi_{|\partial \Omega} = 0. \tag{19}
\]

Because eigenfunctions are square-integrable, we look for solutions in Hilbert space, i.e. \(\psi \in H_0^1(\Omega)\). Here, the notation \(H_0^1(\Omega)\) means the space of all functions with derivatives continuous and subject to Eq. (19). By integration by parts, the weak form of Eq. (14) can be derived: \(\forall u \in H_0^1(\Omega)\),
\[
P(u, \psi) = k^2 Q(u, \psi), \tag{20}
\]
in which, the bilinear forms \(P(\cdot, \cdot)\) and \(Q(\cdot, \cdot)\) are defined as: \(\forall u, v \in H_0^1(\Omega)\),
\[
P(u, v) = \int_{\Omega} \left[ \nabla u \cdot \left( A \nabla v \right) - \frac{u}{\alpha \beta} \nabla (\alpha \beta) \cdot \nabla v \right] dr, \tag{21}
\]
\[
Q(u, v) = \int_{\Omega} n^2(r) uv dr. \tag{22}
\]

Based on Eq. (20), we develop FEM to calculate the spectrum of \(\mathcal{H}_0\). We remark here that the theory presented in this letter is not restricted for only dielectric cavities. In fact, the presenting theory in this letter is applicable to any refractive index distributions, including largely deformed cavities, multiple cavities, random media and even gradually varied \(n(r)\) etc.

In calculating the spectrum of \(\mathcal{H}_0\), we set the parameters \(R_0/r_0 = 3\) and \(d/r_0 = 1\) where \(r_0\) is the cavity radius. The damping function is set as
\[
\sigma(r) = \begin{cases} 0 & r \leq R_0, \\ (r - R_0)^4 & R_0 < r \leq R_0 + d, \end{cases} \tag{23}
\]
where the region \(r > R_0 + d\) is cut off.

In the first calculation, we consider circular-shape cavity with radius \(r_0 = 1\). The refractive index inside cavity
is \( n_1 = 2 \) and outside cavity is \( n_0 = 1 \). We calculate the eigenvalues of \( \tilde{H} \), plotted in Figure 2.

For the circular-shape cavity, eigen-solutions also can be analytically solved and they are called whispering-gallery modes (WGMs) \([17]\). The eigenvalues of WGMs are given by solving the transcendental equation \([18, 21]\):

\[
J_m'(n_1 kr_0) J_m(n_1 kr_0) = n_0 H'_m(n_0 kr_0) H_m(n_0 kr_0),
\]

where \( J_m \) and \( H_m \) are Bessel function of \( m \)th order and first-type Hankel function of \( m \)th order, respectively. For each integer \( m \), roots of Eq. (24) can be found and rearranged in absolute-value ascending order, indexed by integer \( l \). Then each mode could be referred by the mode number \((m, l)\), where \( m \) is called azimuthal order and \( l \) is called radial order.

By solving Eq. (24), we find eigenvalues of WGMs for \( m = 1, 2, 3, 4, 5 \), plotted in Figure 2. The eigenvalues of \( \tilde{H} \) agrees perfectly with the eigenvalues via solving Eq. (24), and the maximum relative error \( |\Delta k/k| < 1.4 \times 10^{-4} \). The result shows that the non-Hermitian Hamiltonian Eq. (17) constructed for optical resonance system is very effective.

In the second calculation, we apply the effective Hamiltonian to quad-cosine cavity to study mode transition near exceptional points (EPs). The phenomenon of EPs happens when the matrix representation of the quantum system is in Jordan form \([42]\), meaning that algebraic multiplicity is larger than geometric multiplicity. EPs could happen only in non-Hermitian systems, because Hermitian quantum systems in matrix representation are always diagonalizable.

The quad-cosine cavity is expressed in polar system as

\[
R(\theta) = r_0 [1 + \epsilon \cos(4\theta)],
\]

where cavity radius \( r_0 = 1 \) and \( \epsilon \) is the deformation parameter. The refractive index inside the cavity is \( n_1 = 1.6366 \) and outside the cavity is \( n_0 = 1 \).

By varying the deformation parameter \( \epsilon \), we study evolution of two modes with index \((24, 1)\) and \((20, 2)\). Although each mode is associated with clockwise and counter-clockwise (2-fold) degeneracy, we only consider one pair of the two modes, and the behavior of the other pair is similar.

We calculate the eigenvalues of \( \tilde{H} \) for \( \epsilon \) varying from 0.0021 to 0.0024, as shown in Figure 3. We find that \( \epsilon = \epsilon_{EP} = 0.002215 \) is a second-order exceptional point, where eigenvalues of the two modes coalesce.

The evolution of mode distribution is shown in Figure 4. The two modes are distinctly different in small deformation \( \epsilon = 0.0021 \) and highly coupled in large deformation \( \epsilon = 0.0024 \). The turning point is the exceptional point \( \epsilon = \epsilon_{EP} \), where the eigen distribution also coalesce, see the middle panel in Figure 4. The successful application in EPs demonstrates a general validity of the effective Hamiltonian.

To summarize, we apply the PML technique to construct the non-Hermitian Hamiltonian for optical resonance problem for the first time. The main mechanism is to introduce at far field region an absorbing layer free of reflection. We perform complex stretching to transform the eigenfunctions from exponential-growth into exponential-decay. By building up the non-Hermitian Hamiltonian, the optical resonance systems is assimilated to quantum systems. We calculate eigenvalues of the non-Hermitian Hamiltonian in the circular cavity and the results agree well with analytical results, which validates the effectiveness of the non-Hermitian Hamiltonian. We also apply the Hamiltonian to quad-cosine cavity to study mode evolution around exceptional points. The proposed non-Hermitian Hamiltonian is not limited to single-cavity systems, but applies to optical resonance systems with arbitrary refractive index distribution.

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