

Coupled mode theory in non-Hermitian optical cavities

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Abstract: We study the coupling of mode in time for non-Hermitian cavities. Using variational principle, we provide a self-consistent approach to study the mode hybridization in non-Hermitian cavities from the first-principle of Maxwell's equations. We first extend the reaction concept for time reversal adjoint system using the scalar inner product. We apply our theory to the non-Hermitian parity-time symmetric cavities, and obtain excellent agreement with results obtained by finite element fullwave simulations. In contrast, the conventional coupled mode theory using complex inner product fails to capture the bifurcation of the dispersion of parity-time symmetric cavities, as non-Hermiticity increases. Our theory may have potential applications in non-Hermitian optical systems.

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1. Introduction

Variational principle provides a self-consistent approach to study various optical problems, and plays an important role in electromagnetics [1, 2], as well as in the development of coupled mode theory (CMT) [3–8], and many other related numerical approaches, i.e., finite element method (FEM) [9] and method of moment (MOM) [10] and so on. Variational principle works extremely well for Hermitian electromagnetic problems, due to the nice properties of the associated Hilbert space, and the positive definite resulting matrix. On the other hand, non-Hermitian coupled systems in optics, i.e., waveguides, cavities, or coupled waveguide cavities, are ubiquitous, which is due to the fact that materials losses/gain, or/and the exclusion of radiation modes in the truncated mode sets are not negligible. For instance, the joule losses of the plasmonic systems not only shift the resonances, but also destroy the mode orthogonality in the modal expansion under the scheme of complex inner product. In open optical systems, i.e., leaky mode waveguides [11, 12] and finite quality (Q)-factor cavities, the radiation losses can be significant such that the out-going field amplitude grows exponentially, as the detection point is away from the field concentration region.

Despite extensive usage and dramatic success of Hermitian CMT in coupled waveguide and cavities, the extension to non-Hermitian CMT is not straightforward. Non-Hermitian problems in general refer to truncated space, in which the dynamics, or equation of motion of subsystem is of interest, while all the rest degrees of freedom (DOFs) of the full system are integrated out. In lossy optical materials, the details of how the materials interact with light are integrated out, yielding a linear integrated factor to describe the overall absorption or gain. As for leaky wave system, it is obvious that the DOFs of the full radiation continuum are too large to include in the system that is under study. Though the aforementioned non-Hermitian problems have been proved to be very interesting and counter-intuitive, they also impose certain challenges in theoretical modeling and numerical simulations. The major challenge is to define an orthogonal and complete mode set that is associated to the operator that describes the non-Hermitian optical problems, i.e., the subsystem of interest, in which the variational principle can be applied.

There has been extensive work in the field of open electromagnetic system, in which the characteristic features, i.e., eigen-frequencies, or propagation constants, may be a complex number. For instance, quasinormal modes or quasimodal expansion has been developed to study the normalization [13–16] as well as the scattering properties [17, 18] of resonant structures. Using time reversal solution as the adjoint system, Haus and his co-workers studied the coupling of

mode in time for the coupled cavities with radiation losses based on the conservation of cross energy [19].

Despite those significant advances in understanding the normalization and coupling of modes in open cavities, to the best of our knowledge, yet a self-consistent approach of studying mode coupling of non-Hermitian cavities from the first principle of Maxwell's equations rather than phenomenological basis [20], is in lack. In [21], the authors develop a self-consistent approach of studying mode hybridization of non-Hermitian waveguides from reaction conservation. In this paper, we extend the approach of constructing coupled mode formulism from reaction conservation to non-Hermitian coupled optical cavities by introducing time reversal solution as adjoint, instead of counter-propagating modes in waveguides. In contrast to Haus's work, our formulation targets directly on the eigen-frequency (ω) of coupled cavities with intrinsic material losses, instead of ω^2 of optical cavities with radiation losses, in which the post-selection on the branches of the square root of ω^2 needs to be performed [19].

The paper is organized as follows. In Section 2, we extend the reaction concept for time reversal system. Subsequently, we construct the generalized temporal CMT (GTCMT), and discuss the orthogonality of cavity modes in the scheme of scalar inner product. In Section 3, we use GTCMT to study the mode hybridization of coupled non-Hermitian cavities. In contrast, we also give the results by the conventional temporal CMT (CTCMT) and fullwave simulations, as well as comparisons with phenomenological models (PMs). Finally, Section 4 concludes the paper.

2. Formulation of mode coupling in non-Hermitian cavities

2.1. Adjoint system of non-Hermitian cavities: time reversal solution

Variational principle, or extremizing principle, in electromagnetics in general is to seek stationary solutions of some functional of Maxwell's equations for specific structures, which is deeply related to a conserved physical quantity. Such a conserved quantity sets up the framework, in which the extremizing principle shall be built. In Hermitian optical waveguides, two distinct conserved quantities can be found: optical power, or reaction between two distant sources which interact through waveguide modes. In contrast, in non-Hermitian waveguides, only the reaction conservation can be used to construct variational principle [21]. We refer further details between variational principle and CMT and other numerical solvers, i.e., MOM and FEM, to Berk and others [1, 2, 9, 10, 22]. In the following, we first discuss the concept of reaction between the original system and its time reversal partner, and its application in building CMT for coupled non-Hermitian cavities.

We consider two sets of cavity modes, which are time reversal to each other. The time reversal partners share the same spatial dependence on fields, but up to a sign difference. Concretely, electric field \mathbf{E} and magnetic current density \mathbf{M} hold even, while magnetic field \mathbf{H} and electric current density \mathbf{J} become odd, i.e., $\bar{\mathbf{T}}[\mathbf{E}(t), \mathbf{H}(t), \mathbf{J}(t), \mathbf{M}(t)]^T = [\mathbf{E}(-t), -\mathbf{H}(-t), -\mathbf{J}(-t), \mathbf{M}(-t)]^T$, as the time reversal operation $\bar{\mathbf{T}}$ is applied [23]. The original definition of reaction [24] between two sources \mathbf{S}_a and \mathbf{S}_b sharing the same time dependence, can be trivially extended to the case where \mathbf{S}_a and $\bar{\mathbf{T}}\mathbf{S}_b$ share opposite time dependence. In this case, the reaction is given by

$$(\bar{\mathbf{T}}\mathbf{F}_b, \mathbf{S}_a) = \int dV [\bar{\mathbf{T}}\mathbf{E}_b \quad \bar{\mathbf{T}}\mathbf{H}_b] \sigma \begin{bmatrix} \mathbf{J}_a \\ \mathbf{M}_a \end{bmatrix}, \quad (1)$$

where the metric tensor $\sigma = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{pmatrix}$, the original source $\mathbf{S}_a = [\mathbf{J}_a, \mathbf{M}_a]^T$ and the time reversal field $\bar{\mathbf{T}}\mathbf{F}_b = [\bar{\mathbf{T}}\mathbf{E}_b, \bar{\mathbf{T}}\mathbf{H}_b]^T$, which is generated by source $\bar{\mathbf{T}}\mathbf{S}_b$. Thus the corresponding

reaction conservation between source S_a and $\bar{T}S_b$ is given by

$$(\bar{T}\mathbf{F}_b, S_a) + (\bar{T}S_b, \mathbf{F}_a) = \iint dS [\mathbf{E}_a \times \mathbf{H}_b - \mathbf{E}_b \times \mathbf{H}_a], \quad (2)$$

$$\text{where } (\bar{T}S_b, \mathbf{F}_a) = \int dV \begin{bmatrix} \bar{T}J_b & \bar{T}M_b \end{bmatrix} \sigma \begin{bmatrix} \mathbf{E}_a \\ \mathbf{H}_a \end{bmatrix}.$$

Evidently, reaction needs to be corrected based on the even or odd property of the time reversal operation on the fields. As we extend the surface of the volume containing all sources to infinity, the surface integral vanishes, which yields the reciprocity theorem for time reversal solution as follows,

$$(\bar{T}\mathbf{F}_b, S_a) + (\bar{T}S_b, \mathbf{F}_a) = 0. \quad (3)$$

Equation (3) is the reaction conservation for time reversal adjoint system, and also the foundation for studying the mode coupling in time in this paper. It also imposes certain constraints on the material parameters as given by $\epsilon_r = \epsilon_r^T$ and $\mu_r = \mu_r^T$, which is consistent with requirement of reciprocity medium and could be lossy or active.

2.2. GTCMT and mode orthogonality in coupled non-Hermitian cavities

In coupled cavities, the original unperturbed fields are given by $\phi = [e_{0,m}, \mathbf{h}_{0,m}]^T e^{i\omega_{0,m}t}$, where $e = \{e_x, e_y, e_z\}$, $\mathbf{h} = \{h_x, h_y, h_z\}$. Given a small perturbation to the adjoint system, the adjoint perturbed fields can be seen as the linear combination of the unperturbed fields of the adjoint system, i.e., $\bar{T}\psi = \bar{T}\{\sum_n a_n e_{0,n}, \sum_n a_n \mathbf{h}_{0,n}\}^T e^{i\omega t}$. If we replace the sources in Eq. (3) using Maxwell's equations, Eq. (3) can be reformulated as follows,

$$(\bar{T}\psi, \bar{H}\phi) + (\bar{T}(\bar{H}^\# \psi), \phi) = 0, \quad (4)$$

where $\bar{H} = \bar{W}^{-1} \bar{L}$, $\bar{H}^\# = \bar{W}^{-1} \bar{L}^\#$, $\bar{L} = \begin{pmatrix} \nabla \times & ik_{0,m} \mu_{r,0} \\ -ik_{0,m} \epsilon_{r,0} & \nabla \times \end{pmatrix}$, $\bar{L}^\# = \begin{pmatrix} \nabla \times & ik \mu_r \\ -ik \epsilon_r & \nabla \times \end{pmatrix}$, and $\bar{W} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$. In our unit, we use normalized frequency, i.e., $k_{0,m} = \omega_{0,m}/c$ and $k = \omega/c$, therefore the vacuum wavenumber essentially is the targeted quantity that we are interested in.

We use Eq. (4) to construct GTCMT, in the similar procedure as proposed in [21]. Considering the case that a small perturbation is given to the imaginary part of ϵ_r , i.e., $\epsilon_r = \epsilon_{r,0} + i\Delta\epsilon$, we have

$$\sum_n a_n [b_{mn} - i(k - k_{0,m})p_{mn} - ik\kappa_{mn}] = 0, \quad (5)$$

where $b_{mn} = \int dV [\nabla \cdot (e_{0,n} \times \mathbf{h}_{0,m}) - \nabla \cdot (e_{0,m} \times \mathbf{h}_{0,n})]$, $p_{mn} = \int dV [\epsilon_{r,0}(e_{0,n} \cdot e_{0,m}) - \mu_{r,0}(\mathbf{h}_{0,n} \cdot \mathbf{h}_{0,m})]$ and $\kappa_{mn} = \Delta\epsilon \int dV (e_{0,n} \cdot e_{0,m})$. For $\Delta\epsilon = 0$, we have

$$b_{mn} = i(k_{0,n} - k_{0,m})p_{mn}. \quad (6)$$

It is easy to see that b_{mn} is reduced to zero if the cavity wall tends to infinity. For $k_{0,m} \neq k_{0,n}$, the orthogonality relation $p_{mn} = 0$ holds, meaning the cavity modes with different frequency are orthogonal. Inserting Eq. (6) back to Eq. (5) yields

$$\sum_n a_n [(k_{0,n} - k)p_{mn} - k\kappa_{mn}] = 0. \quad (7)$$

Equation (7) is the GTCMT propose in this paper, which is valid to study the mode hybridization of Hermitian and non-Hermitian cavities.

In contrast, we provide the CTCMT by the complex conjugate inner product [19] for comparison. In this case, Eq. (4) becomes

$$(\psi^*, \bar{H}\phi) + ((\bar{H}^\# \psi)^*, \phi) = 0, \quad (8)$$

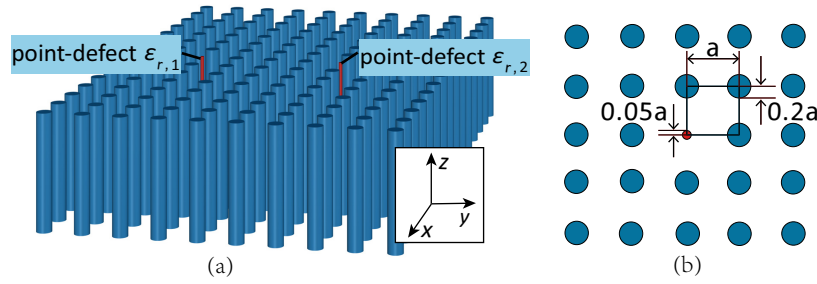


Fig. 1. Coupled single mode cavities in photonic crystal structures. Each individual point-defect can support a monopole state. (a) The 3D sketch of photonic crystal. The rods are periodic along x and y directions, and assumed to extend indefinitely in the z direction. (b) The structure parameters. The crystal constant is a and the rods radii are $0.2a$. The radius of each defect rod is reduced to $0.05a$.

where $*$ denotes the complex conjugate. In analogy with the above procedure, we have

$$\sum_n a_n [b_{mn} - i(k_{0,m} \epsilon_{r,0} - k^* \epsilon_{r,0}^*) e_{mn} - i(k_{0,m} \mu_{r,0} - k^* \mu_{r,0}^*) h_{mn} + ik^* \kappa_{mn}] = 0, \quad (9)$$

where $b_{mn} = \int dV [\nabla \cdot (\mathbf{h}_{0,n}^* \times \mathbf{e}_{0,m}) + \nabla \cdot (\mathbf{h}_{0,m} \times \mathbf{e}_{0,n}^*)]$, $e_{mn} = \int dV (\mathbf{e}_{0,n}^* \cdot \mathbf{e}_{0,m})$, $h_{mn} = \int dV (\mathbf{h}_{0,n}^* \cdot \mathbf{h}_{0,m})$ and $\kappa_{mn} = \Delta \epsilon^* \int dV (\mathbf{e}_{0,n}^* \cdot \mathbf{e}_{0,m})$. For $\Delta \epsilon = 0$, we have

$$b_{mn} = -i[(k_{0,n}^* \epsilon_{r,0}^* - k_{0,m} \epsilon_{r,0}) e_{mn} + (k_{0,n}^* \mu_{r,0}^* - k_{0,m} \mu_{r,0}) h_{mn}]. \quad (10)$$

Inserting Eq. (10) back to Eq. (9) yields

$$\sum_n a_n [(k_{0,n}^* - k^*) p_{mn} - k^* \kappa_{mn}] = 0, \quad (11)$$

where $p_{mn} = \int dV [\epsilon_{r,0}^* (\mathbf{e}_{0,n}^* \cdot \mathbf{e}_{0,m}) + \mu_{r,0}^* (\mathbf{h}_{0,n}^* \cdot \mathbf{h}_{0,m})]$. We will show GTCMT works fine for both Hermitian and non-Hermitian cavities, but CTCMT fails for non-Hermitian cavities in the next section. As a side remark, we show the non-Hermiticity of the coupled cavities will destroy the mode orthogonality. Considering the imaginary parts of the eigen-frequencies ($k_{0,m}$, $k_{0,n}$) and material functions ($\epsilon_{r,0}$, $\mu_{r,0}$), are very small, we can further simplify Eq. (10) by keeping the leading terms as follows,

$$b_{mn} = -i(k_{0,n}^R - k_{0,m}^R) Q_{mn} - 2k_{0,n}^R (\epsilon_{r,0}^I e_{mn} + \mu_{r,0}^I h_{mn}), \quad (12)$$

where $Q_{mn} = \int dV [\epsilon_{r,0} (\mathbf{e}_{0,n}^* \cdot \mathbf{e}_{0,m}) + \mu_{r,0} (\mathbf{h}_{0,n}^* \cdot \mathbf{h}_{0,m})]$, and the superscript R stands for the real part and I the imaginary part, respectively. For well located cavity mode, b_{mn} goes to zero, which is similar to Eq. (6). However, the presence of gain or loss will break the mode orthogonality in the scheme of complex inner product in Eq. (12), in contrast to the scheme of scalar inner product, where the mode orthogonality preserves even in the non-Hermitian cavities.

3. Results and discussions

In this section, we compare CTCMT and GTCMT with fullwave simulations for analyzing the mode hybridization of two coupled single mode cavities. We also present the results by PMs, i.e., two parameters fitting (TPF) and four parameters fitting (FPF). The structure is sketched in Fig. 1, which is formed by introducing two point-defects to the 2D photonic crystal. The rods in the x and y directions are 21×21 . Each point-defect supports a monopole bound state in the TM band gap. By placing two defects with distance of several lattice constants, one can easily

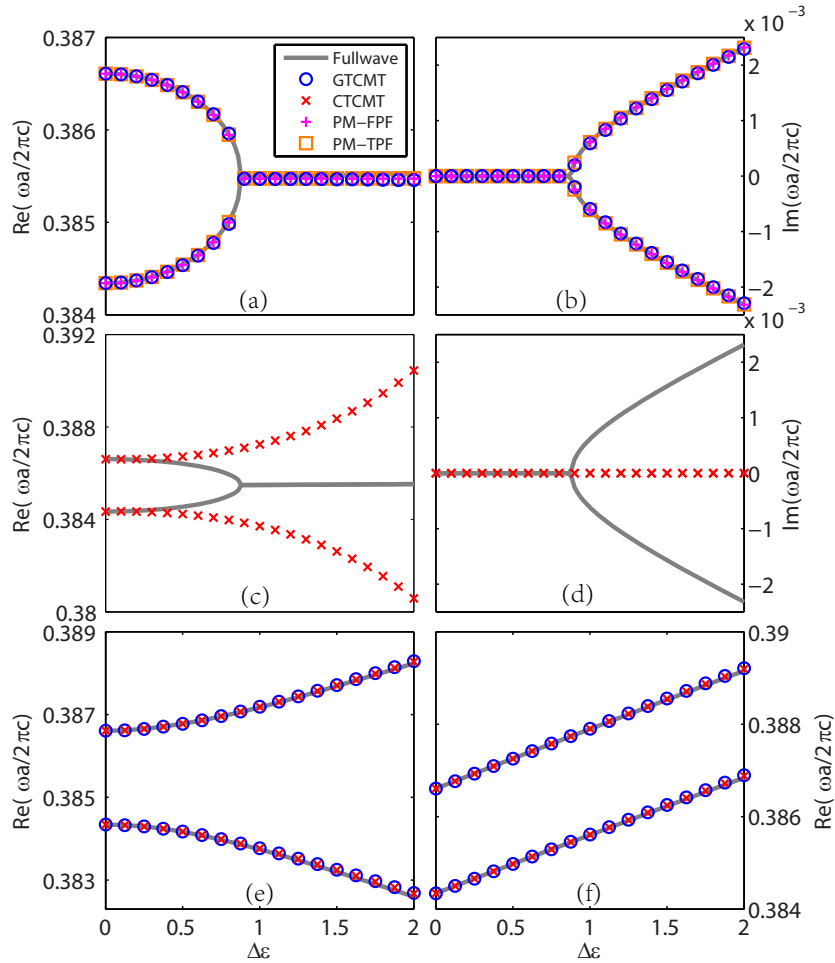


Fig. 2. Real part (a, c, e, f) and imaginary part (b, d) of eigen-frequency versus $\Delta\epsilon$. The relative permittivities of the point-defects are given as follows: $\epsilon_{r,1} = \epsilon_{r,0} + i\Delta\epsilon$, $\epsilon_{r,2} = \epsilon_{r,0} - i\Delta\epsilon$ in (a), (b), (c) and (d); $\epsilon_{r,1} = \epsilon_{r,0} + \Delta\epsilon$, $\epsilon_{r,2} = \epsilon_{r,0} - \Delta\epsilon$ in (e) and $\epsilon_{r,1} = \epsilon_{r,0} - \Delta\epsilon$, $\epsilon_{r,2} = \epsilon_{r,0} + \Delta\epsilon$ in (f). The structure parameters are given by Fig. 1(b), and the original relative permittivity of the rods $\epsilon_{r,0} = 8.9$. We compare the results obtained by four different approaches with the results obtained by fullwave simulations. CTCMT (GTCMT) is derived from the first principle based on complex (scalar) inner product. PM-TPF (PM-FPF) is the phenomenological model which we need to fit two (four) parameters based on fullwave simulations or experimental measurements.

create a pair of odd and even supermodes in the coupled system [25]. It is necessary to rewrite Eq. (7) as an eigenvalue problem as given by

$$\tilde{\mathbf{H}}a = k\tilde{\mathbf{W}}a, \quad (13)$$

where $\tilde{\mathbf{H}} = \begin{pmatrix} k_{0,1}p_{11} & k_{0,2}p_{12} \\ k_{0,1}p_{21} & k_{0,2}p_{22} \end{pmatrix}$, $\tilde{\mathbf{W}} = \begin{pmatrix} p_{11} + \kappa_{11} & p_{12} + \kappa_{12} \\ p_{21} + \kappa_{21} & p_{22} + \kappa_{22} \end{pmatrix}$, $a = [a_1, a_2]^T$. The initial $k_{0,1}$ and $k_{0,2}$ of the odd and even supermodes are provided by COMSOL simulations, and the elements p_{mn} and κ_{mn} are calculated by projecting the fields as explained in previous section.

Figure 2(a) and 2(b) show the evolution of the eigen-frequencies of two coupled cavities with balanced gain and loss. Increasing $\Delta\epsilon$ increases the non-Hermiticity, leading to the phase transi-

tion in the eigenstates of the system. Consequently, the eigen-frequencies of the two supermodes get closer and closer until an exceptional point (EP), where they become identical. Beyond the EP point, the real part of the eigen-frequency remains the same, but the imaginary part of the eigen-frequency splits gradually. We can see the results obtained by our GTCMT (blue open circle) have an excellent agreement with the the results by fullwave simulations (gray solid line), which are implemented in Comsol Multiphysics 5.2 [26]. For comparison, we reformulate Eq. (11) as

$$\tilde{\mathbf{H}}a = k^* \tilde{\mathbf{W}}a, \quad (14)$$

where $\tilde{\mathbf{H}} = \begin{pmatrix} k_{0,1}^* p_{11} & k_{0,2}^* p_{12} \\ k_{0,1}^* p_{21} & k_{0,2}^* p_{22} \end{pmatrix}$, $\tilde{\mathbf{W}} = \begin{pmatrix} p_{11} + \kappa_{11} & p_{12} + \kappa_{12} \\ p_{21} + \kappa_{21} & p_{22} + \kappa_{22} \end{pmatrix}$. Notably, CTCMT (red cross) is valid just for small $\Delta\varepsilon$, which is not able to capture the EP point in non-Hermitian cavities, as shown in Fig. 2(c) and 2(d).

Next, we consider the Hermitian case, where the perturbation emerges in the real part of ϵ_r . Figure 2(e) shows the case that $\Delta\varepsilon$ increases with the opposite sign in two cavities. In this case, the two eigen-frequencies are further separated from each other as $\Delta\varepsilon$ increases. Figure 2(f) shows the case that $\Delta\varepsilon$ increases with the same sign in two cavities. In this case, both the two eigen-frequencies gradually increase as $\Delta\varepsilon$ increases. In Fig. 2(e) and 2(f), the imaginary part of the eigen-frequency remains zero. It is clear that both GTCMT (blue open circle) and CTCMT (red cross) agree well with the the results by fullwave simulations (gray solid line). Our GTCMT is valid to capture the EP point in non-Hermitian systems. However, there is certain discrepancy of the real part of the eigen-frequency between GTCMT and fullwave simulations beyond the EP point. As shown in Fig. 2(a), GTCMT can't extract the slowly growing feature of the real part of the frequency beyond the EP point. We attribute the discrepancy to the non-linear behavior of the coupled system for larger magnitude of gain/loss, while our coupled mode model is designed only for linear systems. More details about non-linear behavior of the coupled system is beyond the scope of this paper.

Table 1. Comparisons between the CMT derived from the first principle and two-band PMs

Models	GTCMT	CTCMT	PM-TPF	PM-FPF
Coupled equation	$\tilde{\mathbf{H}}a = k\tilde{\mathbf{W}}a$	$\tilde{\mathbf{H}}a = k^*\tilde{\mathbf{W}}a$	$\tilde{\mathbf{H}}a = ka$	$(\tilde{\mathbf{H}} + \tilde{\mathbf{\Gamma}})a = ka$
	see Eq. (13)	see Eq. (14)	$\tilde{\mathbf{H}} = \begin{pmatrix} k_{0,1} & i\kappa_{12} \\ i\kappa_{21} & k_{0,2} \end{pmatrix}$	$\tilde{\mathbf{H}} = \begin{pmatrix} k_{s,0} & \kappa_{12} \\ \kappa_{21} & k_{s,0} \end{pmatrix}$ $\tilde{\mathbf{\Gamma}} = \begin{pmatrix} -i\gamma_1 & 0 \\ 0 & -i\gamma_2 \end{pmatrix}$
Modal basis	Odd and even supermodes	Odd and even supermodes	Odd and even supermodes	Single cavity modes
Coupling mechanism	Perturbation from gain/loss	Perturbation from gain/loss	Perturbation from gain/loss	Evanescent coupling
Constraints	Reaction conservation	Cross energy conservation	$\kappa_{12} = \kappa_{21}$	$\kappa_{12} = \kappa_{21}$ $\gamma_1 = -\gamma_2$
Underlying principle	First principle	First principle	Phenomenological observation	Phenomenological observation

To get a comprehensive impression of our model and PMs, we give a comparison on similarities and differences of four approaches, as shown in Table. (1). Evidently, all the resultant interesting phenomena by GTCMT, i.e., bifurcation, are simply the consequences of the reaction conservation, which is rigorously derived from the first principle. Thus, our model can be used as a tool of studying new phenomena in non-Hermitian systems, or designing non-Hermitian optical devices. In comparison, PMs rely on the known results, i.e., the location of EP point in the

parameter space for TPF, and location of EP point as well as magnitude of mode splitting in FPF for fitting. Thus, PMs can hardly be used for predictions or designing purposes, although they work perfectly well in describing the parity-time (\mathcal{PT}) symmetric optics in unbroken/broken phases and the transition, as seen in Fig. 2(a) and 2(b).

4. Conclusions

In conclusion, we have theoretically studied the mode coupling in time in non-Hermitian cavities, from the first principle of Maxwell's equations instead of phenomenological observations. The model essentially relies on the reaction conservation, which provides a solid foundation of constructing coupled mode theory for non-Hermitian cavities from variational principle. We introduce the time reversal operation \bar{T} in reaction to account two independent sources sharing opposite frequency, i.e., the original and its adjoint problem as the complete dual space for constructing our theory from perturbation. Interestingly, we found that each individual mode in the complete mode set of the coupled non-Hermitian cavity can be orthogonal to all the other modes under the scalar inner product adopted here. In contrast, such mode orthogonality in a certain mode set of non-Hermitian cavities is completely lost in the scheme of complex inner product. As an example, we study a pair of non-Hermitian coupled cavities in 2D photonic crystal. Our model is able to capture the feature of bifurcation in \mathcal{PT} symmetric system, where CTCMT fails. Our theoretical model may have potential applications in non-Hermitian cavities, or coupled waveguide cavity structures.

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