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Engineering of the Fano resonance spectral response with non-Hermitian metasurfaces by navigating between exceptional point and bound states in the continuum conditions

Supplementary Material

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1. Operation at the exceptional point

The exceptional point corresponds to the PT-symmetry phase transition when the operating point of the system in the CDP (the two-dimensional κ - δ space) evolves along the path compelled by the relation:

$$\frac{\delta}{\kappa} = -\frac{\gamma_0}{\eta} = -\frac{2\sqrt{\gamma_1\gamma_2}}{\gamma_2 - \gamma_1}$$
 S1

The corresponding situation is depicted in Figs S1(a,b). The coordinates { κ , δ } of exceptional points EP. and EP₊ occurring for negative and positive values of coupling coefficient are then { η ,- γ_0 } and {- η , γ_0 }, respectively. As illustrated in Figs. S1(a) and S2(a), we observe a coalescence of the real parts of the eigenfrequencies [Re(ω_+)=Re(ω_-)] for the points situated on the interval [EP.,EP₊] of the dotted line in Fig. S1 joining these exceptional points. This situation corresponds to the broken phase of PT symmetry occurring when κ |<| η |, i.e. in a weak coupling regime. On the other hand, for the rest of the points of this line, those situated outside the interval [EP.,EP₊], a coalescence of the imaginary parts of the eigenfrequencies [Im(ω_+)=Im(ω_-)] presenting the condition of passive PT-symmetry is observed.

Note, however, that there are an infinite number of trajectories that pass through the EP. Since the sensitivity of generic devices is commonly expected to be greatly increased by an abrupt change in eigenfrequencies, the optimal path is the one that offers the fastest splitting of eigenfrequencies in the vicinity of the EP. From the conservation of the trace of the Hamiltonian matrix, it can be directly inferred that the maximum splitting of modes eigenfrequencies corresponds to the case of the PT-symmetry phase transition path, which therefore presents an optimal trajectory through the EPs with respect to the points of the CDP not being on the PT-symmetry phase transition path.



Fig. S1: Logarithmic scale colormap representation of real and imaginary components of eigenfrequencies difference $\Delta = \omega_+ \cdot \omega_-$. Parameters of the coupled resonators system used in numerical modeling: $\omega_1 = 10$, $\gamma_1 = 0.8$, $\gamma_2 = 0.2$. All values are given in normalized frequency units. Dotted line at angle φ corresponds to the evolution along PT-symmetry phase transition path. Bold dots indicate exceptional points. a) Re(Δ); b) Im(Δ).

The corresponding solutions for these latter are those of the non-Hermitian Hamiltonian not belonging to the class of PT-symmetry. Contrary to the case of PT-symmetry, their eigenfrequencies are just complex. This is illustrated in Fig. S2 on the example of path $\kappa_- \kappa_+$ (dash-dotted line in Fig. S1) corresponding to the modulation of coupling strength and for the path δ_+ - δ_- (dashed line in Fig. S1) that corresponds to the modulation of detuning between resonators. As evident, the splitting of eigenfrequencies is smaller compared to the PT-symmetry phase transition path, which indeed represents the optimal trajectory through the EP. However, as pointed out in [1,2], the divergent sensitivity of eigenvalues does not necessarily lead to an arbitrarily high sensitivity. The reason for this is related to the coalescence of the eigenstates around the EP, which exactly cancels out the singularity in the susceptibility.



Fig. S2: Evolution of real (a) and imaginary (b) components of eigenfrequencies along different paths in the κ - δ plane (the CDP): dotted line - PT-symmetry phase transition path given by a generalized evolution parameter $\rho = \kappa/\cos(\phi)$; dashed line - $\delta = \rho \sin(\phi)$, $\kappa = \cosh(-\eta)$; dash-dotted line - $\delta = \cosh(-\eta)$. The parameters of the coupled resonators system used in the numerical modeling are the same as those in Fig. S1.

2. Dark mode operation

The way to further sharpen the variation of the spectral response is to make the Fano resonance asymmetrical in order to obtain a cliff-like behavior. This can be achieved if the frequency $\hat{\omega}$ corresponding to the maximum of EIT where S₁₁=0 is very close to the one of

the frequencies $\breve{\omega}_{\pm}$ where $S_{12}=0$. To find the condition satisfying this requirement we use again the property of universality of the solutions and consider a particular example when $k\approx 0$. As noted above, in this case $S_{12}=0$ when $\breve{\omega}_{\perp}\approx \omega_{1}$ and $\breve{\omega}_{\perp}\approx \omega_{2}=\omega_{1}+2\delta$. The absorption losses are neglected ($\chi_{1}=\chi_{2}=0$). As follows from Eq. (16) the maximum of EIT is fulfilled when:

$$\hat{\omega} = \omega_1 + 2 \frac{\delta \gamma_1 - \kappa \gamma_0}{\overline{\gamma}} = \omega_2 - 2 \frac{\delta \gamma_2 + \kappa \gamma_0}{\overline{\gamma}}$$
(S2)

Since k≈0 it follows then that $\hat{\omega} \approx \omega_1$ when $\gamma_1 \ll \gamma_2$ or $\hat{\omega} \approx \omega_2$ when $\gamma_2 \ll \gamma_1$. Such a situation corresponds to a system of two predominantly radiatively coupled oscillators (i.e. k≈0), with very dissimilar radiative losses. The operation point is located in the near vicinity of the DM where Im(ω .)=0, also identified as bound state in the continuum (BIC). It corresponds to the blue diagonal wedge forming an angle ψ with the abscissa-axis, and close to the CDP ordinate-axis, as shown in Fig. S3.



Fig. S3: Logarithmic scale colormap representation of the imaginary part of the antisymmetric mode eigenfrequency Im(ω -). Parameters of the coupled resonators system used in numerical modeling: ω_1 =10, γ_1 =0.999, γ_2 =0.001. All values are given in normalized frequency units. Dotted line corresponds to the PT-symmetry phase transition path. Black bold dots indicate exceptional points. The bold white dots on ordinate axis correspond to the points in κ - δ space whose spectral responses are shown in Fig. S4. The bold black and cyan dots correspond to the points in κ - δ space on the PT-symmetry phase transition path whose spectral responses are shown in Fig. S5.

For a given particular choice $\gamma_2 \ll \gamma_1$ when the radiation rate of one resonator tends towards zero, the BIC path approaches the δ -axis, i.e. $\psi \approx -\pi/2$, while the PT-symmetry path approaches the κ -axis. The evolution of the spectral response corresponding to this case as a function of the frequency detuning δ is shown in Fig. S4.



Fig. S4: Scattering matrix coefficients spectral response at different points along κ =0 ordinate path shown in Fig. S3. a) δ =-0.5; b) δ =-0.-75. Parameters of the coupled resonators system used in numerical modeling: ω_1 =10, γ_1 =0.999, γ_2 =0.001. All values are given in normalized frequency units.

The evolution of the spectral response along the PT-symmetry phase transition path for this case where $\gamma_2 \ll \gamma_1$ which almost corresponds to the abscissa axis is represented in Fig. S5. As can be seen, the spectral response is perfectly symmetric with respect to the EIT peak frequency, as was also the case for the PT-symmetric phase-transition path shown in Fig. 3 of the main material corresponding to the balanced situation, whereby $\gamma_1 = \gamma_2$.



Fig. S5: Scattering matrix coefficients spectral response at different points along PT-symmetry phase transition path shown in Fig. S3. a) $\rho = \overline{\gamma} - EP$; b) $\rho = 1.5 \overline{\gamma} - PT$ -symmetric. Parameters of the coupled resonators system used in numerical modeling: $\omega_1=10$, $\gamma_1=0.999$, $\gamma_2=0.001$. All values are given in normalized frequency units.

3. Impact of absorption losses

To take into account how absorption losses affect the optimal design, we consider the situation most frequently encountered in practice where both plasmonic resonators are made of the same metal, i.e. $\chi_1 = \chi_2$. The eigenfrequencies of the effective Hamiltonian are then:

$$\omega_{\pm} = \frac{\omega_1 + \omega_2}{2} + j(\overline{\gamma} + \chi) \pm \sqrt{(\delta + j\eta)^2 + (\kappa + j\gamma_0)^2}$$
(S4)

where $\chi = (\chi_1 + \chi_2)/2$. As it can be seen the discriminant in Eq. (S4) is the same as in Eq. (11). The isometric properties of the Hamiltonian solutions given by Eq. (S4) are therefore not affected by the presence of absorption losses. On the other hand, the homothetic

properties of the Hamiltonian are lost since the eigenfrequencies now depend on the $\chi/\overline{\gamma}$ ratio.

From a general physical point of view, the ultimate sharpness of the resonance that can be achieved is determined by the level of absorption losses. In other words, this means that the only resonances observable in the system are those associated with eigenfrequencies for which:

$$\operatorname{Im}(\omega_{-}) \geq \chi \tag{S5}$$

A general overview of the solutions to Eq. (S5) can be obtained from a mere observation, in Fig. 2(a) of the main material, of the distribution in the CDP of the antisymmetric mode eigenfrequency imaginary part. As it can be seen, the blue colored diagonal wedge corresponding to values of $\text{Im}(\omega_{-}) < 0.001$ occurs only in the near vicinity of the line defined by Eq. (S3), the line corresponding to the BIC condition. The width of this region is smallest along the PT-symmetry phase transition path line, which is perpendicular to that of the BIC. It gradually widens when moving along the BIC path away from the origin point.

The physical meaning of the solutions satisfying Eq. (S5) is that for the resonant behavior to be observed, the "effective detuning" between the two resonators must be greater than the minimum resonance width imposed by the absorption losses. To formalize this mathematically, we can take advantage of the isometric properties of the system and consider again the special case when $\gamma_1=\gamma_2$. As mentioned previously it corresponds to the situation where the angle $\varphi=\pi/2$ while $\psi=0$. For this particular example the evolution parameter ρ coincides with δ . As shown in the Appendix B of the main material, the following expression holds for the detuning δ needed between two resonators as a function of the level of absorption χ

$$\delta = \rho = \sqrt{2\chi(\overline{\gamma} - \chi)} \tag{S6}$$

Within the limits of low absorption losses ($\chi << \overline{\gamma}$), the following approximate expressions can be used to provide a better insight into the behavior described by Eq. (S6):

$$\rho = \sqrt{2\chi\overline{\gamma}} \tag{S7}$$

We may introduce the ratio $Q = \overline{\gamma} / \rho$ as the measure of the spectral sharpness of the EIT resonance. Based on Eq. (S7), we can easily deduce that to obtain even a very modest $Q \approx 10$, the level of absorption losses must be as low as $\chi \approx \overline{\gamma} \times 10^{-2}$. This explains the inherent difficulty in achieving highly resonant behavior using plasmonic resonators in the optical and even in the upper THz domain, where metal-related ohmic losses are becoming important.

As also evident, what matters is not the level of absorption losses *per se*, but rather the product $\chi \overline{\gamma}$ of absorption and radiation losses. The ability to control radiation losses that depend on the dipole moment of individual antenna-type resonators therefore provides a degree of freedom for EIT resonance quality factor engineering. The evolution of the spectral response along PT-symmetry phase transition path as function of resonators detuning and for a fixed level of absorption losses $\chi=0.2 \overline{\gamma}$ is illustrated in Fig. S6.

As can be seen in Fig. S6(a), the EIT feature visible in Fig. 3(a) of the main material when ρ =0.01, disappears completely in the presence of sizable absorption losses. As shown in Fig. S6(b), the EIT becomes clearly visible when $\rho \approx \text{Im}(\omega)$. The contrast of the EIT increases as the operating point moves along the PT-symmetry phase transition path away from the origin, but at the cost of an increase in spectral width. Note that in the broken phase up to the EP, i.e. when $\rho = \overline{\gamma} = (\gamma_1 + \gamma_2)/2$, the shape of the absorption spectrum is that of a single Lorentzian line [see Fig. S6(c)]. Beyond the EP, i.e. in the PT-symmetrical phase shown in Fig. S6(d), the resonances of the real parts of the eigenfrequencies do not merge and the absorption spectrum rather corresponds to the superposition of two detuned Lorentzian lines.



Fig. S6: Scattering matrix coefficients spectral response at different points along PT-symmetric path in the presence of absorption losses: a) $\rho=0.01$ – broken PT-symmetric phase; b) $\rho=0.6 \overline{\gamma}$ – broken PT-symmetric phase meeting condition $\rho\approx Im(\omega_{-})$; c) $\rho=\overline{\gamma}$ – EP; d) $\rho=1.5 \overline{\gamma}$ – PT-symmetric phase. Parameters of the coupled resonators system used in numerical modeling: $\omega_{1}=10, \gamma_{0}=\gamma_{1}=0.5, \chi=0.1$. All values are given in normalized frequency units.

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