PT-symmetric metasurfaces: wave manipulation and sensing using singular points

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Abstract

We investigate here active metasurfaces obeying parity–time (PT) symmetry and their sensing applications, taking advantage of singularities unique to non-Hermitian systems, such as the spontaneous PT-symmetry-breaking point (exceptional point or EP) and the coherent perfect absorber–laser (CPAL) point. We show theoretically that a PT-symmetric metasurface sensor may provide enhanced sensitivities compared to traditional passive sensors based on metamaterial/ metasurface resonators, because the singular point of one-way zero reflection arising from the EP or the CPAL-related sharp resonance may result in dramatically modulated scattering responses or resonance offsets. We demonstrate the proposed concept with realistic metasurface sensors based on photopumped graphene metasurfaces that simultaneously offer terahertz optical gain and (bio) chemical sensing functions. The proposed PT-symmetric metasurfaces may impact not only loss compensation and extraordinary manipulation of electromagnetic waves, but also practical sensing and detection applications.

1. Introduction

Ever since parity–time (PT) symmetry in quantum systems was discovered by Bender in 1998, there have been numerous studies investigating its exotic physical implications [1–5]; a non-Hermitian Hamiltonian can counterintuitively have a real eigenspectrum once the system is invariant under simultaneous parity (P) and time-reversal (T) transformations [1, 2]. Interestingly, given the antilinear character of the PT operator, the Hamiltonian and PT operator do not always share the same eigenvectors. As a matter of fact, beyond a certain non-Hermiticity threshold, called an exceptional point (EP), an abrupt phase transition can occur and the spectrum becomes complex. At the EP, eigenvalues and eigenvectors of the non-Hermitian system may converge simultaneously [1–5]. Although the concept of PT-symmetric quantum systems is still a matter of debate [6], its analogues in classical wave systems, such as electromagnetics and acoustics [3–5, 7–31], have been demonstrated experimentally, thanks to formal similarities between the Helmholtz and Schrödinger equations. Optical systems have emerged as versatile platforms for exploring PT-symmetry because in this spectral range there are several experimentally feasible ways to realize distributed gain and loss. So far, PT-symmetric electromagnetic systems have unveiled a number of new applications, including unidirectional propagation phenomena (e.g., invisibility, tunneling and negative refraction) [11, 12, 28, 29], planar focusing [30], beam switching [26, 27], coherent perfect absorbers–lasers [8, 14, 15] and optical isolators and circulators [11, 20, 22, 23]. Very recently, the concepts of PT-symmetry have been extended into lumped-element electronic circuits [32, 33] and transmission-line networks [29, 30], opening new avenues for developments of innovative imaging [30] and communication [32] systems with high speed and low noise.

In this paper, we will investigate PT-symmetric systems comprising a gain/loss metasurface pair, as shown in figure 1(a), and its practical realization in the THz regime, as shown in figure 1(b). Such paired amplifying and attenuating metasurfaces, linked by an electrical distance, may constitute the most compact and simplest possible PT-symmetric wave system supporting exotic and anomalous physics, such as unidirectional...
reflectionless transparency [12, 13] and a coherent perfect absorber–laser (CPAL) [14, 15]. This system is characterized by a PT-symmetric distribution of surface admittance, $j Y_i = j Y_i^*$, [30] where $Y_i$ represents the surface admittance of the $i$th metasurface. This implies that the input admittance seen on either side must have the same susceptance and oppositely signed conductance of the same magnitude. Moreover, we will show theoretically that PT-symmetric metasurfaces, when used as sensors, may offer greater modulation depth, greater spectral resolution and larger resonance shifts when compared to traditional passive metasurface/metamaterial-based sensors [34–36]. In particular, when the PT-symmetric metasurface operates near the EP or CPAL point, any small change in the metasurface admittance can result in dramatically altered scattering properties, associated with the bifurcation of eigenvalues of the scattering matrix. Here, we will demonstrate the concept of a PT-symmetric sensor with practical graphene metasurfaces, as shown schematically in figure 1, which simultaneously provide sensing functions and THz optical gain (when pumped by a near-infrared or visible laser), a necessary condition for the PT symmetry [28]. In this scenario, an optically pumped (active) graphene metasurface may exhibit a negative surface conductance $Y_2 = -G$, opposite to a positive surface conductance of a resistive metallic filament $Y_1 = G$. It has recently been proposed that optically pumped graphene may allow population inversion due to cascaded optical photon emissions, and, thanks to the gapless feature of graphene, interband transition near the Dirac point may result in the THz lasing effect [37–42]. In seemingly unrelated fields of study, resonant perfect absorbers based on plasmonic [34–36] or graphene [43–46] metamaterials/metasurfaces have been investigated extensively for optical sensing applications. However, the major challenge of these passive sensors resides in how to improve their sensitivity and their low modal quality factor (Q-factor), which is inherently limited by energy dissipation at the resonance.

In the following, we will extend the concept of PT symmetry to generalized sensors based on metamaterials and metasurfaces, with a focus on practical implementation in the THz spectrum using graphene-based metasurfaces. The sensing mechanism resides in the unique chemically tunable conductivity of graphene, for which the admittance of the graphene metasurface may be continuously and instantaneously varied by $n$- or $p$-type doping due to surface adsorbates (e.g. reactive gas, molecular, bacterial and chemical species [43, 44]). In the following, we will present the theory and design practice for PT-symmetric graphene metasurfaces that find useful applications for not only extraordinary manipulation of THz waves, such as EP-related unidirectional scattering and CPAL phenomena, but also useful applications in sensitively detecting gas, chemical or biological agents on the graphene surface.

2. PT-symmetric metasurface pairs

Figure 1 (a) shows the PT-symmetric system constituted by a pair of metasurfaces with isotropic, homogeneous surface admittance $Y_1 = G_1 + jB_1$ and $Y_2 = G_2 + jB_2$, separated by an electrical distance $x = kd$, where propagation constants and characteristic admittances for outside medium (free space is assumed here) and dielectric spacer are $(k_{00}, Y_0) = (\omega \sqrt{\varepsilon_0/\mu_0}, \sqrt{\varepsilon_0/\mu_0})$ and $(k, Y) = (s k_{00}, s Y_0)$, $d$ is the physical length of dielectrics or air gap, and $s$ is a dimensionless parameter (if the dielectric medium is non-dispersive and lossless, including free space, $\{s \in \mathbb{R} : s \geq 1\}$); we adopt a time-harmonic field of the form $e^{j\omega t}$ throughout this study. As a weak constraint of the PT-symmetric system, $j Y_1$ and $j Y_2$ must be complex conjugates to each other, namely

$$\begin{align*}
(j Y_1)^* &= j Y_2, \\
(j Y_2)^* &= j Y_1,
\end{align*}$$

Thus, the propagation constants and characteristic admittances for outside medium and dielectric spacer are $k = s^2 k_{00}$ and $Y = s^2 Y_0$, respectively. In the THz regime, the optically pumped graphene metasurface represents an active metasurface ($G_2 < 0$), while the metallic filament represents a resistive sheet ($G_1 > 0$).
$G_2 = -G_1 = -\gamma Y_0, \{ \gamma \in \mathbb{R} \} \text{ and } B_1 = B_2 = \chi Y_0, \{ \chi \in \mathbb{R} \}$. In the transmission-line model (figure 1(a)), the equivalent voltage and current at the port $i$, $(V_i, I_i) = (V^+ + V^-, I^+ - I^-)$, are defined based on tangential electric and magnetic fields $(E^{+/→}, H^{+/→})$ [47], and they can be related by the admittance matrix $Y$ as

$$
\begin{pmatrix}
V^+_i \\
V^-_i
\end{pmatrix} = Y^{-1}
\begin{pmatrix}
I^+_i \\
I^-_i
\end{pmatrix},
$$

where

$$
Y = \begin{pmatrix}
G_1 + jB_1 - jY \cot(x) & jY\csc(x) \\
jY\csc(x) & G_2 + jB_2 - jY \cot(x)
\end{pmatrix}.
$$

where $+$ and $-$ represent the forward (backward) propagating waves.

For a forward-propagating source wave, the closed-loop analysis for this system is illustrated in figure 2(a). We note that the excitation port can be seen as a negative conductance $-Y_0$ because while a positive admittance represents energy dissipation, a negative admittance implies an energy source. Likewise, in such normal-mode analysis, the output port is terminated by free-space admittance $Y_0$. By applying Kirchhoff’s law, the condition for the existence of normal mode can be characterized by solving the following equation

$$
\text{Det}[Y_{ext} + Y] = 0,
$$

where

$$
Y_{ext} = \begin{pmatrix}
-Y_0 & 0 \\
0 & Y_0
\end{pmatrix}.
$$

It is clear that if $G_2 = -G_1 = -\gamma Y_0$ and $B_2 = B_1 = \chi Y_0$, the system is PT-symmetric (space–time reflection symmetry); namely, in the closed-loop analysis (figure 2(a)), the input admittance at port 1, $Y_{in,1} = [(\gamma - 1) + j\chi] Y_0$, and that at port 2, $Y_{in,2} = [-(\gamma - 1) + j\chi] Y_0$ satisfy the condition: $Y_{in,1} = (jY_{in,2})^\ast$ [30]. For given design parameters $(\gamma, \chi, s, x)$, normal modes (resonances) may exist if the determinant in equation (2) is equal to zero, which is true when the dimensionless gain–loss parameter (or non-Hermiticity parameter [32]) $\gamma$ satisfies

$$
\gamma = 1 \pm \sqrt{s^2 + 2\chi s \cot(x) - \chi^2}.
$$

The validity of PT-symmetry would require the gain–loss parameter to be real, namely $s^2 + 2\chi s \cot(x) - \chi^2 > 0$. Assuming that the surface susceptances of both metasurfaces are zero $(\chi = 0)$, excitation of the normal mode requires the condition $\gamma = 1 \pm s$, which is interestingly independent of the electrical distance $x$. Moreover, $\gamma > 0 (\gamma < 0)$ implies that the incident plane wave first hits the loss (gain) surface. We note that when the two metasurfaces are suspended in free space $(s = 1)$, normal modes exist at $\gamma = 0$ and 2; however, $\gamma = 0$ implies the trivial case of plane-wave propagation in free space.

When a backward-propagating source wave is launched, as sketched in figure 2(b), equation (2b) should be modified as $Y_{ext} = \begin{pmatrix}
Y_0 & 0 \\
0 & -Y_0
\end{pmatrix}$. In this scenario, resonance exists if $\gamma$ satisfies

$$
\gamma = -1 \pm \sqrt{s^2 + 2\chi s \cot(x) - \chi^2},
$$

and $s^2 + 2\chi s \cot(x) - \chi^2 > 0$. For purely amplifying/attenuating surfaces with $\chi = 0$, the resonance condition becomes $\gamma = -1 \pm s$, and $\gamma > 0 (\gamma < 0)$ implies that the incoming wave first hits the gain (loss) surface. It is interesting to note that in the closed-loop analysis (figure 2(b)), the input admittance in port 1 and
that in port 2 satisfy the general PT condition $jY_{in1} = (jY_{in2})^*$, where $Y_{in1} = [(\gamma + 1) + j\chi]Y_0$ and $Y_{in2} = [- (\gamma + 1) + j\chi]Y_0$ for a backward-propagating source wave. The scattering matrix $S$ is commonly used to analyze an $N$-port transmission-line network coupled to a discrete set of scattering channels [47], where the incoming wave enters via the input channels, interacts in the network and exits via the output channels. For the one-dimensional PT system depicted in figure 1(a), $S$ relates the fields (voltages) incident on the ports and those reflected from the ports:

$$\begin{pmatrix} V_2^+ \\ V_1^+ \end{pmatrix} = S \begin{pmatrix} V_2^- \\ V_1^- \end{pmatrix}, \quad S = \begin{pmatrix} t_1 & r_2 \\ r_1 & t \end{pmatrix}$$

(5)

where $r_1$ ($r_2$) is the reflection coefficient for a THz wave incident from port 1 (2) and $t$ is the transmission coefficient; $t$ is independent of the direction of incidence due to the reciprocal nature of the system. We note that $S$ can be determined from the admittance matrix $Y$ [47], and from equations (1) and (5) it is given by

$$S = C(I + \sqrt{z}Y\sqrt{z})^{-1}(I - \sqrt{z}Y\sqrt{z}),$$

(6)

where $C = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $z = \begin{pmatrix} Y_0^{-1} & 0 \\ 0 & Y_0^{-1} \end{pmatrix}$. From equation (6), the scattering matrix elements for the PT-symmetric metasurface in figure 1(b) can be derived as

$$S = \begin{pmatrix} 1 - \gamma^2 + s^2 - \chi (\chi - j2) + 2s (\chi - j) \cot(x) \\ 1 - \gamma^2 + s^2 - \chi (\chi - j2) + 2s (\chi - j) \cot(x) \end{pmatrix}$$

$$= \begin{pmatrix} j2 s \csc(x) \\ j2 s \csc(x) \end{pmatrix}$$

(7)

Assuming that the design in figure 1(a) comprises a pair of resistive/amplifying metasurfaces with zero susceptance ($\chi = 0$) and a normal dielectric spacer ($s \geq 1$), it is found from equation (7) that if $\gamma = s + 1$ and $\sin(x) = s/2(s + 1)$, then one may obtain unidirectional scattering properties, with $|n_2| = |t| = 1$ and $|n| = 0$. On the other hand, if $\gamma = s - 1$, $\sin(x) = s/2(s - 1)$ and $s > 2$, one may obtain the second type of unidirectional reflectionless propagation, with $|n_2| = |t| = 1$ and $|n| = 0$. Such results clearly characterize the unidirectional reflectionless transparency in a PT system: for a certain value of $\gamma$, zero reflection is obtained on only one side of the pairwise gain/loss system or the other. We should note that the above results are consistent with equations (3) and (4) (assuming $\chi = 0$) obtained from the closed-loop analysis, which well characterize resonances producing zero reflection coefficient.

Figure 3(a) shows the loci of complex scattering coefficients on a polar diagram for this PT-symmetric system with $s = 1$, $\chi = 0$ and $x = \sin^{-1}(1/4)$, while $\gamma$ is varied; each color in the legend represents a different normalized surface conductance. It is seen that the reflection coefficients $r_2$ and $r_1$ are, in principle, different. A condition of special interest resides in the exceptional point ($\gamma = 2$), where one may obtain unidirectional reflectionless transparency with $|n_2| = 0$ and $|n| = 1$, with unitary transmission for light incident from both sides, $|t| = 1$. Such a property is rather independent of the separation between the two metasurfaces. For instance, the scattering matrix for $\gamma = 2$ and arbitrary $x$ is given by

Figure 3. (a) Scattering coefficients and (b) corresponding eigenvalues of $S$ (complex domain) as a function of gain–loss parameter $\gamma$ for PT-symmetric metasurfaces in figure 1(a).
$$S = \begin{pmatrix} e^{ix} & -2 + 2e^{2ix} \\ 0 & e^{ix} \end{pmatrix}.$$  

(8)

It can be straightforwardly demonstrated that the scattering matrices in equations (7) and (8) indeed satisfy the condition of PT symmetry [13, 14]:

$$S^*(\omega) = \mathcal{P}\mathcal{T} S(\omega) \mathcal{P}\mathcal{T} = S^{-1}(\omega),$$

(9)

where $\mathcal{P} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $T = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, and $\mathcal{K}$ is the complex conjugate operator. In the one-dimensional PT system, the transition between symmetry and symmetry-breaking can also be characterized by tracing the evolutions of eigenvalues of $S$, $\lambda_1$ and $\lambda_2$ [13]. We notice that equation (9) can be satisfied in two possible ways: either each eigenvalue is itself unimodular, or the eigenvalues form pairs with reciprocal moduli, corresponding to symmetric and symmetry-broken scattering behaviors, respectively [13]. In the exact PT-symmetric phase, $\mathcal{P}\mathcal{T}$ and $S$ share the same eigenstates, and eigenvalues of $S$ must be nondegenerate and unimodular, $|\lambda_1,2| = 1$, implying that there is no net amplification or dissipation. On the other hand, in the broken PT-symmetric phase, eigenstates are not themselves PT-symmetric, and two eigenvalues are non-unimodular and related by $\lambda_1 = 1/(\lambda_2)^\ast$. Interestingly, there exists a transitional point, called the exceptional point, where eigenvalues and eigenvectors of $S$ are degenerate, $\lambda_1 = \lambda_2 = 1/(\lambda_2)^\ast$. From equations (8) and (9), one may obtain

$$r_2^* r_1^* = 1 - |r|^2$$

and

$$\lambda_{1,2} = t \pm \sqrt{n^2 r^2} = \frac{\pm \sqrt{(\gamma^2 - 1)^2 - 2s(\gamma^2 + 1) + s^2} - j2s \csc(x)}{1 + s^2 - \gamma^2 - j2s \cot(x)},$$

(10)

Figure 3(b) presents the complex eigenvalues of $S$ as a function of $\gamma$ for the PT system in figure 3(a). It is seen that when $\gamma > 2$ ($\gamma < 2$), eigenvalues are unimodular and nondegenerate (reciprocal moduli), implying that the PT symmetry is exact (broken). In addition, the two eigenvalues collapse into one at the EP ($\gamma = 2$); such degeneracy results in unidirectional reflectionless propagation with $n_1 = 0$ and $r_1 = 0$. Results presented in figure 3(b) are consistent with the evolution of the transmission coefficient in figure 3(a).

It is worth mentioning that the EP, representing the asymptotic behavior of eigenvalues of $S$, should be correlated to results derived from the closed-loop analysis (equation (3)), since $S$ and $Y$ are linked to each other through the transformation presented in equation (6). Applying the resonance conditions obtained from the closed-loop analysis to $S$ will result in a triangular matrix, with either $r_1$ or $r_2$ being zero. We note that the closed-loop normal-mode analysis based on the admittance matrix $Y$ (or impedance matrix $Z = Y^{-1}$) can also be written into the effective Hamiltonian form, as reported in [32, 33], which provides an alternative way to study PT-symmetric electronic systems. In Hamiltonian systems, the exact (broken) PT-symmetric phase, indicated by purely real (imaginary) eigenfrequencies, would result in narrow resonant dips (broad resonance) in the reflection spectrum. This is different from the previous scattering-matrix modeling, however, which studies the evolution of eigenvalues of $S$ at real frequencies. Although the closed-loop analysis (related to the Hamiltonian) and the scattering-matrix modeling have different definitions for their eigenstates, as $S$ and $Y$ are designed to characterize different physical quantities, both methods should be able to clearly indicate transitions of PT phases because, inherently, $S$ and $Y$ can be transformed into each other using equation (6).

In the PT-symmetric system, there exists another singular CPAL point, where eigenvalues of $S$ go to either zero or infinity, $|\lambda_{1,2}| = 0, \infty$, corresponding respectively to the coherent perfect absorber mode or the lasing mode [13–15]. At such a point, the PT system simultaneously behaves as a perfect absorber that absorbs the incoming coherent waves and as a laser oscillator that emits outgoing coherent waves. We note that the proposed metasurface configuration can also produce CPAL operation, and its required conditions are derived as

$$\chi = 0, \quad \gamma = \sqrt{1 + s^2}\quad \text{and} \quad x = n\pi/2,$$

(11)

where $n = 1, 3, 5 \cdots$. We should note that a directional transparency with $|\lambda_{1,2}| = 1$ is obtained when $n = 2, 4, 6$, which is in some sense similar to a resonant loss–gain compensation medium. Such a CPAL mode exists only in the broken PT-symmetric phase [13–15]. Applying results in equation (11) to equation (2) also leads to a non-zero determinant. Figures 4(a) and (b) present eigenvalues in complex numbers using absolute-value notation as a function of $\gamma$ for the PT-symmetric metasurfaces with $\chi = 0$, $s = 1$, and $x = \pi/2$. It is seen that the CPAL operation can be achieved when $\gamma = \sqrt{2}$, consistent with equation (11). In the vicinity of the CPAL point, one may obtain huge outgoing scattering waves.

Next, we consider the effect of a reactive perturbation ($\chi \rightarrow \chi + \Delta \chi$) in the PT-symmetric system comprising at least one chemically/physically sensitive metasurface. The PT-symmetric metasurface, when operating around the EP and CPAL singularities, may constitute an ultrasensitive sensor, for which any small change in metasurface admittance (impedance) may cause bifurcations in eigenvalue and may therefore
remarkably modulate scattering responses. Figure 5(a) presents evolutions of eigenvalues for the PT system in figure 3(a), with \( \gamma = \sqrt{2} \) and \( \chi \) of the active metasurface being varied from a negative value (inductive perturbation) to a positive value (capacitive perturbation); here we assume that the system initially operates at the EP \( \chi = 0 \). Figure 5(b) is similar to figure 5(a), but for a pair of identical passive metasurfaces \( Y_1 = Y_2 = 2 \) with the susceptance of one metasurface being perturbed. From figures 5(a) and (b), it is seen that for the same value of \( \Delta \chi \), eigenvalues of the PT system can have a more dramatic splitting than a passive sensor that lacks the EP-related singularity. Such results suggest that a PT-symmetric metasurface sensor may enhance the modulation depth of scattering signals, particularly for \( r_1 \) and therefore provide better sensitivity. This argument will be demonstrated with realistic graphene metasurface sensors in the next section. Similarly, a PT sensor operating around the CPAL point may be expected to display ultrahigh sensitivity to reactive fields on metasurfaces. Ideally, admittance perturbations around the CPAL point may enable eigenvalues to change radically from infinity to a rather low value, leading to considerable changes in scattering coefficients, as shown in figure 4(c). In this figure, the evolutions of eigenvalues are studied for the PT-symmetric metasurfaces in figure 4(a) with \( \gamma = \sqrt{2} \), while the susceptance of the active metasurface is varied slightly \( Y_1 = 2 \), \( Y_2 = (-2 + j \chi ) Y_0 \) and \(-0.3 \leq \chi \leq 0.3\). It is surprisingly seen that, at the CPAL point, eigenvalues of \( S \) show quite a dramatic dependence on \( \chi \). However, we should notice that strong scattering fields in the lasing condition could cause the system to access the nonlinear regime, where stability and harmonic balance must be taken into consideration.

Tracing the shift of the resonant peak with respect to the reactive energy perturbation has been a common sensing mechanism for electromagnetic and optical sensors [34–36]. Traditional plasmonic or metasurface sensors usually consist of a passive, tunable metasurface separated from the ground plane (e.g. a thick metal layer) by a proper electric distance [34–36, 43, 44]. The ground plane is necessary to break the field symmetry and
achieve perfect absorption at the operating frequency [45]. In these devices, resonant absorption occurs when the surface susceptibility of the metasurface cancels out the input admittance yielded by the grounded dielectric substrate, which is given by $B_d = -jY_0 \cot(k_d d)$ [45]. In general, the distance between the metasurface and the metallic ground is sub-wavelength, and therefore $B_d$ can be approximately modeled as a surface inductance $L_d = \mu_0 d$ (or $B_d = (j\omega L_d)^{-1}$) mounted in parallel to the metasurface susceptibility $B_s$ which, in general, can be decomposed into a surface capacitance $C_s$ and surface inductance $L_s$ [45–49]. If the loss is moderately low, the resonance frequency is given by $\omega_0 \approx 1/\sqrt{C_s (L_s + L_d)}$, which leads to $B_s(\omega_0) + B_d(\omega_0) = 0$. In the proposed PT-symmetric metasurfaces, the reflection dip can be correlated with the EP, and, as can be understood from equations (7) and (8), the gap between the metasurface and the resistive sheet has no effect on the resonance frequency, as long as the admittance of the active, self-resonant metasurface is $-2Y_0$. Since it is physically possible to maintain a constant gain over a finite frequency range (surface conductance $G_s = -2Y_0$), the reflection dip occurs at the frequency where the metasurface reaches its self-resonance, i.e. the net surface susceptibility of the metasurface approaches zero, $B_s(\omega_0) = 0$. As a result, the resonance frequency of the proposed PT-symmetric metasurface is given by $\omega_0 = 1/\sqrt{C_s}$, which may provide a greater fractional frequency shift $\Delta \omega_0/\omega_0$ in response to the reactive energy perturbation ($\Delta L_s$ or $\Delta C_s$), when compared to passive metasurface sensors with $\omega_0 \approx 1/\sqrt{C_s (L_s + L_d)}$. In the following, we will demonstrate that PT-symmetric metasurfaces, if combined with sensing functions, such as those of graphene metasurfaces, may outperform conventional passive sensors in terms of figures of merit, including the modulation depth of the scattering signal, the spectral resolution and the sensitivity related to resonance-offset effects.

3. Active graphene metasurfaces and PT-symmetric THz systems

Graphene represents a novel 2D material platform extending plasmonics to the mid-infrared and even terahertz regimes, with the Drude weight tuned by electrostatic gating, chemical doping or elastic modulation [45–59]. It has been reported that the conductivity of photodoped graphene $\sigma$ can have a negative real part that gives an optical gain at THz frequencies [37–42]. When graphene is optically pumped, the interband transitions and the cascaded optical-phonon emission could lead to photoexcited electron–hole pairs near the Dirac point, splitting the Fermi level into two quasi-Fermi levels $E_{F\uparrow}, E_{F\downarrow} = \pm \epsilon_F$ [37–42], as illustrated in figure 6. Since the relaxation time for intraband transitions $\tau \approx 1$ ps is shorter than the recombination time $\tau \approx 1$ ns for electron–hole pairs [60], the population inversion can be achieved [37–42]. Once the interband emission of photons in the gapless graphene prevails over the intraband Drude absorption, a negative conductivity can be obtained for THz photons. Detailed expressions for $\sigma$ can be found in the appendix. Figure 6 presents $\text{Re}[\sigma]$ as a function of frequency for a graphene monolayer photopumped to different quasi-Fermi levels at temperature $T = 3$ K; here the conductivity of unpumped graphene with a Fermi level $\epsilon_F$ is also presented for comparison. It is seen that under the optical excitation, $\text{Re}[\sigma]$ can be negative and its bandwidth depends on the quasi-Fermi level controlled by the intensity of pump light.

Here, we consider a practical PT-symmetric THz system consisting of an optically pumped graphene metasurface (gain) and a metal filament (loss), illuminated by a normally incident transverse magnetic (TM) wave with the electric field polarized perpendicular to graphene ribbons, as shown in figure 1(b). The loss portion of this PT system can be readily realized with a metallic filament of thickness $t \ll \lambda_0$, whose surface conductance is given by $Y_s = \sigma_0 t$, where the Drude conductivity $\sigma_0(\omega) = \sigma_0/(1 + j\omega\tau) \approx \sigma_0$ and a relaxation
The delay time $\tau \sim 10^{-14}$ s is assumed for common metals [61]. Here we choose a nichrome (NiCr) filament with $\sigma_m = 6.7 \times 10^5$ [S m$^{-1}$] [61] and $t = 7.9$ nm, which has a surface conductance of $2Y_0$ over a broad THz range. To satisfy the constraint of PT symmetry, the susceptance of the graphene metasurface resulting from the kinetic inductance must be conjugately canceled out with capacitive elements, which could be, for instance, graphene-ribbon arrays shown in figure 1(b). For the normally incident TM plane wave, the equivalent surface admittance of a graphene-ribbon array with a sub-wavelength period can be expressed as [45–49]

$$Y = \frac{1}{\sigma(1 - \vartheta)} - \frac{1}{\xi Y_0 \ln [\csc(\pi\vartheta/2)]},$$

(12)

where $\vartheta$ represents the ratio between the gap $g$ and period $a$ of the graphene-ribbon array ($\vartheta = g/a$), $\xi(\omega) = 2\omega n/\pi c = 4n/\lambda c$, $c$ is the speed of light and $\lambda$ is the wavelength. The imaginary part in the denominator of equation (12) accounts for the net contribution of the kinetic inductance per unit cell $L_K = \text{Im}[\sigma]/\omega(1 - \vartheta)|\sigma|^2$ and the geometric capacitance per unit cell $C_{GS} = \varepsilon_0 2\pi \ln [\csc(\pi\vartheta/2)]/\pi$ [62, 63], which are in series with the resistance per unit cell $R_i = \text{Re}[\sigma]/(1 - \vartheta)|\sigma|^2$; equation (12) can also be recast as $Y = [R_i + j(\omega L_K - 1/\omega C_{GS})]^{-1}$. Given the conductivity of graphene at the operating frequency $\sigma(\omega_0, \varphi)$, the optimal set of dimensionless parameters $\vartheta$ and $\xi$, leading to conditions for the observation of the EP $(\text{Re}[Y(\omega_0)] = -2Y_0$ and $\text{Im}[Y(\omega_0)] = 0$), can be derived as

$$\vartheta = 1 + \frac{2Y_0 \text{Re}[\sigma(\omega_0)]}{|\sigma(\omega_0)|^2},$$

(13a)

$$\xi = -\frac{(1 - \vartheta)|\sigma(\omega_0)|^2}{\text{Im}[\sigma(\omega_0)] Y_0 \ln [\csc(\pi\vartheta/2)]}.$$  

(13b)

As discussed earlier, such an active graphene metasurface with admittance of $-2Y_0$ at the resonance, when paired with a metallic filament with admittance of $2Y_0$, may access the EP of the PT-symmetric system.

Next, we consider a practical PT-symmetric sensor implemented by an active graphene metasurface, which exhibits the EP-related unidirectional reflectionless propagation at the frequency $\omega_0/2\pi = 2$ THz. The design parameters for the graphene metasurface are $(\vartheta, \xi) = (0.21, 0.095)$, as determined by equation (13), and the photopumped quasi-Fermi level $\varepsilon_F = 20$ meV; the thickness of the nichrome filament is $t_{ni} = 7.9$ nm and air gap size $d = 6.03$ $\mu$m. Such a design results in a pair of amplifying/attenuating surfaces with admittance $Y = \pm 2Y_0$, which are separated by an electrical distance $x(\omega_0) = \sin^{-1}(1/4)$. Figures 7(a) and (b) present the calculated amplitude and phase of the scattering coefficients, $\eta_1$, $\eta_2$ and $t$, against frequency for this PT-symmetric THz system. It is clearly seen that at the EP (2 THz), the system is unidirectionally transparent with $|t| = 1$, $|\eta_1| = 0$ and $|\eta_2| = 1$. Due to the fact that the conductivity of graphene and the metasurface admittance are dispersive, the condition for PT symmetry cannot be fulfilled over a finite frequency interval, but only at a specific frequency point $\omega_0$, as a result of causality and Kramers–Kronig relations [64]. Figure 7(c) presents the eigenvalues of $S$ as a function of frequency for this PT system, showing that when the operating frequency shifts away from the EP, the degenerate eigenvalues may quickly split into complex ones, accompanied by dramatic changes in scattering properties (figure 7(a)). It is seen from figure 7(b) that the phase of $\eta_1$ experiences an abrupt change of $\pi$; due to this step-function-like behavior in phase, the reflection coefficient $r_1$ is zero at the EP, where the delay time $\tau_{\text{delay}} = \partial \arg(r_1)/\partial \omega$ becomes a delta function, and hence the backscattered waves are trapped for an infinitely long time and can be completely absorbed by the resistive component (lossy nichrome filament).
Because of its atomic thickness and low density of states, graphene exhibits interesting conduction properties that are sensitive to \( n-/p \)-type doping (e.g. gas and (bio)chemical species attached on its surface). So far, several chemically specific, label-free graphene sensors have been proposed. In these devices, \( n-/p \)-type doping may change the transconductances of graphene field-effect devices [65–69] or the optical properties of graphene plasmonic sensors [43, 44, 56]. Here, we combine the concept of PT-symmetric graphene metasurfaces with graphene-enabled (bio)chemical sensing. We consider a sensing device based on the PT-symmetric graphene metasurface in figure 7, which initially achieves the EP at 2 THz, with a sharp dip in the reflection spectrum (\( r_1 \)). Once the graphene metasurface is chemically doped, the symmetry of susceptances between active and passive metasurfaces will be broken (also the gain–loss balance is slightly broken), resulting in the splitting of \( \lambda_{1,2} \) at the EP frequency and therefore a related change in the reflection coefficient \( r_1 \).

Figure 8(a) presents the evolution of complex eigenvalues of \( S \) as a function of the shift in the quasi-Fermi level \( \Delta E_F \) at 2 THz for the graphene-based PT-symmetric metasurfaces in figure 7(a), under \( n \)-type (\( p \)-type) doping that causes a shift in quasi-Fermi level \( \Delta E_{F_n} = \Delta E_F \) (\( \Delta E_{F_p} = -\Delta E_F \)). Reflection \( r_1 \) and transmission \( t \) spectra for the PT-metasurface sensor system in (a), with different doping levels. (c) Reflection spectrum for the conventional graphene metasurface sensor, whose design parameters and initial conditions are similar to those of the PT sensor in (b), but the metallic filament is replaced by a mirror.

In the frequency range of interest (i.e. low THz), chemical doping primarily modulates the effective susceptance of the graphene metasurface because \( \text{Re}\{\sigma\} \) has a relatively flat dispersion, as can be seen in figure 6. As long as the surface conductance of the active graphene metasurface is close to \(-2Y_0\), the separation between the metasurface and the metal filament has no effect on the resonance frequency, as can be understood from equation (8). Therefore, the frequency offset of the dip in reflection depends mostly on the self-resonance of the metasurface, at which its net surface susceptance is zero, \( jB_0 = 0 \). Such a condition suggests that the resonance frequency is \( \omega_0 \approx \sqrt{\frac{k}{k}} \). Figures 9(a) and (b) present the shift in resonance frequency \( \Delta\omega/\omega_0 \) as a function of...
of \( \Delta \varepsilon_F \) (or the induced density of charged impurities \( n_{\text{imp}} \) in graphene) for the active, PT-symmetric metasurface sensor (figure 8(b)) and the passive one (figure 8(c)); here we also plot the self-resonance frequency of the metasurface (the frequency at which zero net susceptance is obtained, \( B_j \approx 0 \) for different \( \Delta \varepsilon_F \)). It is seen that the self-resonance frequency of the metasurface agrees excellently with the resonance frequency of the PT sensing system. On the other hand, for a passive metasurface sensor, the resonant absorption, corresponding to a reflection dip, occurs when the susceptance of the metasurface cancels out the susceptance input into the grounded dielectric substrate, \( B_d = -j \chi_0 \cot(k_d d) \). Since the distance between the metasurface and the ground is generally short, \( B_d \) can be modeled as an effective inductance \( L_d = \mu_d d \) mounted in parallel to the metasurface, \( B_d = (j \omega L_d)^{-1} \). In this case, if the loss is moderate, the resonance frequency is given by \( \omega_0 \approx \sqrt{C_{\text{GS}}(L_K + L_d)} \). As can be expected, the active, PT sensor with \( \omega_0 \approx \sqrt{C_{\text{GS}} L_K} \) may provide a greater frequency offset with respect to \( L_K \) perturbation (via chemical doping) than the passive one. Overall, figures 8 and 9 clearly demonstrate that a PT sensor operating in the vicinity of the EP, if combined with sensing functionalities (possible with metasurfaces formed from nanomaterials), can potentially outperform conventional passive photonic and plasmonic sensors.

Finally, we note that the proposed PT-symmetric graphene metasurfaces can also achieve CPAL effects with singularity-enhanced sensing functions. Figure 10(a) shows the PT-symmetric graphene metasurface with design parameters: the geometric parameters of the metasurface, \( \theta = 0.15, \xi = 0.059 \), the photopumped quasi-Fermi level \( \varepsilon_F = 15 \) meV, the thickness of nichrome filament \( t_{\text{fil}} = 5.6 \) nm and the size of the air gap \( d = 37.5 \) \( \mu \)m. Such a setup leads to the CPAL phenomenon at the design frequency \( \omega_0 / 2\pi = 2 \) THz. (b) Evolutions of eigenvalues of the scattering matrix as a function of operating frequency for this system.
Figure 11. (a) Reflection \( r \) and (b) transmission \( t \) spectra for the PT-symmetric sensor system in figure 10, with different doping levels. (c) Magnitude of reflection coefficient \( r \) against the change in quasi-Fermi level \( \Delta\varepsilon_F \) at the design frequency \( \omega_0/2\pi = 2 \text{ THz} \) (CPAL point). The inset in (c) shows the evolutions of eigenvalues of the scattering matrix as a function of \( \Delta\varepsilon_F \) at 2 THz; the CPAL phenomenon occurs at \( \Delta\varepsilon_F = 0 \).

ultra-narrowband and sharply peaked scattering response in figure 10(a) is particularly desired to develop ultrasensitive and ultrahigh-resolution optical sensors.

Figures 11(a) and (b) respectively present the calculated reflection and transmission spectra for the PT-symmetric metasurface in figure 10 at different doping levels. It is seen that the CPAL point, existing at \( \Delta\varepsilon_F = 0 \text{ meV} \), is highly sensitive to the value of \( \Delta\varepsilon_F \) that perturbs the metasurface admittance. Even a small shift in the quasi-Fermi level may dramatically vary the local transmission and reflection properties around the design frequency (2 THz). Figure 11(c) reports the reflection amplitude \( |r| \) against \( \Delta\varepsilon_F \), clearly showing that when the system operates at the singular CPAL point, the reflection amplitude can be dramatically modulated by \( \Delta\varepsilon_F \). The inset of figure 11 presents evolutions of eigenvalues as a function of \( \Delta\varepsilon_F \) at 2 THz, showing that eigenvalues vary quite remarkably for a small change in graphene’s carrier density, which alters the metasurface admittance. The extraordinarily large modulation depth in the scattering response, taking advantage of the CPAL-related singularity, may greatly enhance the sensitivity of graphene-based photonic sensors. We should note that, due to strong fields at the CPAL point, the operation will be complicated by the higher-order nonlinearities of graphene [70], which could make scattering responses intensity-dependent and bistable. For simplicity, in this work we ignore the nonlinearities of graphene, which will be studied elsewhere. Nonetheless, we note that within the vicinity of the CPAL point where the system could be conditionally stable, the modulation depth of the scattered signal is still quite large. The strongly modulated scattering responses around the CPAL point, together with the chemically sensitive admittance of the graphene metasurface, offer the unique possibility to make an ultrasensitive THz sensor.

4. Conclusions

We have presented PT-symmetric systems based on a pair of metasurfaces with balanced gain–loss distributions. We have studied such systems by using two different approaches: the closed-loop analysis related to the admittance or impedance matrix (analogous to an effective Hamiltonian [32]) and scattering-matrix eigenproblems. We found that although their eigenstates and therefore PT phases have different definitions, physical properties revealed by both approaches are intrinsically linked, because a mathematical transformation exists between scattering-matrix and admittance-matrix representations of the system. Moreover, we proposed the use of a PT-symmetric metasurface for sensing applications, taking advantages of the EP- or CPAL-related singularity that leads to dramatic eigenvalue degeneracy/splitting in response to perturbations of the metasurface admittance. Finally, we have shown that in the THz spectrum, the proposed PT-symmetric system may be realized with optically pumped graphene metasurfaces, which simultaneously provide THz plasmon gain and (bio)chemical sensing functions, thanks to graphene’s tunable, chemically sensitive conductivity. With the known analytical expression for the surface admittance of a graphene metasurface, we have put forward an efficient and accurate analytical method for designing PT-symmetric THz systems with exotic scattering properties produced by EP- and CPAL-related singularities. Our theoretical results show that in PT-symmetric graphene sensors, even a light chemical doping may result in greatly modulated scattering properties. Our results unveil a critical first step in breaking the limitations on sensitivity of numerous electromagnetic sensors based on plasmonic, metasurface and metamaterial devices.
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Appendix. Photodoping and its relation to pump intensities

The nonequilibrium conductivity of graphene modeled from Green’s functions, taking into account both intraband and interband transitions $\sigma = \sigma_{\text{intra}} + \sigma_{\text{inter}}$, is given by

$$\sigma_{\text{intra}} = \frac{g^2}{\pi \hbar^2} \frac{1}{\omega - i \tau} \left[ \int_0^\infty \varepsilon \left( \frac{\partial F_1(\varepsilon)}{\partial \varepsilon} - \frac{\partial F_2(-\varepsilon)}{\partial \varepsilon} \right) d\varepsilon \right]$$

(A1)

$$\sigma_{\text{inter}} = -\frac{g^2}{\pi \hbar^2} \left( \omega - i \tau^{-1} \right) \int_0^\infty \frac{F_2(-\varepsilon) - F_1(\varepsilon)}{(\omega - i \tau^{-1})^2 - 4 \varepsilon^2/\hbar^2} d\varepsilon,$$

(A2)

where $F_1(\varepsilon) = \left[ 1 + e^{(\varepsilon - E_F)/k_B T} \right]^{-1}$, $F_2(\varepsilon) = \left[ 1 + e^{(\varepsilon - E_F)/k_B T} \right]^{-1}$, $q$ is the electric charge, $\varepsilon$ is the energy, $\hbar$ is the reduced Planck constant, $k_B$ is the Boltzmann constant, $T$ is the temperature, $\omega$ is the angular frequency and $\tau$ is the momentum relaxation time of charge carriers (here we assume $\tau = 1$ ps, which is consistent with experimental results). By solving the integral in equation (A1), $\sigma_{\text{intra}}$ can be written in a compact form:

$$\sigma_{\text{intra}} = -\frac{g^2}{4\hbar} \ln \left[ 1 + e^{\tau/\hbar k_B T} \right] \left( \frac{\tau}{1 + \omega^2 \tau^2} - \frac{\omega}{\omega^2 + \tau^2} \right).$$

(A3)

Re[$\sigma_{\text{inter}}$] in equation (A2) could be negative, but this must compete with the positive Re[$\sigma_{\text{intra}}$]. For instance, in the THz spectral range, Re[$\sigma_{\text{inter}}$] can be approximately expressed as [37]

$$\text{Re}[\sigma_{\text{inter}}] \approx \frac{g^2}{4\hbar} \tanh \left( \frac{h\omega - 2\varepsilon_F}{4k_B T} \right),$$

(A4)

which can be negative if $h \omega < 2\varepsilon_F$. The equilibrium and nonequilibrium conductivities would converge to a similar form in low-frequency (e.g. microwaves) and high-frequency (e.g. mid-infrared) regimes. In the visible and near-infrared spectral ranges, where the photon energy $h\Omega_0 \gg \varepsilon_F$ and $h\Omega_0 \gg k_B T$ only the interband contribution is important and the optical conductivity becomes

$$\sigma = \frac{q^2}{4\hbar} \tanh \left( \frac{h\omega - 2\varepsilon_F}{4k_B T} \right) \approx \frac{q^2}{4\hbar}. (A5)$$

As is known from (A4) and (A5), the magnitude of Re[$\sigma$] is bounded by the physical limit of $\pm q^2/4\hbar$.

Under equilibrium conditions, the electron density $n_0$ and hole density $p_0$ in graphene, as functions of Fermi energy $E_F$, can be obtained from integration of the density of states weighted by the Fermi–Dirac distribution as [56]

$$n_0(E_F) = -\frac{2}{\pi} \left( \frac{k_B T}{6\hbar v_F} \right) L_2 \left[ -e^{-q k_B T/(k_B T)} \right],$$

(A6)

$$p_0(E_F) = -\frac{2}{\pi} \left( \frac{k_B T}{6\hbar v_F} \right) L_2 \left[ -e^{q k_B T/(k_B T)} \right],$$

(A7)

where the dilogarithm $L_2$ is a special case of the polylogarithm $L_n(z)$ for $n = 2$. For pristine graphene with $E_F = 0$, the carrier densities are obtained as

$$n_0(0) = p_0(0) = \frac{\pi k_B T}{6\hbar v_F} \left( \frac{k_B T}{\hbar v_F} \right)^2,$$

(A8)

where $v_F$ is the Fermi velocity in graphene. The carrier densities for n- or p-doped graphene with $|E_F| \gg k_B T$ can be derived as

$$n_0(E_F) = p_0(-E_F) = \frac{|E_F|^2}{\pi \hbar^2 v_F^2}.$$ (A9)

Under near-infrared and visible illumination, the excess electrons and holes are generated in pairs ($\delta n = \delta p$), and the total carrier densities become $n = n_0 + \delta n$ and $p = p_0 + \delta p$. The density of photoexcited carriers is given by
\[ \delta n = \delta p = \frac{\alpha I_{ph} \tau_r}{h \Omega_0}, \]  
(A10)

where \( \alpha \) is the optical absorptance, \( I_{ph} \) and \( h \Omega_0 \) are the intensity and photon energy of the pump light, and \( \tau_r \) is the recombination lifetime for electron–hole pairs (typically \( \tau_r \approx 1 \text{ ns} \)). Under weak optical excitation, i.e. \( \varepsilon_F \ll k_0 T \), the normalized densities of excess carriers are derived as

\[ \frac{\delta n}{n_0} = \frac{\delta p}{p_0} \approx \frac{12 \ln 2}{\pi^2} \frac{\varepsilon_F}{k_0 T}. \]  
(A11)

From equations (A10) and (A11), the quasi–Fermi levels \( E_{\text{F}n}, E_{\text{F}p} = \pm \varepsilon_F \), as functions of the intensity of pump light, are given by

\[ \frac{\varepsilon_F}{k_0 T} = \frac{\pi}{2 \ln 2} \left( \frac{\hbar v_F}{k_0 T} \right)^2 \frac{I_{ph} \tau_r}{h \Omega_0}. \]  
(A12)

On the other hand, under intense optical excitation, i.e. \( \varepsilon_F \gg k_0 T \), the normalized densities of excess carriers are derived as

\[ \frac{\delta n}{n_0} = \frac{\delta p}{p_0} \approx \frac{6}{\pi^2} \left( \frac{\varepsilon_F}{k_0 T} \right)^2 - 1. \]  
(A13)

From equations (A10) and (A13), \( \varepsilon_F \), as a function of intensity of pump light, is given by

\[ \frac{\varepsilon_F}{k_0 T} = \sqrt{\frac{\pi^2}{6} \left( 1 + \frac{\delta n}{n_0} \right)} \approx \sqrt{\frac{\pi^2}{6} + \pi \left( \frac{\hbar v_F}{k_0 T} \right)^2 \frac{\tau_r I_{ph}}{h \Omega_0}}. \]  
(A14)

In the near-infrared and visible ranges, \( h \Omega_0 \gg \varepsilon_F \) and \( h \Omega_0 \gg k_0 T \), and therefore the optical conductivity \( \sigma \), based on equation (A5), can be expressed as

\[ \sigma (\Omega_0) = \frac{q^2}{4 \hbar} \tanh \left( \frac{h \Omega_0 - 2 \varepsilon_F}{4 k_0 T} \right) \approx \frac{q^2}{4 \hbar}, \]  
(A15)

which leads to a constant optical absorption \( \alpha \approx (q^2/4h) / 4 \Omega_0 \approx 2.3\% \) over a broad near-infrared and visible spectral range. For instance, assuming a pump source at \( \Omega_0/2\pi = 193 \text{ THz} \) and the recombination time \( \tau_r = 1 \text{ ns} \), an energy splitting of \( \varepsilon_F = 15 \text{ meV} \) at \( T = 3 \text{ K} \) requires the pump intensity \( I_{ph} \) = 146 mW mm\(^{-2}\). Such an intensity is fairly reasonable at telecommunication wavelengths.

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