Topological bands and triply-degenerate points in non-Hermitian hyperbolic metamaterials

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Introduction. Hyperbolic metamaterials (HMMs), an unusual class of electromagnetic metamaterials, have found important applications in various fields due to their distinctive properties. A surprising feature of HMMs is that even continuous HMMs can possess topological edge modes. However, previous studies based on equal-frequency surface (analogy of Fermi surface) may not correctly capture the topology of entire bands. Here we develop a topological band description for continuous HMMs that can be described by a non-Hermitian Hamiltonian formulated from Maxwell’s equations. We find two types of three dimensional non-Hermitian triply-degenerate points with complex linear dispersions and topological charges ±2 and 0 induced by chiral and gyromagnetic effects. Because of the photonic nature, the vacuum band plays an important role for topological edge states and bulk-edge correspondence in HMMs. The topological band results are numerically confirmed by direct simulation of Maxwell’s equations. Our work presents a general non-Hermitian topological treatment of continuous HMMs, paving the way for exploring interesting topological phases in photonic continua and device implementations of topological HMMs.

Hyperbolic metamaterials (HMMs), an unusual class of electromagnetic metamaterials, have found important applications in various fields due to their distinctive properties. A surprising feature of HMMs is that even continuous HMMs can possess topological edge modes. However, previous studies based on equal-frequency surface (analogy of Fermi surface) may not correctly capture the topology of entire bands. Here we develop a topological band description for continuous HMMs that can be described by a non-Hermitian Hamiltonian formulated from Maxwell’s equations. We find two types of three dimensional non-Hermitian triply-degenerate points with complex linear dispersions and topological charges ±2 and 0 induced by chiral and gyromagnetic effects. Because of the photonic nature, the vacuum band plays an important role for topological edge states and bulk-edge correspondence in HMMs. The topological band results are numerically confirmed by direct simulation of Maxwell’s equations. Our work presents a general non-Hermitian topological treatment of continuous HMMs, paving the way for exploring interesting topological phases in photonic continua and device implementations of topological HMMs.

Recent results by developing a topological band description, along with the bulk-edge correspondence, for continuous HMMs. Our main results are:

i) An effective non-Hermitian Hamiltonian for HMMs is derived from Maxwell’s equations. Symmetry analysis shows the physics can be described by three bands (i.e., a spin-1 system). Proper gyromagnetic or chiral field opens a band gap between the upper and the other two bands except at k = 0, which is a non-Hermitian triply-degenerate point (TDP) [31–33] with complex linear band dispersions (i.e., a topological semimetal). The complex bulk spectrum exhibits an exceptional cone with the TDP as cone vertex. TDPs were studied recently in solid state [31, 32] and ultracold atomic systems [33], but have not been explored in photonic materials or any non-Hermitian systems, and their real linear dispersions are very different from non-Hermitian TDPs. The topological charge of the TDP at k = 0 is ±2 (0) for chiral (gyromagnetic) effect. For any fixed nonzero k_z, the HMM is a 2D Chern insulator, and the TDP emerges as the band gap closing point at k_z = 0.

ii) There exist surface states connecting the single TDP to infinity for both cases (change ±2 or charge 0), which are illustrated through topological edge states in both 3D and 2D Chern insulators with fixed k_z using the bulk-edge correspondence. More importantly, the
topological edge states can only be found in the common band gap of the HMMs and vacuum because unlike electrons in solid-state materials, photons can propagate in the vacuum, forming vacuum band structures outside the HMMs. The edge states are purely real and do not suffer loss as the complex bulk, which, combining with the unique properties of HMMs, enable the design of novel optical devices such as topological lasing.

iii) Our theoretical predictions on topological bands and chiral edge states of HMMs are confirmed by numerically solving the Maxwell’s equations using COMSOL simulations.

Non-Hermitian Hamiltonian and topological invariant.

The HMMs can be described by the source-free Maxwell’s equations with the following constitutive relation

$$D = \epsilon E + i\gamma H, \ B = \mu H - i\gamma E,$$

based on the symmetrized Condon set [34], where $\epsilon$, $\mu$ and $\gamma$ are 3x3 permittivity, permeability and chirality tensors. Without gain and loss, they satisfy $\mu^T = \mu$ and $\epsilon^T = \epsilon$. The chirality term can be written as $\gamma = \text{Tr}(\gamma) I/3 + N$ with $I$ the identity matrix and $N$ a real-valued symmetric trace-free tensor. The chiral and gyromagnetic effects for HMMs can be induced by nonzero $\gamma$ and imaginary non-diagonal terms in $\epsilon$ or $\mu$, respectively. The Maxwell’s equations can be recast to a linear-transformation form $H|\Psi\rangle = \omega|\Psi\rangle$, with

$$H = \begin{pmatrix} \epsilon & i\gamma \\ -i\gamma & \mu \end{pmatrix}^{-1} \begin{pmatrix} 0 & p \\ -p & 0 \end{pmatrix}, \ |\Psi\rangle = \begin{pmatrix} E \\ H \end{pmatrix},$$

where $p_{[mn]} = \varepsilon_{mn\ell} \nabla_{\ell}$ is an antisymmetric tensor operator ($p_{[\nu]} = -p$) defined through the Levi-Civita symbol $\varepsilon_{mn\ell}$. In the limit $\gamma \to 0$, Eq. (2) reduces to the Hermitian formalism in previous works [18, 19, 29] if $\epsilon$ and $\mu$ are positive-definite. In the context of HMMs, the Hamiltonian in Eq. (2) is generally non-Hermitian and possesses complex eigenvalues, therefore the topological classifications for Hermitian systems [35–37] do not apply.

The Hamiltonian has 6 bands, which appear in pairs $(\omega, -\omega)$ due to the symmetry $\Pi H \Pi^{-1} = -H$, where the symmetry operator $\Pi$ is defined as the composite of chiral symmetry $C$ and the operation $\gamma \to -\gamma$. Here $C = \sigma_z \otimes I_3$ and $\sigma_z$ represents Pauli matrix in the $(E, H)$ space. In addition, the state at $(k, \omega)$ represents the same physical state as that at $(-k, -\omega)$ due to the symmetry $H(-p) = -H(p)$, which holds for arbitrary $H$. When combined together, these symmetries dictate that only three bands are independent. Here we consider three bands with $\Re(\omega) \geq 0$ ($\Re$ takes the real part), which form an effective spin-1 system. Note that one band is a zero-energy $(\omega = 0)$ flat band, which represents the static solutions $E = \nabla d(r)$ and $H = \nabla b(r)$. Interestingly, the three bands are always (tripy) degenerate at $(k, \omega) = 0$ for arbitrary $H$, independent of $\epsilon, \mu, \text{and } \gamma$.

The energy spectra for a non-Hermitian Hamiltonian are generally complex, and the topological invariants can be defined by either eigenvalues or eigenstates. The eigenvalue-based winding number for a closed loop in momentum space is defined as $[38, 39]$

$$C_w = \oint_{C} \arg[\omega(k)],$$

which is generally trivial and irrelevant to the topological edge modes for HMMs discussed here. On the other hand, the bands for HMMs are separable in the complex plane, therefore winding number $W = \frac{1}{2\pi} \int_{C} dk \cdot \mathcal{A}(k)$ and the Chern number $C = \frac{1}{2\pi} \oint_{C} ds \cdot \mathcal{F}$ based on eigenstates are well-defined and quantized, which can be used to characterize the topological properties of HMMs. Here $S^1$ is a closed 1D loop and $S$ can be a closed 2D sphere $S^2$ (or infinite plane $\mathbb{R}^2$) in the momentum space, $\mathcal{A}(k) = -iL (\langle \Psi(k)|\nabla_k|\Psi(k)\rangle)_{L}$ and $\mathcal{F} = \nabla \times \mathcal{A}(k)$ are the Berry connection and Berry curvature respectively, and $|\Psi(k)\rangle_{L} (|\Psi(k)\rangle_{R})$ is the right (left) eigenstate [39] of the Hamiltonian. Among the three bands, the zero-energy flat band is topologically trivial, while the other two nonzero bands possess opposite topological invariants. Hereafter we only plot the two nonzero-energy bands with $\Re(\omega) > 0$ for better visualization.

Charge ±2 TDPs from chiral effects.

Without chiral and gyromagnetic terms and assume $\epsilon = \text{diag}(\epsilon_x > 0, \epsilon_y > 0, \epsilon_z < 0)$ and $\mu = I$ for hyperbolic dispersion, there is one degenerate line along the $k_z$ axis between the two upper non-zero bands with $\epsilon_x = \epsilon_y$, as shown in Figs. 1(a). The degenerate line possesses a non-trivial winding number (defined by the highest band) $W = 2$ for a closed loop encircling the line [30]. The corresponding

![FIG. 1: Typical band structures for HMMs. (a) A HMM with $(\epsilon_x, \epsilon_y, \epsilon_z) = (4, 4, -3)$ exhibits a degenerate line along $k_z$ axis between two nonzero bands. (b) The degenerate line (except $k = 0$) in (a) is lifted by $\gamma = \text{diag}(1, 0, 0)$. (c) Corresponding gapped topological bands in 2D $k_x$-$k_y$ plane for $k_z = 1$. See SM [30] for the imaginary bands. The dashed green circle is the exceptional ring. (d) The 3D exceptional cone in momentum space at $k_z \geq 0$.](image)
band structure in the $k_x$-$k_y$ plane with a fixed non-zero $k_z$ contains a quadratic band touching point with winding number $W = 2$ at $(k_x, k_y) = (0, 0)$, which is computed on a closed circle enclosing the degenerate point. The band structures for $\epsilon_x \neq \epsilon_y$ are presented in SM [30].

The degeneracy between two non-zero bands along the $k_z$ axis (except at $k = 0$) can be lifted by breaking inversion symmetry using a chiral term (Fig. 1(b) with $\gamma = \text{diag}(1, 0, 0))$. For a fixed $k_z \neq 0$, the gap at the quadratic band touching point is opened, yielding 2D Chern insulators with opposite Chern numbers $-1$ and $+1$ for $k_z < 0$ and $k_z > 0$ because the inversion symmetry along the $z$ axis is broken (Fig. 1(c)). Note here the 2D Chern number is always defined by the upper band that is fully gapped except at $k = 0$. The 2D Chern number is integrated over the 2D infinite plane $\mathbb{R}^2$ in momentum space at constant $k_z$ and is quantized in continuous limit (see SM [30] for a proof). The lower non-zero band transitions from real to imaginary eigenenergies along an exceptional ring with coalesced eigenstates (the green circle in Fig. 1(c)). Such an exceptional ring at finite $k_z$ shrinks to a point at $k = 0$, resulting in a 3D exceptional cone with the cone vertex at $k = 0$ (Fig. 1(d)).

The origin $k = 0$ is a TDP with linear band dispersions (Fig. 1(b) and [30]), which, for the lower band, can appear in either real or imaginary spectrum along different momentum directions. Such a non-Hermitian TDP is quite different from the real TDPs in electronic and cold atomic Hermitian systems [31–33]. At $k_z = 0$, the band gaps for 2D Chern insulators close, yielding a topological charge $C = +2$ of the TDP that is equivalent to the change of 2D Chern number across $k_z = 0$. Here the topological charge is evaluated on a closed surface $S^2$ enclosing $k = 0$. Because there is only one charge $+2$ TDP in the HMM due to its continuous translational symmetry, there should be surface states connecting the TDP to infinity. We consider an open boundary condition along the $y$ direction with a semi-infinite HMM in $y < 0$ and the vacuum (i.e., $\mu_y = \epsilon_v = I$) at $y > 0$, and the surface state is solved as Dyakonov wave [40]. Within the scope of this work, we find that the surface wave only has real energy despite the complex bulk spectrum. The obtained surface states in the $k_x$-$k_z$ plane connect two bulk bands and vanish at the TDP. Because the band gap appears at different $\omega$ regions for different $k_z$, the commonly used surface spectral density at a fixed $\omega$ is not good for describing the surface states of continuous HMMs. For a fixed $k_z \neq 0$, the chiral edge states propagate along opposite directions (i.e., opposite velocities $d\omega/dk_z$) for $k_z > 0$ and $k_z < 0$ (Fig. 2(a)) because of their opposite bulk Chern numbers of 2D insulators. Although the lower band is purely imaginary in part of the momentum space, the edge states only connect to purely real parts.

**Charge 0 TDP from gyromagnetic effects.** The degenerate line in Fig. 1(a) can also be gapped out by the gyromagnetic effect, leading to another type of TDP at $k = 0$. We consider the gyromagnetic effect that is induced by a magnetic field along the $z$ direction, which yields a pure imaginary non-diagonal term $\epsilon_{xy}$ ($\epsilon_{yz} = -\epsilon_{xy}$ to keep $\epsilon$ Hermitian). The resulting band structure is similar as Fig. (1b) (see Fig. (3b)). However, the Chern numbers for 2D bands in the $k_x$-$k_y$ plane are $+1$ for both $k_z > 0$ and $k_z < 0$ because the magnetic field along the $z$ direction, although breaks the time-reversal symmetry, still preserves the inversion symmetry along the $z$ axis. The Chern number changes sign with the sign of $\epsilon_{xy}$, i.e., $\text{sign}(\Im(\epsilon_{xy}))$ (3 takes the imaginary part). Although the band topology does not change across $k_z = 0$, the band gap still closes, leading a topological TDP at $k = 0$ with charge $0$ due to opposite Berry flux for $k_z > 0$ [30].

Because of the same topology, the edge states for $k_z > 0$ and $k_z < 0$ propagate along the same direction (Figs. 2(b),3(b)). We see for a given $k_x$ and $\omega$ at the edge, there could be two surface states with opposite $k_z$. In Fig. 2(c), we show these two edge modes along $k_z$ for a fixed $k_x$, which start from the lower band and gradually approach the upper band. As a comparison, there may be only one edge mode along $k_z$ for a fixed large $k_x$ with the chiral effect [30]. Such double edge modes originate from topologically trivial 2D bands in the $k_y$-$k_z$ plane for a fixed $k_x$, which gives zero or even numbers of edge modes with opposite chirality.

We remark that when both gyromagnetic and chiral effects are considered, their competition would drive a transition between charge-2 and charge-0 TDPs. An example is shown explicitly in SM [30].

**Bulk-edge correspondence with vacuum bands.** Unlike electronic materials, vacuum is not an insulator for photons and there exist photonic bands for vacuum (although topologically trivial), i.e., the free space continu-
Simulation results are shown in Fig. 4. In panel (a), vacuum and bulk bands, respectively (Fig. 3(a)). The dashed green curve is the vacuum band, which is two-fold degenerate. Two dashed curves (from top to bottom) give the frequencies of the line source in COMSOL simulations shown in Fig. 4(c,a).

(b,c) 3D band structures with edge states for $\epsilon_{xy} = 2i$ and $\epsilon_{xy} = 3.5i$, respectively. The red surfaces represent chiral surface waves and the green one is the vacuum band.

Because of its direct contact with the edges of HMMs, vacuum effects should be taken into account for edge states and bulk-edge correspondence. Here we illustrate the vacuum effects using gyromagnetic effects. For a small $\epsilon_{xy}$ term, the vacuum band is higher than both bulk bands of the HMM (the vacuum band was not shown in Fig. 2(b,c) for this reason). With increasing $|\epsilon_{xy}|$, the band gap between the two non-zero bulk bands increases and the upper band would surpass the vacuum bands at a certain value of $|\epsilon_{xy}|$, after which the edge mode connects to the vacuum band, instead of the upper band, as shown in Fig. 3(a). This is because photons cannot localize at the boundary of the HMM after they diffuse into vacuum. Since the vacuum band is topologically trivial, the physical properties of the surface waves like chirality are preserved.

In Fig. 3(b,c), we plot the 3D band structures with edge modes for both weak ($\epsilon_{xy} = 2i$) and strong ($\epsilon_{xy} = 3.5i$) gyromagnetic effects in the $k_x$-$k_z$ plane, which show similar features as Figs. 2(b) and 3(a). Note that the vacuum band crosses ($k, \omega$ $= 0$ and does not intersect with the non-zero upper HMM band away from the TDP because both bands increase linearly with respect to $|k|$. The surface states, starting from the TDP, always fill the common gap between the lower HMM band and either the upper HMM or vacuum bands, depending on which has the lower energy. For a given $\epsilon_{xy}$, only one band (upper HMM band (Fig. 3(b)) or vacuum band (Fig. 3(c)) for weak and strong gyromagnetic effects, respectively) is connected by the surface states.

Numerical simulations. The above topological band properties and corresponding edge states in continuous HMMs can be further confirmed through COMSOL Multiphysics. Here we choose three different values of line source frequency $\omega_I = 0.9, 1$ and $1.45$, which correspond to band energies below the vacuum band, overlapping with the vacuum band, and overlapping with both the vacuum and bulk bands, respectively (Fig. 3(a)). The simulation results are shown in Fig. 4. In panel (a), when $\omega_I$ just lies below the vacuum band, the surface wave moves along the positive direction and is robust to any scattering process. When we increase $\omega_I$ a little bit so that it overlaps with the vacuum band, the surface wave is scattered into vacuum at defective points and source (panel (b)). If $\omega_I$ overlaps with both vacuum and bulk bands, as well as the gapless surface state, the electromagnetic waves diffuse into the entire space while the right side has a stronger field intensity (panel (c)). Finally, since the chirality of edge states is determined by sign$(3(\epsilon_{xy}))$, the surface wave indeed travels along the opposite direction when the gyromagnetic term is changed to an opposite sign in Fig. 4(d).

Here, we mainly concern the simulations with gyromagnetic terms while the chirality cases are studied in Supplementary Materials [30].

Discussions and conclusion. We have considered a HMM with hyperbolicity on the permittivity tensor, which, however, is not necessary for the existence of chiral surface wave. For instance, a HMM with $\epsilon = I$ and $(\mu_x > 0, \mu_y > 0, \mu_z < 0)$ may also exhibit chiral surface waves under proper time-reversal (or inversion) symmetry breaking. Besides $\epsilon_{xy}$, the gyromagnetic effects can also be generated by non-diagonal terms in $\mu$. Indeed, a purely imaginary $\mu_{xy}$ induces chiral surface waves in a similar way, which, however, becomes topologically trivial (gapless) upon passing the critical point $\Im(\mu_{xy}) = \pm \sqrt{\mu_x \mu_y}$ [30].

For experimental considerations, the chiral effects exist in a range of natural materials [41] while the advances of metamaterials allow us to synthesize strong chiral media [42]. To achieve gyromagnetic effects, magnetic materials can be mixed during fabrication and one commonly used material is Yttrium-Iron-Garnet [20].

The topological band theory described here can be applied to various parameter regions and many interesting effects, such as gain and loss [43], disorder, bian-
isotropy terms with more general $\gamma$ tensor, remain to be explored. The hyperbolic band dispersion of the topological HMMs opens a new avenue for studying negative refraction with topological edge states as well as topological lasing. In particular, the topological edge states in HMMs may be used to design a topological-semimetal laser. By tuning the structure of HMM and gyromagnetic/chiral field, the topological edge mode can be promoted to the lasing mode, rendering a highly efficient single-mode laser, which is robust to local disorders and defects. Note that although the bulk spectrum of HMMs could be complex, the topological edge spectrum is purely real. Thus it does not suffer from the inherent loss, which is the primary roadblock to the insertion of bulk HMMs into practical technologies. Because of the important and unique properties of HMMs like broad-band spontaneous emission enhancement (thus, the lasing threshold would be very small) and the ability to support propagations of large-momentum waves [2], the topological-semimetal laser may outperform recently emerged topological insulator laser using photonic crystals [44, 45].

In conclusion, we developed a topological band description for the non-Hermitian continuous HMMs and found two types of non-Hermitian photonic triply-degenerate points (classified by their topological charges) with different surface states. Our work should provide physical understanding of topological phases in HMMs and may inspire further theoretical and experimental investigations on the fundamental properties as well as practical applications of topological photonic continua.

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Here, we provide additional information about the imaginary band structure and the emergence of various nontrivial photonic band touchings including quadratic band touching, Dirac points and the non-Hermitian photonic TDP.

![Figure S1](image_url)

**FIG. S1:** (a) The degenerate line in Fig. 1(a) has a winding number 2 (solid light-blue line). The line splits into two (dashed light orange lines) in the \(k_y = 0\) plane for \((\epsilon_x, \epsilon_y, \epsilon_z) = (1, 4, -3)\), each of which has a winding number 1. (b,c) The distributions of Berry curvature on closed unit spheres containing charge-2 and charge-0 TDPs. We choose \((\epsilon_x, \epsilon_y, \epsilon_z) = (4, 4, -3)\). Two types of TDPs are induced by \(\gamma = \text{diag}(1, 0, 0)\) and \(\epsilon_{xy} = -\epsilon_{yx} = 2i\), respectively. (d) Similar as Fig. 2(a), but the edge states are calculated along the \(k_z\) direction with \(k_x = 1\) (dashed red curve) or \(k_x = -1\) (solid red curve).

As plotted in Fig. 1(a) in main text, the degenerate line has a winding number 2. In fact, when \(\epsilon_x > \epsilon_y\) (\(\epsilon_x < \epsilon_y\)), the single line splits into two degenerate lines, each carrying a winding \(W = 1\) in \(k_x = 0\) (\(k_y = 0\)) plane. These has been illustrated in the projected 2D plane in Fig. S1(a), where the corresponding winding number \(W\) has been labelled. Regardless of the number and the winding of the degenerate lines, they can be gapped out by either chiral or gyromagnetic effects, rendering two types of TDPs, whose topological charge distributions (Berry curvatures) are plotted in Fig. S1(b) and (c) respectively.

For the charge-2 TDP (Fig. S1(b)), four regions with outgoing Berry flux contribute significantly to the total Chern number while the Berry curvature in other regions is close to 0. For the charge-0 TDP (Fig. S1(c)), the Berry curvature is still significant in the four regions, but the outgoing Berry flux on the top half of the sphere cancels with the incoming flux on the bottom half, yielding zero net Berry flux, thus vanishing topological charge. Different from the charge-0 TDP, the 2D band topology for the charge-2 TDP is also non-trivial in the \(k_y\)-\(k_z\) plane (with fixed \(k_x \neq 0\)). For a large \(|k_x|\), we may only find one chiral surface wave at \(k_z = 1\) (\(k_z = -1\)) represented by the dashed (solid) red curve in Fig. S1(d).

![Figure S2](image_url)

**FIG. S2:** (a,b,c) The imaginary bands for Figs. 1(a,b,c) in the main text. (d,e) Two winding 1 degenerate lines and corresponding Dirac points at \(k_z = 1\) for the HMM with \((\epsilon_x, \epsilon_y, \epsilon_z) = (1, 4, -3)\). (f) The degenerate lines and Dirac points in (d,e) can be gapped by proper fields and two bands become topologically non-trivial.
In Fig. 1(a,b) in the main text, we show that the degenerate line can be lifted by the chirality term. The chiral effect only changes the real parts of the bands and leaves the imaginary parts unchanged, as shown in Fig. S2(a,b). The upper band (orange) is purely real (i.e., $\Im(\omega) = 0$) and the lower band changes from purely real to purely imaginary at two lines crossing the TDP. Fig. S2(c) shows the imaginary spectrum for Fig. 1 (c), where the upper band is purely real in the entire $k_x$-$k_y$ plane. For any finite $k_z$, the lower band changes from purely real to purely imaginary across an exceptional ring. The exceptional ring forms an exceptional degenerate cone in the 3D momentum space (see Fig. 1(d) in main text and also Fig. S6), which does not prevent defining the band Chern number of the lower band as we will discuss later.

When the winding 2 degenerate line splits into two degenerate lines with winding number 1 (see Fig. S1(a)), the quadratic touching point splits into two charge-1 Dirac points as well, which are depicted in Fig. S2(e). Similarly, the two Dirac points can be gapped with either gyromagnetic or chirality effects (Fig. S2(f)), leading to a nontrivial phase in $k_z \neq 0$ plane.

So far we only plot the two relevant bands for simplicity. To better visualize the non-Hermitian TDP, we plot the full six bands for a chirality-induced charge-2 photonic TDP in Fig. S3. Clearly, the full bands, both real and imaginary parts, are symmetric to $\omega = 0$ as expected.

![Fig. S3](image)

**Fig. S3:** (a) and (b) Real and imaginary spectra in the $k_x$-$k_y$ plane with $k_y = 0$. (c) and (d) Real and imaginary spectra in the $k_x$-$k_y$ plane with $k_z = 0$. The parameters are $\epsilon = (4, 4, -3)$, $\mu = 1$ and $\gamma = (1, 0, 0)$.

We first consider the $k_y = 0$ plane and the real/imaginary spectra are plotted in Figs. S3(a,b). The top/bottom band is purely real and shows linear dispersions along arbitrary directions in the plane. The middle dispersive bands form a cone structure along $k_z/k_x$ in the real/imaginary part, which is distinct from the Hermitian TDPs in either electronic [32] or atomic [33] systems. Similar bands are observed at the $k_x = 0$ plane because the type-I HMM shows dielectric properties in both $x$ and $y$ directions.

For the $k_z = 0$ plane, the photonic TDP also mixes both real and imaginary bands, but does not show the cone structure. As shown in Figs. S3(c,d), the middle flat band is two-fold degenerate. For the top and bottom bands, each has a purely real and purely imaginary branches. All of them are linear along any direction in the $k_x$-$k_y$ plane.

**Band gap and quantization of Chern number**

As discussed in the previous section, there is a TDP locating at the origin with proper gyromagnetic/chiral fields. When $k_z$ deviates from 0, the degeneracy is lifted, which is essential for the non-trivial topology. However, we have not proven that the TDP is the only degeneracy along $k_z$.

We prove this by analytically finding the energy gap. We first consider the gyromagnetic case with non-zero $\epsilon_{xy} = ia_\epsilon$ and $\epsilon_{yx} = -ia_\epsilon$. Without loss of generality, we take $\epsilon_\epsilon = \epsilon_y > 0$ and $\epsilon_\epsilon < 0$ and find the gap size is proportional to $|k_z/\sqrt{a_\epsilon + \epsilon_\epsilon}|$. Similarly, we can find the band gap $k_z \sqrt{|\epsilon^2_\epsilon - \epsilon_\epsilon^2 + \sqrt{\epsilon^2_\epsilon (\epsilon^2_\epsilon - \epsilon_\epsilon^2)}}/(a^2_\epsilon - \epsilon_\epsilon \epsilon_\epsilon)$ for non-zero chiral effects along the $x$ direction $\gamma_x = a_\gamma > 0$. In both cases, the gaps are proportional to $|k_z|$ (linear dependence), therefore would not close at any finite $k_z$.

With a well-defined band gap, we can compute the topological invariant of each band. For a continuous system, the band Chern number can be quantized when the integration range goes to infinity in the momentum space. Here we first provide the numerical results to illustrate the quantization of Chern number. We consider the same case as Fig. 2(a) in the main text and compute the Chern number in different regimes as shown in Tab. S1. The integral range is set as $-k_{\text{max}} \leq k_x, k_y \leq k_{\text{max}}$ and we find that the Chern number indeed converges to a quantized number at sufficiently large $k_{\text{max}}$. By inspecting the distribution of Berry curvature, we find that the main contribution comes near the band gap opening point and the Berry curvature decreases exponentially at large momentum.
While the above numerics only suggest the convergence of Chern number, we can prove that Chern number is strictly quantized in certain cases. In order to show this, we need to prove that the Berry curvature vanishes at infinity, specifically, when \( k_z = k_{z,0} \) is a finite non-zero constant and \( k_x, k_y \to \infty \). It is mathematically challenging to solve the eigenmodes directly and also hard to get any insight due to the complex expressions. In order to circumvent this difficulty, we unitize the linear \( \mathbf{k} \) dependence to convert the eigenvalue problem at infinite momenta to finite momenta. To show how this procedure can be performed, we consider only right eigenvectors (left eigenvectors are similar) and rewrite the eigenvalue problem in cylindrical coordinate as

\[
H(k_r \cos \theta, k_r \sin \theta, k_{z,0})|\Psi\rangle = \omega|\Psi\rangle,
\]

where we do not write the \( \mathbf{k} \)-dependence of \(|\Psi\rangle\) or \( \omega \) explicitly. The cylindrical coordinate is defined by \( k_r = \sqrt{k_x^2 + k_y^2} \) and \( \tan \theta = k_y/k_x \). Due to the linearity of \( p(\mathbf{k}) \), we have \( p(k_r \cos \theta, k_r \sin \theta, k_{z,0}) = k_r p(\cos \theta, \sin \theta, k_{z,0}/k_r) \). The above equation can be rewritten as

\[
H(\cos \theta, \sin \theta, k_{z,0}/k_r)|\Psi\rangle = (\omega/k_r)|\Psi\rangle,
\]

which becomes

\[
H(\cos \theta, \sin \theta, 0)|\Psi\rangle = \omega_0|\Psi\rangle
\]

when \( k_r \to \infty \). Here \( \omega_0 = \lim_{k_r \to \infty} \omega(k_r) \) is a constant since \( \omega(k_r) \) must grow linearly when \( k_r \) is sufficiently large. Since the problem for infinite momentum is converted to one for finite momentum, every quantity can be computed exactly.

As an illustration, we consider an example with the following parameters: \( \epsilon_x = \epsilon_y = -\epsilon_z > 0 \), \( \epsilon_{xy} = -\epsilon_{yx} = i\chi \), \( \mu = \mu_0 \) and \( \gamma = 0 \). We only consider the case \( \chi^2 < \epsilon^2 \) so that the upper band \( \omega = \sqrt{\frac{\epsilon_x}{\mu_0}} \sqrt{\frac{\epsilon_x^2 + \epsilon_y^2}{\epsilon_z^2 - \chi^2}} \) is purely real and fully gapped from other bands. Note that, once we impose \( k_z = \cos \theta \) and \( k_y = \sin \theta \), the eigenfrequency \( \omega \) reduces to a constant \( \omega_0 = \sqrt{\frac{\epsilon_x}{\mu_0} \sqrt{\frac{\epsilon_x^2 + \epsilon_y^2}{\epsilon_z^2 - \chi^2}}} \) as in Eq. (5). The corresponding normalized right eigenvector is

\[
|\Psi(\theta)\rangle = \frac{1}{\epsilon_z^2 + \epsilon_x \mu_0 - \chi^2} \left( 0, 0, -\frac{k_x \epsilon_x}{\omega}, -\frac{k_x k_y (\epsilon_x^2 - \chi^2)}{k_x^2 + k_y^2}, \frac{k_x (\epsilon_z^2 - \chi^2)}{k_x^2 + k_y^2}, 0 \right)^T,
\]

which leads to vanishing Berry curvature

\[
\mathcal{R} = \langle \partial_{k_x} \Psi(\theta) | \partial_{k_y} \Psi(\theta) \rangle - \langle \partial_{k_y} \Psi(\theta) | \partial_{k_x} \Psi(\theta) \rangle = 0
\]

at any given momentum. This is equivalent to that the Berry curvature vanishes at infinity along any path on the \( k_x-k_y \) plane. In this sense, the \( \mathcal{R}^2 \) momentum space (at finite \( k_z \)) can be compactified into a sphere \( S^2 \), on which the topological classification is the same as that on a torus and the quantization of Chern number is guaranteed. Similar results can be drawn when we have gyromagnetic or chiral effects.

**Topological transitions between two types of TDP**

When the chiral and gyromagnetic effects coexist, the competition between them could drive a transition of the TDP between charge-2 and charge-0. In Fig. S4(a), we plot how the TDP charge changes as a function of the gyromagnetic term \( \epsilon_{xy} \) with fixed chiral term \( \gamma = \text{diag}(1, 0, 0) \). The transition is closely related to the 2D band topology in the \( k_x-k_y \) plane with a fixed \( k_z \). As we increase \( |\epsilon_{xy}| \) (consider \( \Im \epsilon_{xy} < 0 \)), the corresponding 2D Chern number remains unchanged for \( k_z < 0 \), but changes sign for \( k_z > 0 \) (\( k_z < 0 \)). At the transition point, the 2D band gap closes as shown in Figs. S4(b-d), leading to the appearance of degenerate lines in the \( k_z > 0 \) region.

---

TABLE S1: Convergence of Chern number of upper band when the integration range goes to large momentum. The system parameters are \((\epsilon_x, \epsilon_y, \epsilon_z) = (4, 4, -3)\), \( \mu = 1 \) and \( \gamma = \text{diag}(1, 0, 0) \). The Chern number is computed on a plane with constant \( k_z > 0 \).

| \( k_{\text{max}} \) | \( 3 \times 10^0 \) | \( 3 \times 10^1 \) | \( 3 \times 10^2 \) | \( 3 \times 10^3 \) | \( 3 \times 10^4 \) | \( 3 \times 10^5 \) | \( 3 \times 10^6 \) |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| \( C \)          | 0.963996        | 0.997366        | 0.999738        | 0.999974        | 0.999997        | 1.000000        | 1.000000        |
FIG. S4: (a) The charge of the TDP as a function of $\epsilon_{xy}$ with fixed $\gamma = \text{diag}(1,0,0)$. The TDP changes from charge 2 to charge 0 around $-\Im(\epsilon_{xy}) = 1.85$. (b-d) The 2D band structures in the $k_z = 1$ plane with $-\Im(\epsilon_{xy}) = 1, 1.85, 3$ respectively. Other parameters are $(\epsilon_x, \epsilon_y, \epsilon_z) = (4,4,-3), \mu = I$.

Chiral surface wave by chirality effects

With increasing chirality, the HMMs bands may also become higher than vacuum bands. Here we take $\gamma = \text{diag}(1.6,0,0)$ for simulations and the corresponding 2D band structure is plotted in Fig. S5(a).

FIG. S5: (a) Similar to Fig. 2(a) but with chirality $\gamma = \text{diag}(1.6,0,0)$. (b)-(d) COMSOL simulation results for panel (a) with $\omega_I = 0.6, 1, 1.1$ respectively. $k_z = 1$. (e) Similar as panel (b) but for $k_z = -1$.

We consider three different frequencies in COMSOL simulations, similar as those for gyromagnetic effects in the main text. $\omega_I = 0.6$ lies within the common gap and we observe the scattering-free chiral surface wave as shown in Fig. S5(b), whose direction is consistent with the prediction of band theory. As we increase $\omega_I$ to 1, the frequency cuts the vacuum band and the surface wave diffuses into vacuum at defects (Fig. S5(c)). $\omega_I = 1.1$ overlaps with both bulk and vacuum bands and there are no chiral surface waves (Fig. S5(d)). Since the chiral effects break inversion symmetry, the surface wave has opposite chirality at $k_z = -1$, which is also confirmed by the simulation results in Fig. S5(e).

Exceptional degeneracy of the lower band

As we discussed in the main text, away from $k = 0$, the upper band is fully separated from both the lower band and the zero-energy flat band, therefore its topology is well defined. However, the lower band may have zero energy solutions, which are degenerate with the zero-energy flat band in the momentum space. As shown in Fig. 1(c) and Fig. S2(e,f), the lower band (blue) would change from purely real to purely imaginary on an exceptional ring where it is degenerate with the zero energy flat band. Such an exceptional ring exists at any finite $k_z$ plane and thus forms an exceptional (degenerate) cone in the entire momentum space (see Fig. 1 (d) as well as Fig. S6).

To understand such degeneracy, we consider the HMMs without chiral or gyromagnetic effects. Without loss of generality, we consider the line in the $k_y = 0$ plane with a fixed $k_z$. As $k_x$ changes from 0 to $-\infty$, the polarization (linear) of the lower-band states rotates in an opposite direction with respect to the rotation of $k$ (see Fig. S6) due to the metal properties along the $z$ direction, which becomes parallel with $k$ at some critical $k_z$, leading to the zero energy solution through $\nabla \times E = 0$. As $k_x$ changes from 0 to $-\infty$, the lower-band eigenstates change continuously, even across the degenerate points. Therefore these degeneracies do not affect the quantization of the Chern number.

In the presence of chiral or gyromagnetic effects, the changes of the polarization are similar although it is no longer linear. As $k_x$ changes from 0 to $-\infty$, the polarization changes from left-handed (right-handed) elliptical polarization
FIG. S6: Illustration of the exceptional cones (see also Fig. 1 (d)) in the momentum space between the zero flat band and lower non-zero band. The arrows show the directions of the polarizations at different $k$, which become parallel with $k$ on the cone.

to right-handed (left-handed) elliptical polarization. At the degenerate point, the polarization is linear and parallel with $k$. Moreover, we also notice that Berry curvatures of the lower band mainly resides on the real-valued energy region.

**EFS theory: connection to band theory and its incompleteness**

In this subsection, we discuss how the EFS theory [11–13] relates to our topological band theory and why EFS is not suitable for studying topological properties, although it may happen to provide some correct predictions in certain parameter regimes. Finally, we will show a counterexample where the EFS theory gives misleading answers while the prediction of our band theory is correct.

First of all, in both frameworks, the edge states are the same physical states, which are solved from matching boundary condition of Maxwell’s equations along the open-boundary direction. Here we choose it to be the $y$ direction. The electric fields are solved from the master equation

$$ K \times \mu^{-1} K \times E + i\omega(K \times \mu^{-1}\gamma E + \gamma \mu^{-1} K \times E) + \omega^2(\epsilon - \gamma \mu^{-1}\gamma)E = 0, \quad (S8) $$

which can be easily derived from Maxwell’s equations and the constitutive relations listed in the main text.

The topological invariant used in the EFS theory is also Chern number. In general, there are three Chern numbers, corresponding to three EFSs (the middle one may disappear in certain cases, leaving only two EFSs). The middle EFS (Chern number $C_1$) is usually a simple closed 2-manifold while the other two EFSs ($C_2$) stretch to infinity, which are defined by the upper band and lower band in our band theory, respectively. When the middle one contains the origin $k = 0$, it simply gives the charge of the TDP. As a result, we expect to see $|C_1| = 2$ and $C_1 = 0$ for chirality and gyromagnetic effects, respectively. In addition, $|C_2| = 1$ since it should be identical to the 2D Chern number calculated by the real part of lower band in the $k_x$-$k_y$ plane with a fixed $k_z$. An example of EFSs with Chern number and edge states are plotted in Fig. S7(a).

In this sense, EFSs indeed capture certain information of band topology. However, they are insufficient to fully characterize topological properties of HMMs due to the lack of well-defined bulk-edge correspondence and their inability of describing topological phase transitions. In the band theory, we require a gapped band structure to define topological invariant on each band and the difference between band Chern numbers will give the number of edge modes (the Chern number must sum over all bands below Fermi surface for a fermionic system). Nevertheless, there is no direct connection between the number of chiral edge modes and Chern number of Fermi surfaces. Topological phase transitions are usually signaled by gap closing, while the EFS theory may not capture them due to the non-Hermitian nature of HMMs where the gap closing may happen in the complex plane.

Specifically, we find that when a large gyromagnetic effect is introduced via permeability, the band topology becomes trivial with a vanishing band gap. Consequently, there should be no chiral edge state according to our band theory, which is also confirmed by COMSOL simulations. However, the EFS theory still predicts the existence of topological edge states in such parameter region.

We start from a HMM with the permittivity tensor $(\epsilon_x, \epsilon_y, \epsilon_z) = (4, 4, -3)$ and permeability tensor $\mu = I$. The degeneracy in Fig. 1 (a,b) are lifted by the non-diagonal terms $\mu_{xy} = -\mu_{yx}$, which are both purely imaginary. As we indicated in the discussion section of the main text, there is a phase transition point $\mu_{xy} = i$, at which the permeability tensor is not invertible. Therefore we take $\mu_{xy} = 0.9i$ and $1.8i$ across the transition and show the EFSs in Fig. S7(a).
In both cases, the EFSs Chern numbers (from top to bottom) are calculated to be 1, 0 and −1. The corresponding edge state solutions are also plotted. The existence of non-vanishing Chern number suggests that the system should be topologically non-trivial for all $\mu_{xy}$.

For $\Im(\mu_{xy}) < 1$, the EFS theory actually gives the correct prediction (Fig. S7(a1)). However, for $\mu_{xy} = 1.8i$, the EFS theory does not give consistent results for different energies. Two examples with $\omega = 0.6$ and 1 are plotted in Fig. S7(a2,a3). In Fig. S7(a2), there exist two surface waves (one starts from the vacuum), which do not agree with the EFS Chern number and spoil the bulk-edge correspondence in the EFS theory. Furthermore, the results in Fig. 4(a3) for $\omega = 1$ may lead to the impression that it is a topologically non-trivial phase because the surface wave seems to match with the EFS Chern numbers. These types of results lead to incorrect conclusions drawn by authors of [13].

We investigate the same parameter region using the topological band theory. In Fig. S7(b1), we show the 2D band structure at $\mu_{xy} = 0.9i$ and $k_z = 1$, which is indeed topologically non-trivial. Nevertheless, as the gyromagnetic term passes the critical transition point, the band becomes gapless and the band Chern number cannot be defined. Consequently, the system must be trivial and there is no chiral surface wave anymore.

A natural question is why there is only one edge state solution in Fig. S7(a3), while two in Fig. S7(a2)? We explore this question through solving the 2D band structure and the corresponding surface waves with a fixed $\mu_{xy}$ but different $k_z = 1, 2$. The results are plotted in Figs. S7(b2,b3). In Fig. S7(b2), we see a surface wave starts from the vacuum band, inverts its chirality at certain $k_z$, then passes through the imaginary bands of the HMM, and finally approaches $\omega = 1$ at infinity. For $k_z = 2$ shown in panel S7(b3), the surface wave is split by the real bands of the HMM and the end of vertical one intersects with the dash line $\omega = 0.6$. This reveals that two solutions in Fig. S7(a2) actually correspond to one surface wave, which exhibits opposite chirality in different regions of the momentum space. Therefore the unidirectionality of surface wave is spoiled for $\mu_{xy} = 1.8i$. The COMSOL simulations also support such a conclusion, as shown in Fig. S7(c). From top to bottom, we show the total electric field strength at $\mu_{xy} = 0.9i, 1.1i$ and $1.8i$ respectively. Only the first one exhibits chiral surface wave while the remaining two are trivial because the edge states propagate along both directions like plasma surface wave.

Nevertheless, even the surface wave solutions are not taken into consideration, the EFS theory already does not work because it gives non-trivial topological invariants in a trivial region and does not capture the topological phase transition.