Bound states within the radiation continuum in diffraction gratings and the role of leaky modes

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Abstract

We discuss resonant states with diverging $Q$ factor within the radiation continuum based on the anomalous interaction of leaky guided modes and diffracted waves in suitably designed reflection gratings. We show that these trapped optical states can be understood within the framework of leaky-wave theory, which unveils their generation process and dynamics. Our findings reveal an interesting mechanism to realize embedded eigenstates in periodic structures, shedding light on their electromagnetic properties, and offering the possibility to quantitatively predict their occurrence and systematically design optimal structures that support them. The realization of extraordinary optical trapping in open structures may be important for applications that require strongly confined and enhanced fields and high selectivity in angle and frequency.

1. Introduction

In modern science and technology, the ability to confine light and realize optical states with large oscillation lifetime is of paramount importance in a variety of scenarios, such as for filtering, sensing, enhancement of light–matter interactions and long-range optical communications. When an open electromagnetic structure (e.g., an open cavity, or waveguide) is externally illuminated, the presence of highly confined modes often manifests itself in the form of narrow asymmetric resonances, i.e., Fano resonances [1], in the reflection, transmission or scattering spectra. One of the earliest observations of this response was in the spectrum of diffraction gratings, which may exhibit rapid intensity variations known as Wood’s anomalies (see, e.g., [2–4], and references therein). Interestingly, some of these anomalies have been shown to arise from the excitation of complex guided modes, i.e., leaky waves, supported by a periodic grating (see, e.g., [5, 6]), and their asymmetric Fano lineshape can be explained as the result of the interference between such discrete resonant states, corresponding to transverse resonances of the open wave-guiding structure, and the non-resonant reflection background. Although such resonant-type Wood’s anomalies typically have narrow bandwidths, their lifetime (or $Q$ factor) never truly diverges in conventional grating structures, indicating that the mode cannot be ideally confined. This behavior is expected because, if there exist radiation modes (i.e., outgoing plane waves) that fulfill phase matching with a mode of an open wave-guiding structure, such mode becomes leaky and gradually loses its energy in the form of free-space radiation, resulting in finite oscillation lifetime. In particular, transverse momentum matching with propagating plane waves in free space can be fulfilled when the mode, or one of its space harmonics, is a fast wave with phase constant $\beta < k_0$, where $k_0$ is the free-space wavenumber (in other words, when the mode lies within the radiation cone of the dispersion diagram). It is therefore interesting that recent theoretical and experimental investigations [7–16] have shown that specific geometries, e.g., double gratings [7] or photonic crystal slabs [8–13], can actually exhibit Fano scattering resonances with a diverging $Q$ factor, as the supported leaky mode becomes ideally uncoupled from free-space radiation, despite the presence of phase-matched outgoing waves. This effect results in ideal light confinement and the creation of a bound...
optical state within the continuum of radiation modes, also known as *embedded eigenstate* in analogy with similar anomalous states in quantum mechanics [17, 18]. From the physical standpoint, this phenomenon has been explained as the result of destructive interference among different radiation channels [7–16]. In this context, a rigorous treatment in terms of well-established leaky-wave concepts would be important to quantitatively predict the occurrence of such bound states in suitably designed structures, as well as to exploit them for practical applications [6]. In the following, we show that scattering resonances with diverging $Q$ factor can be supported by reflection gratings as an extreme form of Wood’s anomalies, due to the interaction and interference between leaky guided modes and diffracted waves of the periodic structure. Furthermore, we establish simple and general design guidelines to obtain trapped states in realistic grating structures, and we validate our theoretical predictions with numerical simulations.

### 2. Extraordinary optical trapping in diffraction gratings

To make our analysis as general as possible, not limited to a specific class of structures, we model a reflection grating as an impenetrable periodic surface reactance $X_{\text{z}}(z)$, as shown in figure 1(a), an approach originally adopted by Hessel and Oliner in [5] to demonstrate the guided-mode nature of resonant Wood’s anomalies. In other words, $-iX_{\text{z}}(z)$ represents the purely reactive input impedance looking toward the reflection grating (throughout the paper, we assume a time-harmonic dependence $e^{-i\omega t}$). This planar reactive surface is a useful idealization of a large variety of grating structures, including metallic gratings, periodically-grooved grounded dielectric gratings, etc. The diffraction from a periodically modulated reactance sheet can be calculated using a coupled-wave analysis, in which the periodic impedance function is represented as a Fourier series, and the field above the grating is expanded as a sum of spatial Floquet harmonics, as further discussed in the supplementary material. By applying the electromagnetic boundary condition on the impedance sheet, it is then possible to obtain a set of linear equations, conveniently written in matrix form as

$$Z I = V,$$

which can be solved for the amplitude of the different diffraction orders $I_n$ under a given excitation $V$ (see [5] and the supplementary material for details). Even though the illumination smoothly changes as a function of

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Figure 1. (a) Sketch of plane wave diffraction from a periodic reactance sheet modeling a reflection grating (in this model, $-iX_{\text{z}}(z)$ represents the purely reactive input impedance looking toward the reflection grating). (b) Intensity of the specular reflection from a sinusoidally modulated capacitive surface reactance, under TE plane-wave incidence, exhibiting both Rayleigh (dashed curves) and resonant Wood’s anomalies. Brighter colors correspond to higher intensities. Each diffraction order is allowed to propagate in the region below the corresponding dashed curve (the curve for the $n = -1$ order is above the considered wavelength range). The inset shows a detail of the plot corresponding to the black dashed box.

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3 Supplementary material is available online at stacks.iop.org/NJP/19/093011/mmedia.
angle and frequency, the diffraction amplitudes may exhibit rapid variations associated with two classes of Wood’s anomalies: (a) Rayleigh anomalies, occurring when a diffraction order emerges or disappears at grazing angles, i.e., when the transverse wavenumber of the diffracted wave vanishes:

\[
k_{x,n} = \sqrt{k_0^2 - (k_z + 2\pi n/d)^2} = 0,
\]

which corresponds to branch-point singularities on the complex plane of the longitudinal wavenumber \(k_z\) (\(d\) is the grating period); (b) resonant anomalies, occurring when a phase-matched diffraction order of the incident plane wave excites a guided complex mode (leaky wave with complex \(k_z\)) supported by the grating. These modes are source-free solutions of the boundary-value electromagnetic problem and, thereby, their dispersion relation can be obtained by requiring the matrix \(Z\) to be singular. Interestingly, for small values of periodic modulation, the roots of the determinant of \(Z\) can be interpreted as resonances of a transverse equivalent network, formed by the average surface reactance in parallel with the wave impedance for a given angle of incidence and polarization. For example, for TE plane-wave incidence, the approximate condition for resonant Wood’s anomalies reads [5]

\[
-iX_{0,s} + \omega\mu_0/k_{x,n} = 0,
\]

where \(\omega\) is the angular frequency, \(\mu_0\) the free-space permeability and \(X_{0,s}\) the zero order term in the Fourier expansion of the periodic reactance function. It should be stressed, however, that equation (3) only produces real values of \(k_z\), which—in the limit of small modulation—approximately indicate the location of the complex leaky poles on the \(k_z\) plane (essentially neglecting the radiation losses), and the position of the associated resonant anomalies. Instead, for larger values of modulation, as considered in the following, the complex roots of the determinant of \(Z\) need to be numerically evaluated to determine the actual location of the anomalies.

As a relevant example, consider a reflection grating characterized by a sinusoidally modulated surface impedance

\[
Z_s(z) = -iX_s\left(1 + M \cos \frac{2\pi z}{d}\right),
\]

with capacitive reactance \(X_s = -1.2/\mu_0\) and large modulation amplitude \(M = 0.9\) (\(\mu_0\) is the free-space impedance). The diffraction from such a surface can readily be analyzed with the method discussed above (see also supplementary material). The amplitude \(I_0\) of the zero order diffraction (specular reflection) as a function of relative wavelength and incidence angle is plotted in figure 1(b). First- and second-order Rayleigh anomalies are highlighted by dashed lines following equation (2). In addition, a much sharper intensity variation is noticeable near the red dashed line, not accounted for by the dispersion of Rayleigh anomalies. In fact, this is a resonant-type anomaly arising from the excitation of a leaky mode of the structure, which exhibits a typical asymmetric Fano lineshape when plotted as a function of frequency for fixed angle, or vice versa, as we discuss in the following. Most importantly, we observe that the Fano feature gets continuously sharper and sharper as the resonant anomaly approaches the Rayleigh line (inset of figure 1(b)), until it completely disappears when the two anomalies merge, as its \(Q\) factor diverges. This is the signature of a bound optical state, in which—similar to the embedded eigenstates observed in the recent literature [7–16]—radiation loss has disappeared even though the leaky mode lies well within the radiation cone and, thereby, there exist phase-matched outgoing waves.

In order to validate our analytical calculations and further elucidate the peculiar response of the grating, we numerically calculate the amplitude of the different diffraction orders using a commercial finite-element software. In particular, we study the diffraction from an impenetrable periodic reactance sheet, having the same properties as in figure 1, at two different relative wavelengths \(\lambda/d\), as indicated by the dashed arrows in the inset of figure 1(b), close to the value for which the \(Q\) factor is expected to diverge. The computed intensity of the first diffraction orders (up to \(n = \pm 3\)) are reported in figure 2(a), for \(\lambda/d = 0.5\). The specular reflectivity (blue curve) exhibits two marked anomalies, consistent with figure 1(b): (a) an asymmetric Fano resonance around 35°, which—due to energy balance—also influences the spectrum of the \(n = -1\) diffraction order (green curve) (two additional features of this type are visible around 27° and 70°, corresponding to other leaky guided modes weakly excited by the external illumination); (b) a peculiar kink around 30° corresponding to the Rayleigh anomaly at the emergence of the \(n = +1\) diffraction order (red curve). At this point, the derivative of the reflection spectrum is discontinuous, with infinite slope at the left of the kink, due to the vanishing square root in equation (2). As the wavelength is increased, the two anomalies shift towards smaller angles and tend to merge, while the \(Q\) factor of the Fano resonance rapidly grows. As an example, in figure 2(b) we show the numerically computed specular reflectivity around \(\lambda/d = 0.573\), corresponding to the top dashed arrow in the inset of figure 1(b). Consistent with our discussion in the previous paragraphs, the reflection indeed exhibits an extremely narrow asymmetric resonance, as the guided mode supported by the grating is almost completely uncoupled from free-space radiation. A small kink associated with the Rayleigh anomaly is still visible at the left of the resonance peak. Moreover, by changing the angle of incidence by a very small amount from the center of the Fano resonance (angle \(\theta_0\)), the field intensity distribution above the grating dramatically changes, as seen in the insets of figure 2(b). In particular, the fields are extremely enhanced at the Fano resonance, especially near the
grating surface, due to the excitation of a mode of the structure with very large lifetime, hence trapping a large amount of the impinging energy along the periodic structure.

3. Analysis of trapped states on the complex wavenumber plane

The observation of a diverging Q factor in the considered example suggests a general mechanism for the realization of extraordinary optical trapping within the continuum of radiation modes. In fact, such trapped state appears as an extreme form of Wood's anomaly sustained by a diffraction grating under specific conditions, which can be predicted within the framework of leaky-wave theory. As discussed in the previous section, the leaky modes supported by the periodic structure, which are responsible for the resonant anomalies, correspond to the zeros of the determinant $D(k_z)$ of the boundary-condition matrix $Z$ (see supplementary material (footnote 3) for details on the construction of the matrix). Since the zeros of $D(k_z)$ then become the poles of the diffraction amplitudes $I_n$ for a given excitation, according to equation (1), in the following we will refer to leaky zeros or leaky poles interchangeably. Such zeros/poles occur at complex values on the longitudinal-wavenumber $k_z$ plane, as their imaginary part represents the longitudinal attenuation of the mode due to energy leakage in the open half-space above the grating. The modal analysis in the complex plane is complicated by the fact that $D(k_z)$ is a multivalued function due to the square root in the relation between $k_z$ and $k$, leading to a multi-sheeted complex wavenumber plane (which is indeed the case for any open waveguiding structure, as discussed in [6, 19, 20]). Besides, periodicity implies that the number of Riemann sheets is actually finite, two for each space harmonic, which are accompanied by infinite branch cuts emanating from the branch points at $k_z = \pm k_0 - 2\pi n/d$. Interestingly, while in longitudinally homogeneous wave-guiding structures branch-point singularities mark the edges of the fast-wave region at $k_z = \pm k_0$ in periodic structures higher-order branch points fall within the radiation cone of the fundamental space harmonic, and their location can be controlled by suitably choosing the periodicity of the grating. It is also worth noting that only one of the infinite Riemann sheets complies with the radiation condition at infinity (decaying waves toward infinity) for all space harmonics. Intriguingly, forward-propagating leaky modes lie on sheets that do not respect the radiation condition; however, under certain conditions, they can accurately represent the radiation field in limited spatial regions, as extensively discussed in the literature (see, e.g., [6, 19, 20] and references therein).

Figure 2. (a), (b) Numerically computed diffraction intensity versus incidence angle, at a relative wavelength $\lambda/d = 0.5$ and (b) $\lambda/d = 0.573$, corresponding to the white dashed arrows in the inset of figure 1(b). Panel (b) shows a detail of the specular reflectivity over a very narrow angular range around the resonant anomaly. The insets show the steady-state electric field intensity distributions (on the same scale, normalized to the incident intensity), over one period of the periodic structure, at the center of the ultra-narrow Fano resonance (right) and at an angle slightly off-resonance (left).
Figure 3. (a) Four Riemann sheets of the multivalued function $D(k_z)$ (determinant of the boundary-condition matrix $Z$; see supplementary material) on the complex plane of the longitudinal wavenumber $k_z$, showing the branch point of the $n = +1$ diffraction order and, on the bottom (orange) Riemann sheet, a complex zero corresponding to a leaky mode (pole of the diffraction amplitudes). The real axis of the complex plane is marked by branch cuts emanating from infinite branch points, due to periodicity. The function $D(k_z)$ is plotted in logarithmic units. (b) Colliding trajectories of a leaky pole (red curve and dots) and a branch-point singularity (blue curve and dots) as the wavelength is increased. The plotted portion of complex plane is well within the radiation cone of the fundamental space harmonic (i.e., fast-wave region with $|\text{Re}[k_z]/k_0| < 1$). The behavior of the pole at longer wavelengths, after merging with the branch point, is discussed in the supplementary material (see footnote 5).

Figure 3(a) shows four Riemann sheets of the function $D(k_z)$ on a portion of the complex $k_z$ plane (within the fast-wave region, i.e., $|\text{Re}[k_z]| < k_0$), for the example considered in figure 1(b) at a relative wavelength $\lambda/d = 0.5$. A complex zero of the determinant, corresponding to a leaky mode, is visible on the bottom orange sheet, whereas all the sheets exhibit a marked peak along the real axis, which corresponds to the branch point singularity for the $n = +1$ diffraction order, which falls within the fast-wave region due to periodicity, according to equation (2). In addition, multiple branch cuts run along the real axis, emanating from the infinite branch points.

In order to better understand the generation of trapped states as the one observed in figures 1 and 2, it is relevant to study the evolution of leaky poles and branch points as a function of wavelength. Therefore, after having identified the correct Riemann sheet (corresponding to exponential growth in the transverse direction $x$ for the space harmonic of interest, consistent with the nature of forward-propagating leaky modes [6, 19, 20]), we calculate the trajectories of these singularities on the complex plane, which determine the dispersion of Rayleigh and resonant anomalies when the wave-guiding structure is externally illuminated. As seen in figure 3(b), when the wavelength is increased the branch point moves along the real axis towards the origin. The complex leaky pole, with wavenumber $k_z = \beta + i\alpha$, also moves towards lower values of propagation constant, following the branch point. At the same time, it gets closer and closer to the real axis, leading to reduced leakage, which explains the rapid growth of $Q$ factor of the Fano resonances observed in figures 1 and 2. Finally, the leaky pole lands on the real axis exactly at the branch point singularity, i.e., when the $n = +1$ diffraction order emerges at grazing angles (Rayleigh anomaly). In this limit, the leaky mode becomes completely decoupled from free-space radiation, as the fast space harmonic responsible for its leakage vanishes (in other words, the residue of the pole gradually vanishes as it gets closer and closer to the branch point, as shown in the supplementary material (see footnote 3)), leaving only the slow spatial harmonics, which do not radiate. This effect results in the creation of an ideally trapped optical state, existing within the radiation cone. Remarkably, as the leaky pole lands on the real axis, the $Q$ factor of the mode, given by $Q = \beta/2\alpha$, can truly diverge, despite the fact that the structure is electromagnetically open and phase matching can be fulfilled with propagating plane waves. From the point of view of the external excitation, this fact confirms the existence of Wood's anomalies with
unbounded $Q$ factor, in the form of merged Rayleigh and resonant anomalies in suitably designed diffraction gratings.

The above discussion elucidates the nature of the predicted embedded eigenstates in reflection gratings, which can be interpreted as colliding leaky poles and branch points, the latter being located in the radiation cone due to periodicity. In particular, this analysis reveals a new mechanism to obtain bound states within the radiation continuum in periodic structures. Our scheme is different compared to other periodic structures supporting trapped states reported in the literature (e.g., [7, 8]), in which only one space harmonic radiates at the frequency of the embedded eigenstate, and the reflection is purely specular. In addition, our analysis reveals general properties of trapped states, not limited to the specific examples considered in this paper. In particular, the presence of a different singularity within the radiation cone (e.g., a branch point) is a necessary condition for the existence of such embedded eigenstates. In fact, due to passivity, an individual leaky pole cannot exist on the real axis of the complex wavenumber plane, within the fast-wave region, otherwise the diffraction amplitudes $I_n$ would become infinite under finite plane-wave excitation, which is clearly an unphysical result if the structure is passive. Instead, when the complex leaky pole tends to become real as in figure 3(b), another singularity, i.e., a branch point or a scattering zero, needs to be present to cancel the effect of the pole when it finally lands on the real axis, hence respecting passivity. Given the generality of these considerations, we predict that a careful leaky-wave analysis of the structures supporting embedded eigenstates recently reported in the literature would reveal a similar mechanism to cancel the residue of the leaky pole as it becomes real.

Interestingly, given the analogy between leaky waves in open wave-guiding structures and radiation-damped oscillations in open cavities [21], similar considerations also apply to embedded eigenstates in three-dimensional bounded structures, such as spherical scatterers [14, 15]. In the problem of electromagnetic scattering from bounded structures, however, the complex plane of interest is the one of frequency (not of wavenumber in specific directions), which is characterized by a single sheet without branch point singularities. Nevertheless, it was independently shown in [14] and [15] that embedded eigenstates can exist also in this scenario. In fact, a complex pole, corresponding to a natural mode of oscillation (eigenmode) of the bounded open structure, may become real under certain conditions, leading to the realization of a localized optical state that is ideally confined, with diverging lifetime, despite being surrounded by compatible radiation modes (outgoing spherical waves). As discussed above, however, a real scattering pole would violate passivity, as it would imply infinite scattered energy. In fact, it was observed that the pole always lands on the real axis exactly on a scattering zero, which cancels the singularity in order to respect passivity, in direct analogy with the behavior described in this paper for open periodic structures.

4. Practical realization of trapped states in reflection gratings

In the previous sections, we based our analysis and considerations on an idealization of reflection gratings as planar surface reactances. As demonstrated above, this approach is very useful to investigate the properties of Wood’s anomalies and trapped states in a general fashion, not restricted to a specific class of gratings. To complete our study, in this section we demonstrate that trapped states within the radiation continuum can be implemented with realistic grating structures, and we show that their response is indeed consistent with the general principles discussed in the previous sections.

The first option to design a realistic reflection grating supporting trapped states is to directly implement the sinusoidal reactive surface, given by equation (4), that we considered above. This can be done, for instance, by printing an array of metallic strips over a grounded dielectric substrate, following the procedure developed in [22]. However, the generality of the analytical considerations presented above reveals that it is not necessary to implement exactly the reactance profile in equation (4) in order to realize the trapped states observed in figures 1–3. In fact, having elucidated the nature of these trapped states as colliding leaky poles and branch points, we can try to realize them in arbitrary grating structures. As a relevant example, we chose a dielectric grating with modulated ground plane (figure 4(a)) as a practical platform to implement a bound state within the radiation continuum.

As usually done, the guided modes supported by the structure—in the limit of vanishing modulation—are investigated by studying the resonances of the transverse equivalent network. In the considered case, this is simply a segment of transmission line closed by a short circuit (the grounded dielectric slab), connected to a semi-infinite line representing free space. By applying the transverse resonance method [6], the dispersion of the guided modes is then readily obtained. For example, for TE polarization, the dispersion relation reads

$$\frac{1}{\sqrt{k_0^2 - k_z^2}} - \frac{i}{\sqrt{\varepsilon_r k_0^2 - k_z^2}} \tan(t \sqrt{\varepsilon_r k_0^2 - k_z^2}) = 0,$$

(5)
where \( \varepsilon_r \) is the relative permittivity of the dielectric layer and \( t \) its thickness. In the unmodulated case, equation (5) predicts that all guided modes are bound, having real wavenumber with \( \text{Re} [k_z] > k_0 \) (slow waves). However, by introducing a periodic modulation, a mode may become leaky if the periodicity is designed such that at least one of its space harmonic falls within the radiation cone. Most importantly, by combining the dispersion of the fast space harmonics of a guided mode, derived from equation (5), with the dispersion of the branch-point singularities, \( k_s = \pm k_0 - 2\pi n/d \), we are able to design the characteristics of the dielectric grating, namely, permittivity, thickness and periodicity, such that a leaky mode terminates on a branch point within the radiation cone, at the frequency of interest. The properties of the designed grating are reported in the caption of figure 4 (the modulation profile considered in figure 4 is described in the supplementary material (see footnote 3)). The specific shape of the periodic modulation is not important, provided that the perturbation is sufficiently small not to drastically alter the wavenumber of the fundamental space harmonic predicted by equation (5) (for larger modulations the guiding properties of the grating need to be studied with full-wave analysis and numerical simulations, as done for example in [23, 24]). In particular, as depicted in figure 4(a), we choose a smooth modulation, without sharp discontinuities, in order to reduce the excitation of higher-order modes.

Figure 4 shows the numerically computed diffraction intensities versus incidence angle for the designed grating, at a relative wavelength \( \lambda_0/d = 0.59 \) close to value at which the leaky pole is expected to become real. Indeed, a sharp asymmetric resonance is clearly visible near the Rayleigh anomaly at the onset of the \( n = +1 \) diffraction order (around 24°), consistent with the response observed for the idealized grating in figure 2 and the related discussion. In addition, as shown in figure 4(c), the fields on the grating are particularly strong when the incidence angle falls at the center of the Fano resonance, about 10 dB higher than at nearby angles within a range of only one degree. This response further confirms that the designed realistic grating indeed supports a trapped state within the radiation continuum, whose properties can be predicted based on the general considerations presented in the previous sections.

5. Conclusions

In this paper, we have analytically demonstrated that extraordinary light trapping within the radiation continuum can be realized as an extreme form of Wood’s anomaly in diffraction gratings, based on the anomalous interaction of diffracted waves and leaky modes. In particular, we have shown that such trapped states can be interpreted as colliding leaky poles and branch points within the radiation cone, resulting in a mode completely decoupled from free-space radiation, which manifests itself in the diffraction spectrum as a Fano
resonance with diverging Q factor. Our findings unveil a new mechanism for the realization of bound states within the radiation continuum, and offer an appealing platform to predict and design trapped optical states in realistic diffraction gratings, as demonstrated by our numerical simulations. Moreover, the introduction of nonlinearities may further extend the reach of these concepts, by allowing self-trapping of energy into the non-radiating mode under an external excitation that is initially detuned from the trapped state [25]. We are currently working towards an experimental verification of the proposed concepts, which may pave the way for the application of trapped optical states in practical scenarios. On a more general note, our investigations show that leaky-wave concepts are particularly useful to unveil the anomalous physics of open wave-guiding systems, confirming the relevant role of well-established leaky-wave theory in modern science and technology.

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