Anomalous Dispersion Relations by Symmetry Breaking in Axially Uniform Waveguides

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We show that modes of axially uniform waveguides of arbitrary cross section can be made to have anomalous dispersion relations resulting from strong repulsion between two modes. When the axial wave vector k is 0, the two modes have different TE/TM symmetry and thus can be brought arbitrarily close to an accidental frequency degeneracy. For nonzero k, the symmetry is broken causing the modes to repel. When the modes are sufficiently close together this repulsion leads to unusual features such as extremely flattened dispersion relations, backward waves, zero group velocity for nonzero k, atypical divergence of the density of states, and nonzero group velocity at $k = 0$.

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Axially uniform (constant cross section) waveguides have been studied extensively for numerous applications, ranging from optical communications and integrated optics to microwave technology. Lateral confinement of light in waveguides is achieved either by total internal reflection (TIR) as in optical fibers [1], or by the use of a reflective cladding as in metallic waveguides [2], Bragg fibers [3–5], and photonic-crystal fibers [6] (see Fig. 1). Typically, the guided modes of TIR waveguides have dispersion relations $\omega(k)$, frequency versus wave number, that are monotonic curves lying between the light lines associated with the lowest and highest indices of refraction in the structure. On the other hand, reflective-cladding waveguides can have dispersion relations that start from the $k = 0$ axis, as shown in Fig. 1(a). Ordinarily, these modes start with zero group velocity and have monotonically increasing dispersion relations as well.

In this Letter, we show by analytical and numerical methods that reflective-cladding waveguides of arbitrary cross-sectional symmetry can be made to support modes with anomalous dispersion relations, Figs. 1(b)–1(d), that result from strong repulsion between a pair of modes in the vicinity of $k = 0$. We discuss unusual and counterintuitive consequences that include backward waves, a reversed Doppler shift, reversed Cherenkov radiation, atypical singularities in the density of states, and a longitudinal length scale determined purely by the transverse waveguide profile. The results are general because they have their origin in a reflection symmetry shared by all axially uniform waveguides.

Consider a lossless nondispersive isotropic dielectric that is uniform in the z direction: $\epsilon(x, y, z) = \epsilon(x, y)$. The continuous translational symmetry implies that the axial wave vector k is a conserved quantity and that the magnetic field of a mode has the form $\mathbf{H}_k(x, y)\, e^{i(kz-\omega t)}$. The dispersion relation $\omega(k)$ and the field profile $\mathbf{H}_k(x, y)$ are obtained from the eigenvalue equation $\boldsymbol{\Theta}_k \mathbf{H}_k = (\omega^2/c^2)\mathbf{H}_k$, where $\boldsymbol{\Theta}_k = (\boldsymbol{\nabla}_t + ik\hat{\mathbf{z}}) \times (\frac{1}{\epsilon}(\boldsymbol{\nabla}_t + ik\hat{\mathbf{z}}) \times\ )$ and $\boldsymbol{\nabla}_t = (\partial/\partial x)\hat{\mathbf{x}} + (\partial/\partial y)\hat{\mathbf{y}}$.

There are two spatial symmetries that all axially uniform waveguides possess: continuous translational symmetry in the z direction and reflection symmetry through the xy plane. In practice, typical waveguides might have additional symmetries such as rotations around the z axis or reflection into a vertical plane. We first consider waveguides with general nonsymmetric cross section and later deal with additional symmetries.

Let σ_h be the reflection in the transverse xy plane. The dielectric function $\epsilon(x, y, z)$ of a uniform waveguide is obviously symmetric under σ_h. However, the modes of

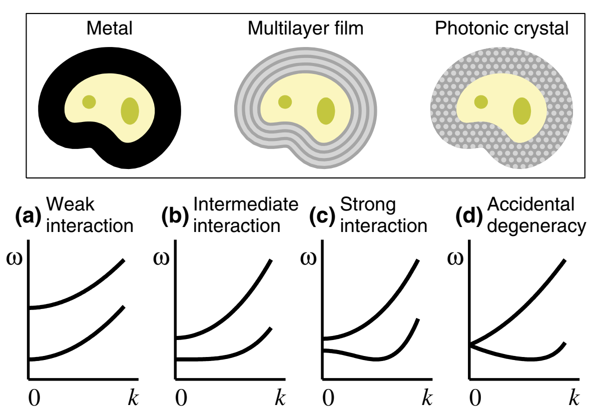

FIG. 1 (color). Top panel: Schematic drawings of the three types of reflective-cladding waveguides that employ metallic, multilayer-film, and photonic-crystal claddings. Bottom panel: Schematic band diagrams showing two neighboring modes as the relative frequency separation is decreased. At $k = 0$ one mode is TE polarized and the other TM polarized (the order is not important). (a) Weakly interacting modes. (b) A stronger interaction leads to a very flat lower band. (c) The repulsion between modes is strong enough to cause a backward wave region in the lower band. (d) Accidentally degenerate modes at $k = 0$ can have nonzero group velocity.

the waveguide are not generally symmetric under σ_h because the axial wave vector k breaks this symmetry. A special case exists for $k = 0$, when the operator $\boldsymbol{\Theta}_k$ still preserves the symmetry of ϵ. At $k = 0$, the modes have to be either even or odd with respect to σ_h. Even modes are said to have transverse electric (TE) polarization because their electric field is contained in the transverse plane; odd modes have transverse magnetic (TM) polarization. It is this symmetry that exists only at $k = 0$ that is responsible for effects presented in this Letter.

Consider now two neighboring TE and TM modes at $k = 0$, as shown in Fig. 1(a). The relative frequency separation between these two modes can be reduced by modifying the dielectric distribution $\epsilon(x, y)$. Because the orthogonality of these two modes at $k = 0$ is guaranteed by the TE/TM symmetry, it is generally possible to make the frequency separation arbitrarily small, as shown in Figs. 1(a)–1(d), including the possibility of creating an accidental degeneracy.

Let us now examine the two modes and their dispersion relations at wave vectors k larger than 0. $\boldsymbol{\Theta}_{k\neq 0}$ is no longer symmetric under reflection through the xy plane, and, since we are considering at this point only waveguides with general nonsymmetric cross section, $\boldsymbol{\Theta}_k$ has no remaining symmetry at $k \neq 0$. The two modes no longer have pure TE or TM polarization and now belong to the same irreducible representation. This leads to a repulsion between the two modes as seen in Fig. 1. The smaller the frequency separation at $k = 0$, the stronger the repulsion becomes.

Waveguides used in practice usually possess additional symmetries. For example, a circular waveguide has continuous rotational symmetry and is symmetric with respect to reflection across planes containing the z axis. In this case, in order to interact, the two modes must be chosen more carefully, such that at $k \neq 0$ the modes belong to the same irreducible representation. Thus, for the circular waveguide, the two modes must have the same angular quantum number. Concrete examples of strongly interacting modes will be given later.

We obtain quantitative results for the behavior of $\omega(k)$ in the vicinity of $k = 0$ by using perturbation theory for the eigenvalue equation for ω^2. We expand $\boldsymbol{\Theta}_k$ in powers of k, and we treat the linear and quadratic terms as perturbations. The approach is similar to the $\mathbf{k}\cdot\mathbf{p}$ method used for electronic band structures. However, the derivation is complicated by the vectorial nature of the electromagnetic eigenvalue problem. Because of the constraint $\nabla \cdot \mathbf{H}(\mathbf{r}) = 0$, the physical modes at $k = 0$ do not form a complete basis in which to expand the modes at $k \neq 0$. The correct perturbation theory in k for electromagnetism was derived recently by Sipe [7]. Since for a nondegenerate mode at $k = 0$ the group velocity is zero, we use second-order perturbation theory to evaluate the second derivative of $\omega_n(k)$ at $k = 0$:

$$\left(\frac{\partial^2\omega_n}{\partial k^2}\right)_{k=0} = \frac{c^2}{\omega_n}\int\left(|\mathbf{E}_t^{(n)}|^2 + \frac{1}{\epsilon}|\mathbf{H}_t^{(n)}|^2\right)dxdy + \frac{c^2}{\omega_n}\sum_{\ell\neq n}\frac{\omega_\ell^2}{\omega_n^2-\omega_\ell^2}\left(\left|\int \hat{\mathbf{z}}\cdot\mathbf{E}_t^{(n)^*}\times\mathbf{H}_t^{(\ell)}dxdy\right|^2 + \left|\int \hat{\mathbf{z}}\cdot\mathbf{E}_t^{(\ell)^*}\times\mathbf{H}_t^{(n)}dxdy\right|^2\right).$$

Here, the index ℓ is summed over all modes of the waveguide, except for the nth mode. The integrals are over the entire cross section. $\mathbf{E}_t^{(n)}$ stands for the transverse part of the normalized electric field for the nth mode at $k = 0$. The right-hand side has two contributions: (i) the first term contains only the field of the nth mode itself and is always positive; (ii) the second term represents the interaction of the mode of interest with the other modes of the waveguide. Contribution (ii) is negative for modes above the mode of interest ($\omega_\ell > \omega_n$) and positive for modes below the mode of interest ($\omega_\ell < \omega_n$). We interpret this term as a repulsion between modes, whose strength diverges as the frequency separation $\omega_n - \omega_\ell$ is taken to zero. Thus, although this term is relatively small for a typical waveguide, we can make it the dominant term by decreasing $\omega_n - \omega_\ell$. Also note that the interaction between two modes is nonzero only for modes of opposite TE/TM polarization.

The first unusual effect that results from the strong mode repulsion is the negative-slope region of the lower mode in Figs. 1(c) and 1(d). Modes for which $v_g = \partial\omega/\partial k$ and $v_\varphi = \omega/k$ have opposite signs are called "backward-wave" modes and were discovered in the context of dielectric-loaded circular metallic waveguides by Clarricoats and Waldron [8]. Based on empirical evidence, their existence has been associated with the near degeneracy of two modes of different polarization [9]. Below the minimum frequency of the backward wave mode there are evanescent modes (not shown in Fig. 1) for which k^2 is not real. The existence of these complex modes has been studied in [10–12]. We believe that this Letter provides the necessary physical intuition for understanding the existence of backward waves and complex modes in waveguides with arbitrary cross section.

We now discuss some remarkable effects based on backward waves. The momentum $\hbar k$ of a photon associated with a such a wave is negative, i.e., it is oriented in the opposite direction to the propagation of the photon. Imagine that an atom placed inside the waveguide absorbs a backward wave photon via an atomic transition. The recoil momentum points towards the direction from which the photon came, which means that negative radiation pressure is being exerted on the atom. Similarly the Doppler shift for light traveling in a backward wave is reversed. Finally, reversed Cherenkov radiation results from resonant radiation of a relativistic electron into a backward wave. While this effect has been discussed before in the context of periodically modulated structures [13,14] and for negative index media [15], it is notable that it can be also obtained in a simple axially uniform waveguide.

Another peculiar feature resulting from strong mode repulsion is the possibility of having zero group velocity at a nonzero value of the wave vector, as in Figs. 1(c) and 1(d). Let $k_0 \neq 0$ be the wave vector where $v_g = 0$. The $(k_0,\ \omega(k_0))$ point of the dispersion relation is qualitatively different from all other points and corresponds to a mode that does *not* transport energy but *does* have moving phase fronts. Moreover, the region of the dispersion relation between 0 and k_0 has all the characteristics of a band in the folded band structure of a medium that has periodicity $\Lambda = \pi/k_0$ in the axial direction — ironically, this longitudinal length scale Λ is determined only by the transverse dielectric profile. To some degree, then, this uniform waveguide behaves as if it had a periodic corrugation in the axial direction. For potential applications, we note that the pitch Λ of this virtual corrugation can be modified dramatically by simply tuning the transverse profile of the waveguide. Also, the flat region of the dispersion relation around the $(k_0,\ \omega(k_0))$ point could be very useful in the field of waveguide nonlinear optics, where a small group velocity enhances nonlinear effects by a factor of c/v_g while the phase-matching criterion can still be satisfied because the wave vector is nonzero.

Another unusual feature is found in Fig. 1(d) for small values of k. If the two interacting modes are exactly degenerate, their group velocities remain constant as $k \to 0$. We can thus have, in an axially uniform waveguide, a propagating mode that has almost no axial phase variation. In terms of practical applications, a regular mode in the neighborhood of $k = 0$ has very small group velocity and thus becomes unusable because both the dispersion and the losses scale inversely with v_g and thus diverge as we approach $k = 0$. The modes in Fig. 1(d) do not have this problem because v_g is roughly a constant in the vicinity of $k = 0$.

The density of states (DOS) associated with the lowest of the two interacting modes varies dramatically between the four situations depicted in Figs. 1(a)–1(d). The contribution of a mode to the DOS is inversely proportional to the group velocity $\partial\omega/\partial k$. More generally, at a singular point the type of Van Hove singularity [16] is determined by the first nonzero derivative of $\omega(k)$. A summary of possible behaviors is presented in Table I, in which the four rows correspond to the four situations shown in Fig. 1. Case (a) is the normal 1D divergence that is associated with the cutoff of a typical mode. In case (b) the mode repulsion is chosen to exactly cancel the second derivative of $\omega(k)$. Also, the third derivative is zero by time-reversal symmetry, which means the first nonzero derivative is $\partial^4\omega/\partial k^4$. This extremely flattened dispersion relation leads to a very strong divergence of the DOS, which could be useful in the design of low-threshold lasers. Also, it would modify the radiative behavior of atoms inside the waveguide [17]. Of course, the cancellation of the second derivative cannot be achieved exactly in experiment. However, it is enough to have a very small second derivative in order to get a very large enhancement of the DOS. In case (c), the second derivative has a negative sign. Also, we have an additional singularity in the DOS coming from the minimum of $\omega(k)$ at a nonzero k [see Fig. 1(c)]. Finally, case (d) corresponds to the accidental degeneracy at $k = 0$ of the two interacting modes. Because the group velocity is constant near $k = 0$, the contribution to the DOS coming from each of the modes is a Heaviside step function. The group velocities of the two modes are equal in magnitude, which means that the total contribution to the DOS is a constant. When the two modes are not exactly degenerate at $k = 0$ they each contribute a peak to the DOS. One can imagine making a waveguide in which the two modes can be tuned in and out of the degeneracy, thus turning on and off the two peaks in the DOS.

TABLE I. Possible Van Hove singularities in the density of states $D(\omega)$ corresponding to the lower mode in Figs. 1(a)–1(d).

	$(\frac{\partial\omega}{\partial k})_0$	$(\frac{\partial^2\omega}{\partial k^2})_0$	$(\frac{\partial^3\omega}{\partial k^3})_0$	$(\frac{\partial^4\omega}{\partial k^4})_0$	$D(\omega)$
(a)	$= 0$	> 0			$(\omega - \omega_0)^{-1/2}$
(b)	$= 0$	$= 0$	$= 0$	$\neq 0$	$(\omega - \omega_0)^{-3/4}$
(c)	$= 0$	< 0			$(\omega_0 - \omega)^{-1/2}$
(d)	$\neq 0$				const

As concrete examples of waveguides supporting modes with anomalous dispersion relations, we have performed numerical simulations for two all-dielectric waveguides as shown in Fig. 2. Both waveguide geometries should be experimentally realizable [4,6,18]. The actual parameters were chosen to exhibit Figs. 1(b) and 1(c) behavior.

The cylindrical Bragg waveguide in Fig. 2(a) confines light by means of a multilayered periodic cladding [4]. We calculate its modes using a transfer matrix approach [3]. We focus on two strongly repelling modes that have angular quantum number unity. At $k = 0$ the lower mode is TE polarized, and the upper mode is TM polarized. The lower mode has a negative group velocity from $k = 0$ to $k_0 = 0.172\,(2\pi c/a)$, with a minimum group velocity $v_g = -0.05c$. It also has a point of zero group velocity at the nonzero wave vector k_0.

In the photonic-crystal fiber [6] of Fig. 2(b) light is confined by the complete band gap of a triangular lattice of holes. The modes of the structure were computed using a freely available frequency-domain solver [19]. We start with the bulk 2D photonic crystal and create a standard core by removing the seven central unit cells [6]. The resulting hollow waveguide supports modes that are similar to those of a hollow metal cylinder. We choose the pair of modes that are analogous to the degenerate pair TE_{01} and TM_{11} of the metal waveguide. Here, they are not

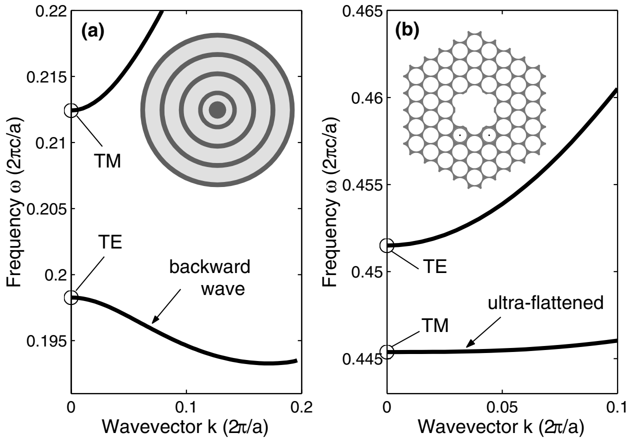

FIG. 2. (a) Dispersion relations of two modes with angular momentum unity for the cylindrical waveguide in the inset. The dark regions have an index of refraction 4.6 (e.g., Te), while the light gray regions have 1.4 (e.g., polymer). Starting from the center, the rod has a radius $0.45a$, the first ring has a thickness $0.32a$, the second one $0.23a$, and the following low/high index layers have thicknesses $0.75a/0.25a$, respectively. (b) Ultraflattened dispersion relation in a photonic-crystal fiber with an index of refraction of 3.5 (e.g., semiconductor). The distance between two neighboring air holes is a and the radius of a normal hole is $0.46a$. The two dotted holes below the fiber core have a modified radius of $0.40a$.

exactly degenerate but have a relatively small frequency separation, which is favorable for a strong mode interaction. However, these modes do not interact because they transform differently under a reflection symmetry across a plane containing the waveguide axis. To allow the modes to interact we break the C_{6v} symmetry of the waveguide by decreasing the radius of two holes below the waveguide core. Thus, we obtain the cross section and dispersion relations of Fig. 2(b). Although backward waves can be obtained here too, we instead choose a value for the radius of the two modified holes such that the lower mode has an extremely flat dispersion relation.

By using higher-order modes, waveguides with a smaller index of refraction contrast can also be made to have anomalous dispersion relations. Because the typical relative frequency separation for these modes is smaller, they require a smaller perturbation in order to be made nearly degenerate. Thus, the high-index component of the waveguide could be made of chalcogenide glasses [18] with an index of up to 2.8. Finally, note that even though the modes in Fig. 2 lie above the light line, if the repulsion is strong enough the anomalous nature of the modes can extend below the light line, leading to backward wave modes that are index guided.

We have shown that repulsion between a pair of modes can result from a reflection symmetry that exists at $k = 0$ and is broken for nonzero k. The strength of the repulsion diverges as the relative frequency separation of the modes is decreased to zero. Although this paper deals only with the band structure of axially uniform waveguides, similar effects should be attainable in more complex systems, such as 2D and 3D photonic crystals.

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