Semi-analytical approach to short-wavelength dispersion and modal properties of photonic crystal fibers

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We consider photonic crystal fibers made from arbitrary base materials and derive a unified semi-analytical approach for the dispersion and modal properties which applies to the short-wavelength regime. In particular we calculate the dispersion and the effective index and comparing to fully-vectorial plane wave simulations we find excellent agreement. We also calculate asymptotic results for the mode-field diameter and the V-parameter and from the latter we predict that the fibers are endlessly single mode for a normalized air-hole diameter smaller than 0.42, independently of the base material.

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Photonic crystal fibers (PCF) are dielectric optical fibers with an array of air holes running along the full length of the fiber. Typically, the fibers employ a single dielectric base material (with dielectric function $\varepsilon_b = n_b^2$) and historically silica has been the most common choice. Recently other base materials have been studied including chalcogenide glass, lead silicate glass, teluride glass, bismuth glass, silver halide, teflon, and plastics/polymers. The fabricated fibers typically share the same overall geometry with the air holes arranged in a triangular lattice and the core defect being formed by the removal of a single air-hole. Obviously, the scalar problem cannot be applied directly to generalize the results to other base materials. The reason is that PCFs made from different base materials do not relate to each other by a linear scaling of the dielectric function, $\varepsilon_b \gg 1$ so that the fraction of electrical field in the air holes is vanishing in the short-wavelength regime. The wave problem has now become scalar, but it should be emphasized that the approach is very different from the usual scalar treatment and recent applications to PCFs in the short-wavelength regime which take the electrical field in the air holes into account. Obviously, the scalar problem posed by Eq. (2) is separable and formally we have that

$$-\nabla^2 \mathbf{E}(\mathbf{r}) = \varepsilon_b \frac{\omega^2}{c^2} \mathbf{E}(\mathbf{r}),$$  \hspace{1cm} (2)$$

with the boundary condition that $\mathbf{E}$ is zero at the interfaces to the air holes. Since the displacement field $\mathbf{D} = \varepsilon \mathbf{E}$ is divergence free we have $0 = \varepsilon \nabla \cdot \mathbf{E} + \mathbf{E} \cdot \nabla \varepsilon \approx \varepsilon \nabla \cdot \mathbf{E}$. In the bulk matrix material the latter equality is exact and the wave equation reduces to

$$-\nabla^2 \mathbf{E}(\mathbf{r}) = \varepsilon \frac{\omega^2}{c^2} \mathbf{E}(\mathbf{r}),$$

which we solve with the boundary condition that $\mathbf{E}$ is zero at the interfaces to the air holes. For the boundary condition to be meaningful it is crucial that $\varepsilon_b \gg 1$ so that the fraction of electrical field in the air holes is vanishing in the short-wavelength regime. The wave problem has now become scalar, but it should be emphasized that the approach is very different from the usual scalar treatment and recent applications to PCFs in the short-wavelength regime which take the electrical field in the air holes into account. Obviously, the scalar problem posed by Eq. (2) is separable and formally we have that

$$\omega = \sqrt{\Omega_{xx} + \Omega_{zz}} = \frac{c}{n_b} \sqrt{\gamma^2 \Lambda^2 - 2 + \beta^2}$$  \hspace{1cm} (3)$$

where $\Omega_z = c\beta/n_b$ is the frequency associated with the longitudinal plane-wave propagation, $\Omega_{xy} = \gamma \times c \Lambda^{-1}/n_b$ is the frequency associated with the transverse confinement/localization, and $\gamma$ is a corresponding dimensionless and purely geometrical number, which only depends on the normalized air-hole diameter $d/\Lambda$. From Eq. (2) it follows that $\gamma$ is an eigenvalue governed by a scalar two-dimensional Schrödinger-like equation

$$-\Lambda^2 (\partial_x^2 + \partial_y^2) \psi(x, y) = \gamma^2 \psi(x, y),$$  \hspace{1cm} (4)$$

with the scalar function $\psi$ being subject to hard-wall boundary conditions at the interfaces to the air-holes, i.e., $\psi = 0$ in the air holes.

The developments in computational physics and engineering have turned numerical solutions of partial differential equations in the direction of a standard task.
For the core modes the problem has been truncated by considering a sufficiently large domain with Dirichlet boundary conditions which for symmetry reasons can be formulated in terms of Neumann conditions. As the normalized air-hole diameter $d/\Lambda$ is increased the localization becomes more tight and as expected the eigenvalue increases. For the fundamental core mode the dashed line shows a third-order polynomial,

$$\gamma_c^2 \simeq \mathcal{A} + \mathcal{B} \frac{d}{\Lambda} + \mathcal{C} \left( \frac{d}{\Lambda} \right)^2 + \mathcal{D} \left( \frac{d}{\Lambda} \right)^3,$$

with $\mathcal{A} = 2.67$, $\mathcal{B} = 12.51$, $\mathcal{C} = -9.45$, and $\mathcal{D} = 13.88$ being fitting parameters.

The recently proposed $V$-parameter $V_{\text{PCF}} \equiv \Lambda(\beta_c^2 - \beta_{cl}^2)^{1/2}$ becomes

$$\lim_{\lambda \ll \Lambda} V_{\text{PCF}} = \sqrt{\gamma_{cl}^2 - \gamma_c^2}$$

and the numerical results shown in Panel (B) agrees nicely with the short-wavelength asymptotic limit of recent simulations on silica-based PCFs. The endlessly single-mode regime defined by $V_{\text{PCF}} < \pi$ exists for $d/\Lambda \lesssim 0.42$ independently of the base material. For more detail on the modal cut-off see Ref. 8 and references therein. Panel (C) shows results for the effective mode-field radius $w_{\text{eff}}$ calculated from $A_{\text{eff}} \equiv \pi w_{\text{eff}}^2$ with the effective area given by

$$\lim_{\lambda \ll \Lambda} A_{\text{eff}} = \frac{\int \int |\psi(x,y)|^2 \int \int |\psi(x',y')|^2}{\int \int |\psi(x,y)|^4}.$$

Here, we employ a finite-element approach to numerically solve Eq. (4) and calculate $\gamma^2$ versus $d/\Lambda$. Panel (A) in Fig. 1 summarizes the results for the fundamental core mode (see inset in Fig. 2), the second-order core mode, and the fundamental cladding mode (see inset in Fig. 3). For the core modes the problem has been truncated by considering a sufficiently large domain with Dirichlet boundary conditions while for the cladding modes we have considered the unit-cell with periodic boundary conditions which for symmetry reasons can be formulated in terms of Neumann conditions. As the normalized air-hole diameter $d/\Lambda$ is increased the localization becomes more tight and as expected the eigenvalue increases. For the fundamental core mode the dashed line shows a third-order polynomial,

$$\gamma_c^2 \simeq \mathcal{A} + \mathcal{B} \frac{d}{\Lambda} + \mathcal{C} \left( \frac{d}{\Lambda} \right)^2 + \mathcal{D} \left( \frac{d}{\Lambda} \right)^3,$$

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$$\lim_{\lambda \ll \Lambda} A_{\text{eff}} = \frac{\int \int |\psi(x,y)|^2 \int \int |\psi(x',y')|^2}{\int \int |\psi(x,y)|^4}.$$
As expected the mode-field diameter decreases as the normalized air-hole diameter is increased and the mode becomes more localized. For \( V_{PCF} = \pi \) we find that \( w_{eff}/\Lambda \approx 0.627 \).

With Eqs. (8) and (11) at hand we have now provided a unified theory of the dispersion relation in the short-wavelength regime for PCFs with arbitrary base materials and Eq. (8) illustrates how geometrical confinement modifies the linear free-space dispersion relation.

In fiber optics it is common to express the dispersion properties in terms of the effective index \( n_{eff} = c\beta/\omega \) versus the free-space wavelength \( \lambda = c2\pi/\omega \). From Eq. (8) it follows straightforwardly that

\[
n_{eff} = n_b \sqrt{1 - \frac{\gamma^2}{4\pi^2 n_b^2} \left( \frac{\Lambda}{\lambda} \right)^2} \tag{8}
\]

which obviously is in qualitative agreement with the accepted view that \( n_{eff} \) increases monotonously with decreasing wavelength and approaches \( n_b \) in the asymptotic short-wavelength limit as reported for e.g. silica-based PCFs. However, how good is the quantitative agreement for different base materials? In Figs. 2 and 3 we employ fully-vectorial plane-wave simulations\(^\text{11}\) to compare Eq. (1) with the predictions of Eq. (8) for the fundamental core and cladding modes, respectively. For the core-modes we have employed a sufficiently large super-cell configuration. As seen there is an over-all good agreement between the fully-vectorial numerical results from Eq. (1) and the semi-analytical predictions of Eq. (8). In the short-wavelength limit \( \lambda \ll \Lambda \) the agreement is excellent, which underlines the high relevance of the present results to large-mode area PCFs. As the index of the base material is increased the agreement is even better (results not shown). As the wavelength \( \lambda \) is increased and becomes comparable to the pitch \( \Lambda \) the quantitative agreement is less good. The reason is well-known from small-core silica-based PCFs where a non-negligible fraction of the electrical field is forced to reside in the air-hole regions and where also vectorial effects of Eq. (1) start to matter.

In conclusion we have shown how a unified description of the short-wavelength dispersion and modal properties is possible. The theory illustrates how the waveguide dispersion originates from the geometrical transverse localization of the mode and the semi-analytical description of the short-wavelength properties is readily applied to PCFs made from any base material.

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