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Designing for beam propagation in periodic and nonperiodic photonic nanostructures: extended Hamiltonian method

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The possibility of radical dispersion in periodic photonic nanostructures has recently generated much interest. However, for applications such as group velocity dispersion compensation and frequency demultiplexing, periodic structures arguably do not offer enough design freedom to achieve the desired input/output dispersion relation over large frequency ranges. In such cases, non-periodic structures could perform much better than periodic structures [1, 2]. One expects that introducing non-uniformities in 2-D and 3-D periodic structures will also allow better control of the device input/output dispersion relations over wider frequency ranges. However, there has been much less study of 2-D and 3-D non-uniform structures due to the difficulty in analyzing them. Hamiltonian optics offers one approach for nonuniform structures, at least for predicting beam paths [3]. In this work, we remove simplifications used previously in [3] and use Hamiltonian optics to design and analyze beam propagation in 2-D periodic structures with slowly varying non-uniformities. Furthermore, we extend the Hamiltonian optics method to analyze the width of a beam propagating in such structures; without such an understanding of beam width and its distortion in periodic and nonperiodic photonic nanostructures, practical design would be very limited. We validate our method with Finite Difference Time Domain (FDTD) simulations, and design a 2-D non-uniform structure that functions as a flat-top frequency demultiplexing device that steers beams in two different frequency ranges to two different locations.

Hamiltonian optics has traditionally been used to describe the optical ray path in a slowly varying dielectric medium [4]. Let $\boldsymbol{X}(\tau)$ and $\boldsymbol{K}(\tau)$ denote the optical beam path in space and the average wavevector along the beam path respectively, where τ is a parameter that varies continuously and monotonically along the beam path. Then the Hamiltonian equations governing the evolution of $\boldsymbol{X}(\tau)$ and $\boldsymbol{K}(\tau)$ are [4]:

$$\frac{d\mathbf{X}}{d\tau}=\frac{\partial H}{\partial \mathbf{k}},\quad \frac{d\mathbf{K}}{d\tau}=\frac{\partial H}{\partial \mathbf{x}},\quad H(\mathbf{x},\mathbf{k})=0, \qquad (1)$$

where $\boldsymbol{x}$ and $\boldsymbol{k}$ are the position vector and the wavevector respectively. For a given $\boldsymbol{x}$, the Hamiltonian H is the dispersion relation minus the frequency. For Eq. 1 to be valid, the characteristic length for the nonuniformities needs to be substantially larger than the actual beam width, and the beam width needs to be substantially larger than the wavelength. With a wavelength around 1.5 μm, we expect to work with devices roughly 150 μm in size, consistent with this approach. At each location in the structure, a local H can be obtained by Bloch wave analysis. With H defined, beam propagation in the structure can be analyzed using the Eq. 1, without the need for time consuming FDTD simulations.

We use the Hamiltonian equations to design a frequency demultiplexing device. The basic structure is a 200 by 200 square lattice of high index rods (n=2.54) in low index background (n=1.56). The gradual non-uniformity in the rod radius steers six beams, equally spaced in frequency, from a single input location on the left side of the structure, to two output locations on the bottom side of the structure, with three beams exiting at each location (Fig. 1). To track the beam path with Eq. 1, the partial derivatives of H need to be calculated. The accuracy of H is important when we actually need to design a device. Therefore, instead of the closed form approximate H used in [3], we calculate H using the iterative eigenmode solver MIT Photonic-Bands package (MPB) [5]. Hundreds of plane wave basis functions are included, rather than the 4 plane wave basis used in [3]. The more accurate calculation comes at the cost of losing the analytical model for H. But, the computational cost of solving Eq. 1 numerically is still insignificant compared to FDTD calculations.

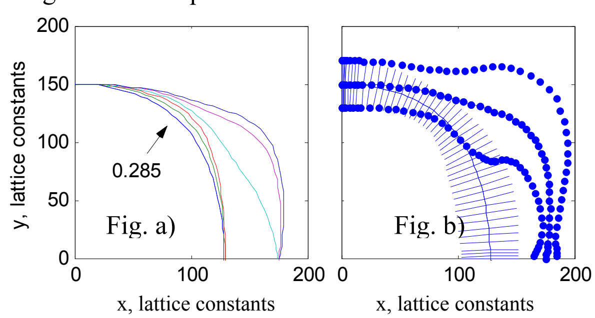

Figure 1. Frequency demultiplexing structure. a) Beam path (Eq. 1) for six frequencies (ωa/c) from 0.28 to 0.285; b) Beam width profile for ωa/c=0.285 (profile of the fence) and ωa/c=0.28 (profile of the 3 dotted lines).

To steer the beams to the desired exit locations, we start with an initial guess for the rod radius distribution $\rho(\boldsymbol{x})$, $\rho(\boldsymbol{x})=a(x^2+y^2)$. The path of the beam with the highest frequency is calculated using Eq. 1, and the coefficient a is optimized until the beam exits at the desired location. Next, on one side of the 1st beam path, $\rho(\boldsymbol{x})$ is varied as a cubic function of $d(\boldsymbol{x})$, where $d(\boldsymbol{x})$ is the shortest distance of each rod to the first beam path. The cubic function is scaled until the 2nd beam exits at the desired location, with the beam path again calculated with Eq. 1. The cubic variation ensures that the path and the width of the 1st beam are not changed in the optimization for the 2nd beam. The optimization process is repeated for the rest of the frequencies sequentially. The final $\rho(\boldsymbol{x})$ directs the six beams to the desired exit locations (Fig. 1a). The decoupling of the design process for different frequencies relies on the spatial separation of the six beams in the device, and is a unique advantage of 2-D devices over 1-D devices.

The iterative process of changing $\rho(\boldsymbol{x})$ and solving for the beam path using (1) takes 10 minutes on a Pentium 4 computer. The FDTD simulation of the beam propagation for a specific $\rho(\boldsymbol{x})$ takes many days on the same machine. Optimizing $\rho(\boldsymbol{x})$ by running an FDTD simulation multiple times would be prohibitively expensive computationally.

We extend the Hamiltonian optics method with equations for the beam width and the radius of curvature in periodic structures with slowly varying non-uniformities. To the best of our knowledge, beam width equations have not previously been proposed for periodic nanostructures. We follow the extension of Hamiltonian optics developed by Poli et. al. [6] for plasmas. Assume a monochromatic field has the form $\boldsymbol{A}(\boldsymbol{x})\exp(-\phi(\boldsymbol{x})+is(\boldsymbol{x}))$. If we expand the complex phase $s(\boldsymbol{x})+i\phi(\boldsymbol{x})$ up to the 2nd order around the beam path, the 2nd derivatives of $s(\boldsymbol{x})$ and $\phi(\boldsymbol{x})$ will give the beam width $W_\alpha(\boldsymbol{x})$, and the radius of curvature $R_\alpha(\boldsymbol{x})$:

$$\frac{\partial^2 s}{\partial\alpha^2} \equiv s_{\alpha\alpha} = \frac{\omega}{cR_\alpha}, \quad \frac{\partial^2 \phi}{\partial\alpha^2} \equiv \phi_{\alpha\alpha} = \frac{2}{W_\alpha^2} \qquad (2)$$

where α is the space coordinate x or y. By substituting the assumed form of the field into Maxwell's equation, ordinary differential equations for the 2nd derivatives of $s(\boldsymbol{x})$ and $\phi(\boldsymbol{x})$ along the beam path are obtained [6]:

$$\frac{ds_{\alpha\beta}}{d\tau} = -\frac{\partial^2 H}{\partial x_\alpha \partial x_\beta} - \frac{\partial^2 H}{\partial x_\beta \partial k_\gamma} s_{\alpha\gamma} - \frac{\partial^2 H}{\partial x_\alpha \partial k_\gamma} s_{\beta\gamma} \qquad (3)$$
$$- \frac{\partial^2 H}{\partial k_\gamma \partial k_\delta} s_{\alpha\gamma} s_{\beta\delta} + \frac{\partial^2 H}{\partial k_\gamma \partial k_\delta} \phi_{\alpha\gamma}\phi_{\beta\delta},$$
$$\frac{d\phi_{\alpha\beta}}{d\tau} = -\left(\frac{\partial^2 H}{\partial x_\alpha \partial k_\gamma} + \frac{\partial^2 H}{\partial k_\gamma \partial k_\delta} s_{\alpha\delta}\right)\phi_{\beta\gamma} - \left(\frac{\partial^2 H}{\partial x_\beta \partial k_\gamma} + \frac{\partial^2 H}{\partial k_\gamma \partial k_\delta} s_{\beta\delta}\right)\phi_{\alpha\gamma}$$

For homogenous media, Eq. 3 reduces to equations for beam width and the radius of curvature of a freely propagating Gaussian beam. For the periodic medium with non-uniformity in our example, Eq. 3 can be solved numerically. We evaluated the 2nd derivatives of H numerically using H calculated from MPB. Fig. 1b shows the beam width calculated for two beams, and verifies that the two chosen output locations are far enough apart. Both beams have a flat phase front at the input and would diverge in vacuum. But, as shown in Fig. 1b, Eq. 3 predicts the beams narrow at some points because the curvature in $\rho(\boldsymbol{x})$ acts like a lens.

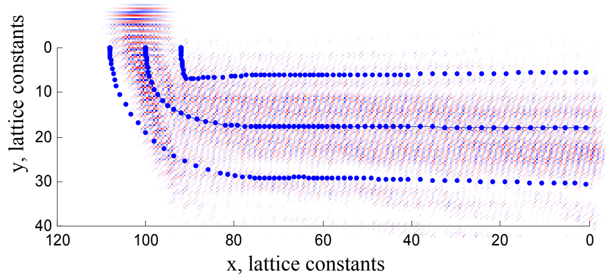

Figure 2. Comparison of the extended Hamiltonian method with FDTD simulation. The center dotted line is the beam path, the dotted lines on each side show the beam width as calculated using Equ. 3. The underlying shading shows the intensity of the e-field from FDTD.

We verify the validity of the proposed extended Hamiltonian method with the FDTD simulation of a smaller structure (100x50 lattice constants) of the same lattice type and index contrast, with a deliberately extremely abrupt beam curvature. The nonuniformity in the lattice causes a beam entering from the upper left corner to turn 90 degrees. The beam path and beam width calculated with Eq. 1 and Eq 3 are plotted over the FDTD simulation results in Fig. 2. 2-D FDTD method with perfectly matched layer boundary conditions [7] is used in the simulation. The two methods are in fairly good agreement. The beam width is under-estimated by our method due to the large nonuniformity of this extreme structure, which challenges the slowly varying approximation.

In summary, we have demonstrated the use of the Hamiltonian optics to design a flat-top frequency demultiplexing device, using an accurately calculated Hamiltonian. We have introduced a set of ordinary differential equations for tracking the beam width in periodic nanostructures with nonuniformities, and confirmed the validity of the equations with FDTD simulations. With Eq. 3, much more can be said about beam propagation in such structures than with Hamiltonian equations alone. We believe this method will enable the quantitative design and analysis of useful devices such as frequency demultiplexers, beam steering devices, and wavelength dependent (e.g., gas) sensors, without resorting to FDTD simulations.

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