

Effective field theory for the nonlinear optical properties of photonic crystalsJ. E. Sipe,¹ Navin A. R. Bhat,¹ Philip Chak,¹ and Suresh Pereira²¹*Department of Physics, University of Toronto, Toronto, Ontario, Canada M5S 1A7*²*Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe, Germany*

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We introduce an effective field theory for the nonlinear optics of photonic crystals of arbitrary dimensionality. Based on a canonical Hamiltonian formulation of Maxwell's equations, canonical effective fields are introduced to describe the electromagnetic field. Conserved quantities are easily constructed and their physical significance identified; the formalism can be easily quantized. We illustrate the approach by considering a periodic Kerr medium, and show how the nonlinear coupled mode and nonlinear Schrödinger equations emerge. We extend the latter to treat optical shock effects, and compare our canonical formulation with earlier treatments.

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I. INTRODUCTION

Current computing capabilities allow for the direct simulation of propagation problems in optics at a level that would have been unthinkable only a few years ago. In particular, calculations of nonlinear optical propagation in photonic crystals and other artificially structured materials by the direct numerical solution of Maxwell's equations are now feasible. And so it becomes even more important now to seek out characterizations of such numerical solutions that allow for their general understanding, and especially for the identification of material and geometric parameters that determine their qualitative nature. This is often done by examining the solutions of approximate equations that describe the electromagnetic field.

The usual approach for uniform media, and materials with weak variations in their linear optical properties, is to construct approximate equations for slowly varying envelope functions that modulate plane waves at a carrier frequency and wave vector [1,2]. In these simple structures, the nonlinear Schrödinger equation (NLSE) has been shown to provide a good description of nonlinear propagation away from a band gap, or within a band gap but at frequencies close to one of the band edges [3], and the nonlinear coupled mode equations (NLCME) serve as a basis for understanding propagation near and even deep within a band gap [4,5].

In other artificially structured materials, such as higher dimensional photonic crystals, there are typically large variations in the linear optical properties of the structure over distances of the order of a wavelength of light. The usual heuristic derivations that lead to the NLSE and NLCME equations here become suspect. Indeed, the approximation that the electromagnetic field can be described by one or a small set of slowly modulated plane waves is clearly physical nonsense. Yet an approach not unlike the heuristic one is possible. The strategy for a photonic crystal is to use slowly varying envelope functions to modulate Bloch waves—i.e., exact solutions of the linear problem—rather than plane waves, and then seek equations for those envelope functions. In the appropriate frequency regimes nonlinear Schrödinger equations and nonlinear coupled mode equations [6] result, with a form similar to those heuristically derived in the limit

of weak variations in the linear optical properties, but with the coefficients “renormalized” to capture how the Bloch wave samples the underlying gain, loss, or nonlinearity. For effective one-dimensional (1D) structures this approach goes back some years [6]; recently [7] it has been generalized to higher dimensional photonic crystals.

These treatments have generally been restricted to dealing with Kerr nonlinearities, and considering only the lowest-order dispersion and diffraction effects. While one can easily envisage extending this approach to consider more general nonlinear and propagation effects, the tedious nature of the derivation is enough to put off even the most enthusiastic practitioner. There are three reasons for this.

First and probably the foremost is the way in which coefficients that characterize the group velocity, group velocity dispersion, and the like, enter in the formalism. In the course of the derivation, slowly varying envelope functions are introduced for all Bloch waves at a given crystal wave vector. One or more of these are assumed large in magnitude; these are sometimes called “principal” terms. The others are of smaller magnitude, which are called “companion” terms, and in the multiple scales analysis are slaved to the principal terms. The dispersion relation coefficients arise through the connection between the principal and companion terms, and a $k \cdot p$ analysis must be done essentially in parallel with the derivation to identify the correct coefficients. Thus a fairly tortuous derivation is required to produce dispersion coefficients in the final equations that are completely expected on simple physical grounds.

Second, because the usual multiple scales approaches proceed by using the assumed form for the electromagnetic field directly in the Maxwell equations, rather than from a Lagrangian or Hamiltonian basis, the conservation laws of the derived dynamical equations, and their connection with underlying symmetries of the problem, are not easy to identify. Indeed, in the case of the nonlinear coupled mode equations there has been confusion and dispute for a number of years over the physical meaning of one of the conserved quantities [8–10].

Third, for full three-dimensional problems any assumption involving envelope functions must respect, at least to an appropriate level of approximation, the fact that the magnetic

field and the electric displacement are divergenceless. In practice this can be addressed by writing the magnetic field in terms of a vector potential and the displacement in terms of a dual potential, and applying the analysis at the level of the potentials [7]. But again more formal complexity is introduced.

In this paper we introduce a different approach that avoids these difficulties. The idea here is to work not with slowly varying amplitudes that modulate Bloch functions, but rather with *effective fields* that are introduced within the context of a canonical formulation of the electromagnetic field in the presence of the photonic structure. To relate these effective fields to the physical electromagnetic fields requires a $k \cdot p$ analysis, but no $k \cdot p$ analysis is needed in deriving the linear dynamics of the effective fields, and to the extent that it enters in the nonlinear dynamics it does so in a very benign way.

So in a sense the dynamics is simplified at the cost of complicating the kinematics. Yet, since the relation between the effective and physical fields can be done once and for all, that cost is very small. The derivation of the dynamical equations proceeds again using multiple scales, but is much easier than in earlier approaches, especially since a divergence-free magnetic field and electric displacement are built into the canonical formulation itself. We will not concentrate here on the formulation of the conditions that would be necessary to make the multiple scales analysis rigorous; that is, we will not display all the length and time scale ratios that must be established as initial conditions and thereafter maintained by the solution of the dynamical equations themselves. This would be done in a way that is now familiar in the literature [6,11,7,12], and indeed in that respect our approach parallels earlier work. Instead we focus on how the difficulties of earlier approaches are avoided. We show how the well-known nonlinear Schrödinger and nonlinear coupled mode equations arise in this approach, assuming a simple Kerr nonlinearity; we leave the extensions to treat new nonlinear propagation effects to future communications.

The starting point is a canonical formulation of Maxwell's equations in the presence of dielectrics, which we assume here are nondispersive and without gain or loss. In earlier communications we used a dual potential to affect this, and on the basis of that we could provide derivations of the NLSE [13] and NLCME [14] equations using such effective fields in the restricted case of one dimension. While that work could be generalized to higher dimensions, we instead use a different canonical formulation of the Maxwell equations that we give in Secs. II and III below. This is an approach free of the introduction of any potential fields at all, and is therefore simpler than the dual potential approach, or others. On the basis of this we introduce our effective fields in Sec. IV, and show how they can be used to derive the NLSE. In Sec. V we turn to the NLCME.

Since our treatment is based on a canonical formulation of the electromagnetic fields, we can easily explore the physical symmetries associated with conserved quantities of the effective fields. This cannot be done in any straightforward way with conserved quantities of the more traditional slowly varying envelope functions. We illustrate this in Sec. VI.

Finally, although our main goal here is to present this approach rather than consider particular applications, in Sec. VII we consider the physics of an additional shock term that can accompany the usual self-phase modulation and group velocity dispersion in the NLSE. This illustrates both how easy the identification of this term is within this approach, and as well how the physics enters differently and more conveniently here than in other, more traditional treatments. We illustrate the use of the equations we derive here with some examples in Sec. VIII; concluding remarks are presented in Sec. IX, and we relegate some of the mathematical details to the Appendix.

Although we will be exclusively concerned with classical fields in this paper, instead of using Poisson brackets we formally employ commutators, moving back and forth freely between the classical and quantum formalism and notation. Similarly we use \dagger interchangeably with $*$ to denote complex conjugation. We do this to point the way towards the generalization of this approach into the quantum domain. The easy ability to do this is yet another advantage of this approach over the more traditional methods. Yet in this paper one can always take

$$\frac{1}{i\hbar}[\dots, \dots] \rightarrow \{\dots, \dots\}$$

to arrive at the actual classical equations intended; at the classical level adopted here the order of field quantities in the various products that appear is irrelevant.

II. CANONICAL FORMULATION OF MAXWELL'S EQUATIONS

The canonical formulation of Maxwell's equations in the absence of free charges, but in the presence of dielectric media, linear and nonlinear, is an old subject in the optics literature that we will not attempt to review here. In many treatments complications arise because one chooses a route to a canonical formulation that begins with a Lagrangian. Yet that is not required. Even in the canonical formulation of a classical system for ultimate use in quantization, one is only required to provide a set of commutators (or Poisson brackets) and a Hamiltonian such that their use leads in the usual way to the desired dynamical equations, and such that the numerical value of the Hamiltonian in the classical theory is equal to the energy. It turns out this is surprisingly easy to do for our problem, as we illustrate below.

As our dynamical equations we take the two curl equations of Maxwell,

$$\frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H}, \quad \frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}, \quad (1)$$

treating the divergence equations

$$\nabla \cdot \mathbf{D} = 0, \quad \nabla \cdot \mathbf{B} = 0, \quad (2)$$

as initial conditions. If these are satisfied at some time, and the fields evolve according to Eq. (1), then they will be satisfied at all later times. Formally one can restrict oneself to

the start to the class of fields $\mathbf{D}(\mathbf{r},t)$ and $\mathbf{B}(\mathbf{r},t)$ that satisfy Eq. (2); in practice, this is most easily done by introducing modes that satisfy Eq. (2), as we do in the following section. Within this framework this suggests that $\mathbf{D}(\mathbf{r},t)$ and $\mathbf{B}(\mathbf{r},t)$ should be thought of as the fundamental fields, and $\mathbf{E}(\mathbf{r},t)$ and $\mathbf{H}(\mathbf{r},t)$ as derived fields.

To be able to integrate Eqs. (1) we need constitutive relations that relate \mathbf{H} and \mathbf{E} to \mathbf{D} and \mathbf{B} . Neglecting magnetic effects we have

$$\begin{aligned}\mathbf{B}(\mathbf{r},t) &= \mu_0 \mathbf{H}(\mathbf{r},t), \\ \mathbf{D}(\mathbf{r},t) &= \varepsilon_0 \mathbf{E}(\mathbf{r},t) + \mathbf{P}(\mathbf{r},t),\end{aligned}\quad (3)$$

where in vacuum $\mathbf{P}(\mathbf{r},t) = 0$, and in a dielectric it must be specified in terms of other fields so that Eq. (1) can be integrated. Historically \mathbf{P} is given in terms of \mathbf{E} , but we want to understand \mathbf{P} as a function of \mathbf{D} :

$$\begin{aligned}P^i(\mathbf{r},t) &= \Gamma_1^{ij}(\mathbf{r})D^j(\mathbf{r},t) + \Gamma_2^{ijm}(\mathbf{r})D^j(\mathbf{r},t)D^m(\mathbf{r},t) \\ &+ \Gamma_3^{ijmn}(\mathbf{r})D^j(\mathbf{r},t)D^m(\mathbf{r},t)D^n(\mathbf{r},t) + \dots,\end{aligned}\quad (4)$$

where we assume that a perturbation approach to the nonlinear optical response will suffice. Here superscripts indicate Cartesian components that are to be summed over if repeated. By allowing the Γ 's to depend on position we allow for an inhomogeneous dielectric, but the response is taken to be local in both space and time. From the point of view of an underlying microscopic theory, this implies that any frequencies of interest are well below any resonant frequencies of the medium [15]. In this limit the Γ 's are invariant under a permutation of their Cartesian components [16]; this we assume as well.

Standard arguments in electromagnetic theory lead to an expression for the energy density [17],

$$h = \int \mathbf{H} \cdot d\mathbf{B} + \int \mathbf{E} \cdot d\mathbf{D}.\quad (5)$$

Note that when Eqs. (4) and (3) are used in this expression we require the permutation symmetry of the Γ 's so that the integration implied in Eq. (5) is independent of integration path, is thus well defined, and can be done. The result for the total energy of the electromagnetic field in the presence of the dielectrics is

$$\begin{aligned}H &= \frac{1}{2\mu_0} \int d\mathbf{r} B^i(\mathbf{r})B^i(\mathbf{r}) + \frac{1}{2\varepsilon_0} \int d\mathbf{r} D^i(\mathbf{r})D^i(\mathbf{r}) \\ &- \frac{1}{2\varepsilon_0} \int d\mathbf{r} D^i(\mathbf{r})\Gamma_1^{ij}(\mathbf{r})D^j(\mathbf{r}) \\ &- \frac{1}{3\varepsilon_0} \int d\mathbf{r} D^i(\mathbf{r})\Gamma_2^{ijm}(\mathbf{r})D^j(\mathbf{r})D^m(\mathbf{r}) \\ &- \frac{1}{4\varepsilon_0} \int d\mathbf{r} D^i(\mathbf{r})\Gamma_3^{ijmn}(\mathbf{r})D^j(\mathbf{r})D^m(\mathbf{r})D^n(\mathbf{r}) + \dots.\end{aligned}\quad (6)$$

To construct a canonical formulation of the electromagnetic field we now simply require a set of Poisson bracket relations (or alternately commutators) that yield the dynamical equations (1) as a consequence of Hamilton's equations using the total energy H as the Hamiltonian. The appropriate equal time commutation relations are

$$\begin{aligned}[D^i(\mathbf{r}), D^j(\mathbf{r}')] &= [B^i(\mathbf{r}), B^j(\mathbf{r}')] = 0, \\ [D^i(\mathbf{r}), B^j(\mathbf{r}')] &= i\hbar \varepsilon^{ijl} \frac{\partial}{\partial r^l} [\delta(\mathbf{r} - \mathbf{r}')],\end{aligned}\quad (7)$$

where ε^{ijl} is the Levi-Civita symbol [18]. Taking these as our fundamental commutation relations, it follows immediately that we recover Eq. (1) using Hamilton's equations

$$\begin{aligned}i\hbar \frac{\partial \mathbf{D}}{\partial t} &= [\mathbf{D}, H], \\ i\hbar \frac{\partial \mathbf{B}}{\partial t} &= [\mathbf{B}, H],\end{aligned}\quad (8)$$

with Eq. (6) as the Hamiltonian.

III. MODE EXPANSION

In the limit of weak nonlinearities it is useful to build on the solutions of Maxwell's equations that obtain in the absence of nonlinearity. To do so, we consider a linear isotropic medium for which we would normally write

$$\mathbf{P}(\mathbf{r},t) = \varepsilon_0 \chi(\mathbf{r}) \mathbf{E}(\mathbf{r},t) = \frac{\chi(\mathbf{r})}{1 + \chi(\mathbf{r})} \mathbf{D}(\mathbf{r},t),$$

so that

$$\Gamma_1^{ij}(\mathbf{r}) = \delta^{ij} \frac{n^2(\mathbf{r}) - 1}{n^2(\mathbf{r})},$$

where we have introduced the local refractive index $n(\mathbf{r})$ as the positive square root of $[1 + \chi(\mathbf{r})]$. The approach outlined here can be easily generalized to linear media with more complicated constitutive relations. We can then write our full Hamiltonian as

$$\begin{aligned}H &= H_0 - \frac{1}{3\varepsilon_0} \int d\mathbf{r} D^i(\mathbf{r})\Gamma_2^{ijm}(\mathbf{r})D^j(\mathbf{r})D^m(\mathbf{r}) - \frac{1}{4\varepsilon_0} \\ &\times \int d\mathbf{r} D^i(\mathbf{r})\Gamma_3^{ijmn}(\mathbf{r})D^j(\mathbf{r})D^m(\mathbf{r})D^n(\mathbf{r}) + \dots,\end{aligned}\quad (9)$$

with

$$H_0 = \frac{1}{2\mu_0} \int d\mathbf{r} B^i(\mathbf{r})B^i(\mathbf{r}) + \frac{1}{2\varepsilon_0} \int d\mathbf{r} \frac{D^i(\mathbf{r})D^i(\mathbf{r})}{n^2(\mathbf{r})}.\quad (10)$$

The linear modes we seek are solutions of the dynamical equations where only H_0 is used as the Hamiltonian. Using this in Eq. (8) we generate the usual linear Maxwell equations

$$\begin{aligned}\frac{\partial \mathbf{D}(\mathbf{r}, t)}{\partial t} &= \frac{1}{\mu_0} \nabla \times \mathbf{B}(\mathbf{r}, t), \\ \frac{\partial \mathbf{B}(\mathbf{r}, t)}{\partial t} &= -\frac{1}{\varepsilon_0} \nabla \times \left[\frac{\mathbf{D}(\mathbf{r}, t)}{n^2(\mathbf{r})} \right],\end{aligned}\quad (11)$$

and look for stationary solutions of these equations,

$$\begin{aligned}\mathbf{D}(\mathbf{r}, t) &= \mathbf{D}_\alpha(\mathbf{r}) e^{-i\omega_\alpha t} + \text{c.c.}, \\ \mathbf{B}(\mathbf{r}, t) &= \mathbf{B}_\alpha(\mathbf{r}) e^{-i\omega_\alpha t} + \text{c.c.},\end{aligned}\quad (12)$$

where c.c. stands for complex conjugate, for which Eq. (11) require

$$\begin{aligned}-i\omega_\alpha \mu_0 \mathbf{D}_\alpha(\mathbf{r}) &= \nabla \times \mathbf{B}_\alpha(\mathbf{r}), \\ i\omega_\alpha \varepsilon_0 \mathbf{B}_\alpha(\mathbf{r}) &= \nabla \times \left[\frac{\mathbf{D}_\alpha(\mathbf{r})}{n^2(\mathbf{r})} \right].\end{aligned}\quad (13)$$

From these we find the so-called ‘‘master equation’’ that $\mathbf{B}_\alpha(\mathbf{r})$ must satisfy,

$$\nabla \times \left[\frac{\nabla \times \mathbf{B}_\alpha(\mathbf{r}, t)}{n^2(\mathbf{r})} \right] = \frac{\omega_\alpha^2}{c^2} \mathbf{B}_\alpha(\mathbf{r}).\quad (14)$$

For $\omega_\alpha \neq 0$, solution of this equation subject to the divergence condition

$$\nabla \cdot \mathbf{B}_\alpha(\mathbf{r}) = 0,\quad (15)$$

together with the $\mathbf{D}_\alpha(\mathbf{r})$ that can be found from Eq. (13), leads to a pair of fields $(\mathbf{D}_\alpha(\mathbf{r}), \mathbf{B}_\alpha(\mathbf{r}))$ that identify a stationary solution of the linear Maxwell equations (1), and that also satisfy the divergence conditions (2). We associate a positive ω_α with each of these solutions, which we call a *mode*. Using the complex conjugate of Eqs. (13), we find that for every mode $(\mathbf{D}_\alpha(\mathbf{r}), \mathbf{B}_\alpha(\mathbf{r}))$ there is another mode

$$(\mathbf{D}_{\alpha'}(\mathbf{r}), \mathbf{B}_{\alpha'}(\mathbf{r})) = (\mathbf{D}_\alpha^*(\mathbf{r}), -\mathbf{B}_\alpha^*(\mathbf{r})),\quad (16)$$

with the same frequency $\omega_{\alpha'} = \omega_\alpha$.

Since the operator on the left-hand side of Eq. (14) is Hermitian, the solutions $\mathbf{B}_\alpha(\mathbf{r})$ associated with different ω_α are orthogonal, and we normalize them according to

$$\int d\mathbf{r} \frac{\mathbf{B}_\alpha^*(\mathbf{r}) \cdot \mathbf{B}_\beta(\mathbf{r})}{\mu_0} = \frac{\hbar \omega_\alpha}{2} \delta_{\alpha\beta},\quad (17)$$

where $\delta_{\alpha\beta}$ indicates a Kronecker delta. For an infinite system such as an idealized photonic crystal, we temporarily assume ‘‘box’’ normalization by taking the integration in such equations to range over a normalization volume. For degenerate modes we use the usual Gram-Schmidt orthogonalization

procedure to guarantee orthogonal modes. From Eq. (13) we then find that the $\mathbf{D}_\alpha(\mathbf{r})$ are orthonormal according to

$$\int d\mathbf{r} \frac{\mathbf{D}_\alpha^*(\mathbf{r}) \cdot \mathbf{D}_\beta(\mathbf{r})}{\varepsilon_0 n^2(\mathbf{r})} = \frac{\hbar \omega_\alpha}{2} \delta_{\alpha\beta}.\quad (18)$$

In terms of these stationary solutions we can write arbitrary \mathbf{D} and \mathbf{B} fields as

$$\begin{aligned}\mathbf{D}(\mathbf{r}, t) &= \sum_\alpha C_\alpha^{(1)}(t) \mathbf{D}_\alpha(\mathbf{r}), \\ \mathbf{B}(\mathbf{r}, t) &= \sum_\alpha C_\alpha^{(2)}(t) \mathbf{B}_\alpha(\mathbf{r}),\end{aligned}\quad (19)$$

where to guarantee the reality (Hermiticity) of $\mathbf{B}(\mathbf{r}, t)$, and $\mathbf{D}(\mathbf{r}, t)$ we require $C_{\alpha'}^{(1)} = (C_\alpha^{(1)})^\dagger$ and $C_{\alpha'}^{(2)} = -(C_\alpha^{(2)})^\dagger$. This can be satisfied by introducing new mode amplitudes a_α with no restrictions, but such that $C_\alpha^{(1)} = a_\alpha + a_{\alpha'}^\dagger$ and $C_\alpha^{(2)} = a_\alpha - a_{\alpha'}^\dagger$. We then have

$$\mathbf{D}(\mathbf{r}, t) = \sum_\alpha [a_\alpha(t) \mathbf{D}_\alpha(\mathbf{r}) + a_{\alpha'}^\dagger(t) \mathbf{D}_\alpha^*(\mathbf{r})],$$

$$\mathbf{B}(\mathbf{r}, t) = \sum_\alpha [a_\alpha(t) \mathbf{B}_\alpha(\mathbf{r}) + a_{\alpha'}^\dagger(t) \mathbf{B}_\alpha^*(\mathbf{r})].\quad (20)$$

Using Eq. (20) in the equal time commutation relations for $\mathbf{D}(\mathbf{r}, t)$ and $\mathbf{B}(\mathbf{r}, t)$, Eq. (7), we find equal time canonical commutation relations for the $a_\alpha(t)$:

$$\begin{aligned}[a_\alpha, a_\beta] &= 0, \\ [a_\alpha, a_\beta^\dagger] &= \delta_{\alpha\beta}.\end{aligned}\quad (21)$$

Substituting the expression (20) into the expression (10) for H_0 we find

$$H_0 = \sum_\alpha \hbar \omega_\alpha a_\alpha^\dagger a_\alpha.\quad (22)$$

The other portions of the full Hamiltonian can be found by substituting the expressions (20) for $\mathbf{B}(\mathbf{r}, t)$ and $\mathbf{D}(\mathbf{r}, t)$ into Eq. (9). Using the Hamiltonian (9) expressed in terms of the mode amplitudes via Eq. (20), the commutation relations (21), and the Heisenberg equations of motion,

$$i\hbar \frac{da_\alpha(t)}{dt} = [a_\alpha(t), H],\quad (23)$$

we recover Maxwell’s equations (1).

We now specialize to a three-dimensional photonic crystal, wherein the index of refraction is periodically varying such that $n(\mathbf{r} + \mathbf{R}) = n(\mathbf{r})$ for any lattice vector \mathbf{R} . The index α then consists of a crystal wave vector \mathbf{k} and a band index m . Passing to the limit of an infinite crystal, the crystal wave

vector \mathbf{k} varies continuously through the first Brillouin zone and, as we show in the Appendix, our field expansions (20) are replaced by

$$\begin{aligned}\mathbf{D}(\mathbf{r},t) &= \sum_m \int d\mathbf{k} [a_{m\mathbf{k}}(t)\mathbf{D}_{m\mathbf{k}}(\mathbf{r}) + a_{m\mathbf{k}}^\dagger(t)\mathbf{D}_{m\mathbf{k}}^*(\mathbf{r})], \\ \mathbf{B}(\mathbf{r},t) &= \sum_m \int d\mathbf{k} [a_{m\mathbf{k}}(t)\mathbf{B}_{m\mathbf{k}}(\mathbf{r}) + a_{m\mathbf{k}}^\dagger(t)\mathbf{B}_{m\mathbf{k}}^*(\mathbf{r})],\end{aligned}\quad (24)$$

our commutation relations (21) are replaced by

$$\begin{aligned}[a_{m\mathbf{k}}, a_{m'\mathbf{k}'}] &= 0, \\ [a_{m\mathbf{k}}, a_{m'\mathbf{k}'}^\dagger] &= \delta_{mm'} \delta(\mathbf{k} - \mathbf{k}'),\end{aligned}\quad (25)$$

with mode functions $(\mathbf{D}_{m\mathbf{k}}(\mathbf{r}), \mathbf{B}_{m\mathbf{k}}(\mathbf{r}))$ normalized according to

$$\begin{aligned}\int d\mathbf{r} \frac{\mathbf{D}_{m\mathbf{k}}^*(\mathbf{r}) \cdot \mathbf{D}_{m'\mathbf{k}'}(\mathbf{r})}{\varepsilon_0 n^2(\mathbf{r})} &= \frac{\hbar \omega_{m\mathbf{k}}}{2} \delta_{mm'} \delta(\mathbf{k} - \mathbf{k}'), \\ \int d\mathbf{r} \frac{\mathbf{B}_{m\mathbf{k}}^*(\mathbf{r}) \cdot \mathbf{B}_{m'\mathbf{k}'}(\mathbf{r})}{\mu_0} &= \frac{\hbar \omega_{m\mathbf{k}}}{2} \delta_{mm'} \delta(\mathbf{k} - \mathbf{k}'),\end{aligned}\quad (26)$$

where the integrals range over all space. We have used Bloch's theorem to write

$$\begin{aligned}\mathbf{D}_{m\mathbf{k}}(\mathbf{r}) &= \sqrt{\frac{\varepsilon_0 \bar{n}^2 \hbar \omega_{m\mathbf{k}}}{16\pi^3}} \mathcal{D}_{m\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} \equiv \frac{\mathbf{d}_{m\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}}}{\sqrt{8\pi^3}}, \\ \mathbf{B}_{m\mathbf{k}}(\mathbf{r}) &= \sqrt{\frac{\mu_0 \hbar \omega_{m\mathbf{k}}}{16\pi^3}} \mathcal{B}_{m\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} \equiv \frac{\mathbf{b}_{m\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}}}{\sqrt{8\pi^3}},\end{aligned}\quad (27)$$

where \bar{n} is a reference refractive index that can be chosen as convenient, and where the $\mathcal{D}_{m\mathbf{k}}(\mathbf{r})$ and $\mathcal{B}_{m\mathbf{k}}(\mathbf{r})$ (see the Appendix) have the periodicity of the lattice,

$$\begin{aligned}\mathcal{D}_{m\mathbf{k}}(\mathbf{r}) &= \mathcal{D}_{m\mathbf{k}}(\mathbf{r} + \mathbf{R}), \\ \mathcal{B}_{m\mathbf{k}}(\mathbf{r}) &= \mathcal{B}_{m\mathbf{k}}(\mathbf{r} + \mathbf{R}),\end{aligned}\quad (28)$$

for any lattice vector \mathbf{R} ; the $\mathbf{d}_{m\mathbf{k}}(\mathbf{r})$ and $\mathbf{b}_{m\mathbf{k}}(\mathbf{r})$ share this property. The constants preceding the periodic functions in Eq. (27) are set so that the periodic functions are normalized according to

$$\begin{aligned}\int_{\text{cell}} \frac{d\mathbf{r}}{V_{\text{cell}}} \mathcal{B}_{m\mathbf{k}}^*(\mathbf{r}) \cdot \mathcal{B}_{m'\mathbf{k}'}(\mathbf{r}) &= \delta_{mm'}, \\ \int_{\text{cell}} \frac{d\mathbf{r}}{V_{\text{cell}}} \frac{\bar{n}^2}{n^2(\mathbf{r})} \mathcal{D}_{m\mathbf{k}}^*(\mathbf{r}) \cdot \mathcal{D}_{m'\mathbf{k}'}(\mathbf{r}) &= \delta_{mm'},\end{aligned}\quad (29)$$

for each \mathbf{k} , where we denote the volume of one unit cell of the medium by V_{cell} . The part of the Hamiltonian describing linear dynamics (10) takes the form

$$H_0 = \sum_m \int d\mathbf{k} \hbar \omega_{m\mathbf{k}} a_{m\mathbf{k}}^\dagger a_{m\mathbf{k}}. \quad (30)$$

Although more general nonlinearities could easily be included, we will here consider only a Kerr nonlinearity with the periodicity of the lattice,

$$\Gamma_3^{ijmn}(\mathbf{r}) = \Gamma_3^{ijmn}(\mathbf{r} + \mathbf{R}).$$

Then the nonlinear part of the Hamiltonian becomes

$$H_{NL} = -\frac{1}{4\varepsilon_0} \int d\mathbf{r} D^i(\mathbf{r}) \Gamma_3^{ijmn}(\mathbf{r}) D^j(\mathbf{r}) D^m(\mathbf{r}) D^n(\mathbf{r}), \quad (31)$$

and the full Hamiltonian is

$$H = H_0 + H_{NL}. \quad (32)$$

In the following section we use Eq. (32) defined in terms of Eqs. (30) and (31) as our Hamiltonian, which we subject to various approximations to describe pulse propagation.

IV. EFFECTIVE FIELDS AND THE NONLINEAR SCHRÖDINGER EQUATION

In this section we use the Hamiltonian formulation of Maxwell's equations in a periodic medium to generate pulse propagation equations in the presence of a Kerr nonlinearity. We will stop our derivation at the level of the nonlinear Schrödinger equation, modified to include a shock term. But equations with higher-order nonlinear, dispersive, and mixed terms could also be derived using the same approach. Our focus here is not the derivation of a new equation relevant in a particular physical situation, but rather to demonstrate that the approach we advocate here makes identification of such equations much easier than has been possible in the past.

To do that it is useful to identify the traditional approach [3,7] in our present notation. One begins with the general expressions (24) for the fields and the mode coefficients (27) to write

$$\begin{aligned}\mathbf{D}(\mathbf{r},t) &= \sum_m \int d\mathbf{k} a_{m\mathbf{k}}(t) \mathbf{D}_{m\mathbf{k}}(\mathbf{r}) + \text{c.c.} \\ &= \sum_m \int \frac{d\mathbf{k}}{\sqrt{8\pi^3}} a_{m\mathbf{k}}(t) \mathbf{d}_{m\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} + \text{c.c.} \\ &= \sum_m f_m(\mathbf{r},t) \mathbf{d}_{m\bar{\mathbf{k}}}(\mathbf{r}) e^{i(\bar{\mathbf{k}} \cdot \mathbf{r} - \omega_{m\bar{\mathbf{k}}}t)} + \text{c.c.},\end{aligned}\quad (33)$$

introducing a set of amplitudes $f_m(\mathbf{r},t)$ associated with each band at a chosen carrier wave vector $\bar{\mathbf{k}}$. The idea is that the effects of the underlying spatial variation in the linear optical properties are contained within the $\mathbf{d}_{m\bar{\mathbf{k}}}(\mathbf{r})$. By "renormalizing" the plane wave used in the uniform medium with this factor, one can hope to identify amplitudes $f_m(\mathbf{r},t)$ that are indeed slowly varying [19], and this is indeed possible [20,6,7].

If one is interested in propagation far from a band gap, or near or in a band gap but close to the band edge, then one of the amplitudes $f_m(\mathbf{r}, t)$ dominates in a multiple scale analysis. It is sometimes called the “principal component,” and the other amplitudes, or “companion components,” are slaved to it. Keeping lowest-order terms in diffraction, group velocity dispersion, and the nonlinearity, a nonlinear Schrödinger equation for the principal component $f_m(\mathbf{r}, t)$ results. We refer to the above-cited works to illustrate how complicated these kinds of derivations of such a simple result can be.

The strategy we adopt here is to avoid working directly with fields such as $\mathbf{D}(\mathbf{r}, t)$ or $\mathbf{E}(\mathbf{r}, t)$, as is done in the expression (33), but to work rather with *effective fields* $g_m(\mathbf{r}, t)$ [21],

$$g_m(\mathbf{r}, t) \equiv \int \frac{d\boldsymbol{\kappa}}{\sqrt{8\pi^3}} a_{m(\bar{\mathbf{k}}+\boldsymbol{\kappa})}(t) e^{i\boldsymbol{\kappa}\cdot\mathbf{r}}. \quad (34)$$

Here we have again picked a reference crystal wavevector $\bar{\mathbf{k}}$, and although the integral in Eq. (34) in principle ranges over the whole Brillouin zone, a smallness parameter in our approach will be the range over $\boldsymbol{\kappa}$ over which contributions from $a_{m(\bar{\mathbf{k}}+\boldsymbol{\kappa})}(t)$ are significant; we will assume that the $g_m(\mathbf{r}, t)$ of interest are slowly varying in space over distances on the order of the lattice spacing. These effective fields are “canonical” in that they satisfy simple equal time commutation relations,

$$\begin{aligned} [g_m(\mathbf{r}, t), g_{m'}(\mathbf{r}', t)] &= 0, \\ [g_m(\mathbf{r}, t), g_{m'}^\dagger(\mathbf{r}', t)] &= \delta_{mm'} \delta(\mathbf{r} - \mathbf{r}'), \end{aligned} \quad (35)$$

which follow directly from the commutation relations (25). However, their relation to the fundamental fields $\mathbf{D}(\mathbf{r}, t)$ and $\mathbf{B}(\mathbf{r}, t)$ is more complicated. Again turning to the expressions for the fields (24) and the mode coefficients (27) we can write

$$\begin{aligned} \mathbf{D}(\mathbf{r}, t) &= \sum_m \int \frac{d\mathbf{k}}{\sqrt{8\pi^3}} a_{m\mathbf{k}}(t) \mathbf{d}_{m\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} + \text{c.c.} \\ &= e^{i\bar{\mathbf{k}}\cdot\mathbf{r}} \sum_m \int \frac{d\boldsymbol{\kappa}}{\sqrt{8\pi^3}} \mathbf{d}_{m(\bar{\mathbf{k}}+\boldsymbol{\kappa})}(\mathbf{r}) a_{m(\bar{\mathbf{k}}+\boldsymbol{\kappa})}(t) e^{i\boldsymbol{\kappa}\cdot\mathbf{r}} + \text{c.c.} \\ &= e^{i\bar{\mathbf{k}}\cdot\mathbf{r}} \sum_m \left(\mathbf{d}_{m\bar{\mathbf{k}}}(\mathbf{r}) g_m(\mathbf{r}, t) + \boldsymbol{\gamma}_{m\bar{\mathbf{k}}}^{(j)}(\mathbf{r}) \frac{\partial g_m(\mathbf{r}, t)}{\partial r_j} + \dots \right) \\ &\quad + \text{c.c.}, \end{aligned} \quad (36)$$

where to obtain the third line we have expanded $\mathbf{d}_{m(\bar{\mathbf{k}}+\boldsymbol{\kappa})}(\mathbf{r})$ about $\boldsymbol{\kappa}=0$ and performed a partial integration, and we have put

$$\boldsymbol{\gamma}_{m\bar{\mathbf{k}}}^{(j)}(\mathbf{r}) \equiv -i \left(\frac{\partial}{\partial k_j} \mathbf{d}_{m\mathbf{k}}(\mathbf{r}) \right)_{\bar{\mathbf{k}}}. \quad (37)$$

While this is formally straightforward, care is required in the very definition of the derivative of that quantity with respect

to \mathbf{k} . After all, if one goes to a numerical code to determine the $\mathbf{d}_{m\mathbf{k}}(\mathbf{r})$ one finds that the code will in general return functions $\mathbf{d}_{m\mathbf{k}}(\mathbf{r})$ that have a random variation in their phase from point to point in the Brillouin zone, even if those points are arbitrarily close. Of course a $\mathbf{D}(\mathbf{r}, t)$ that is slowly varying in space can still result from Eq. (24); this just requires that there be a rapid phase variation of $a_{m\mathbf{k}}(t)$ from \mathbf{k} point to \mathbf{k} point that “undoes” that of $\mathbf{d}_{m\mathbf{k}}(\mathbf{r})$.

This raises an important point. Functions $g_m(\mathbf{r}, t)$ that are slowly varying in space—which clearly requires not only a small range of $|\boldsymbol{\kappa}|$ for significantly contributing $a_{m(\bar{\mathbf{k}}+\boldsymbol{\kappa})}(t)$, but also a smooth variation in their phases—correspond to fields $\mathbf{D}(\mathbf{r}, t)$ that are slowly varying in space only if the phases of the $\mathbf{d}_{m\mathbf{k}}(\mathbf{r})$ are slowly varying as one moves through the Brillouin zone. We will want the slow variation of the $g_m(\mathbf{r}, t)$ to be associated with, and to guarantee, the slow variation of $\mathbf{D}(\mathbf{r}, t)$, and so we require $\mathbf{d}_{m\mathbf{k}}(\mathbf{r})$ that are smooth functions of \mathbf{k} as we move about $\mathbf{k}=\bar{\mathbf{k}}$. To ensure this, we assume that the $\mathbf{d}_{m\mathbf{k}}(\mathbf{r})$ are constructed from their values at $\bar{\mathbf{k}}$ by a $k \cdot p$ expansion. To do this in a way that the $\mathbf{d}_{m\mathbf{k}}(\mathbf{r})$ are analytic functions of \mathbf{k} throughout the *entire* Brillouin zone is not trivial [22]. But since we assume that $|a_{m(\bar{\mathbf{k}}+\boldsymbol{\kappa})}(t)|$ are significant only for small $|\boldsymbol{\kappa}|$ we can use standard $k \cdot p$ theory, modified from its version in electron physics to take into account the differences that arise for photons [23–26]. We will turn to the details of this in a future publication, where we will also consider the nature of such an expansion about a point or line of degeneracy.

So in older approaches the relation (33) of the slowly varying fields $f_m(\mathbf{r}, t)$ to the physical fields of interest was straightforward; in this approach the relation of the effective fields $g_m(\mathbf{r}, t)$ to the physical fields of interest it is more complicated. For applications to finite media, equations such as Eq. (36) would actually have to be implemented to connect fields across interfaces, since it is the Maxwell *saltsu* (boundary) conditions on those physical fields that must be satisfied. But by accepting more complicated relationships between the physical and effective fields, where $k \cdot p$ theory must be used, we drastically simplify the derivation of the dynamical equations for the effective fields. In the linear regime we can completely avoid using $k \cdot p$ theory, and when it does appear in the nonlinear regime it is in a more benign way than in earlier approaches.

To see this, look first at the linear problem. We employ an expansion of the dispersion relation for each band,

$$\omega_{m\mathbf{k}} = \omega_{m\bar{\mathbf{k}}} + (k_i - \bar{k}_i) \omega_{m\bar{\mathbf{k}}}^{(i)} + \frac{1}{2} (k_i - \bar{k}_i) (k_j - \bar{k}_j) \omega_{m\bar{\mathbf{k}}}^{(ij)} + \dots, \quad (38)$$

where the expansion coefficients in the dispersion relation at $\bar{\mathbf{k}}$ appear, with

$$\begin{aligned} \omega_{m\bar{\mathbf{k}}}^{(i)} &= \left(\frac{\partial \omega_{m\mathbf{k}}}{\partial k^i} \right)_{\bar{\mathbf{k}}}, \\ \omega_{m\bar{\mathbf{k}}}^{(ij)} &= \left(\frac{\partial^2 \omega_{m\mathbf{k}}}{\partial k^i \partial k^j} \right)_{\bar{\mathbf{k}}}, \end{aligned} \quad (39)$$

where for simplicity we assume that our bands are nondegenerate at $\bar{\mathbf{k}}$, and we let the number of superscripts signify which derivative is indicated. Using this in our linear Hamiltonian (30), and partially integrating the resulting terms, we find

$$\begin{aligned} H_0 = & \hbar \sum_m \omega_{m\bar{\mathbf{k}}} \int d\mathbf{r} |g_m|^2 + \frac{i\hbar}{2} \sum_m \omega_{m\bar{\mathbf{k}}}^{(i)} \int d\mathbf{r} \left(\frac{\partial g_m^\dagger}{\partial r^i} g_m - \text{c.c.} \right) \\ & - \frac{\hbar}{4} \sum_m \omega_{m\bar{\mathbf{k}}}^{(ij)} \int d\mathbf{r} \left(\frac{\partial g_m^\dagger}{\partial r^j} \frac{\partial g_m}{\partial r^i} + \text{c.c.} \right) + \dots \end{aligned} \quad (40)$$

The linear dynamics for the $g_m(\mathbf{r}, t)$ then follow from

$$i\hbar \frac{\partial g_m}{\partial t} = [g_m, H_0],$$

which is simple to work out because the $g_m(\mathbf{r}, t)$ satisfy the simple commutation relations (35). We find

$$\frac{\partial g_m}{\partial t} = -i\omega_{m\bar{\mathbf{k}}} g_m - \omega_{m\bar{\mathbf{k}}}^{(i)} \frac{\partial g_m}{\partial r^i} + \frac{i}{2} \omega_{m\bar{\mathbf{k}}}^{(ij)} \frac{\partial^2 g_m}{\partial r^i \partial r^j} + \dots, \quad (41)$$

that is, in the linear regime the $g_m(\mathbf{r}, t)$ evolve completely independently. This is *not* true for the $f_m(\mathbf{r}, t)$, since comparing the expressions for $\mathbf{D}(\mathbf{r}, t)$ in terms of the $f_m(\mathbf{r}, t)$, Eq. (33), and the $g_m(\mathbf{r}, t)$, Eq. (36), we see that only approximately do we have

$$f_m(\mathbf{r}, t) \approx g_m(\mathbf{r}, t) e^{i\omega_{m\bar{\mathbf{k}}} t}, \quad (42)$$

to higher order there are contributions from the other $g_{m'}(\mathbf{r}, t)$, since when the $\gamma_{m\bar{\mathbf{k}}}^{(j)}(\mathbf{r})$ are expanded in terms of the $\mathbf{d}_{m'\bar{\mathbf{k}}}(\mathbf{r})$ there will be many nonvanishing terms. We can, of course, write the $\omega_{m\bar{\mathbf{k}}}^{(i)}$ and the $\omega_{m\bar{\mathbf{k}}}^{(ij)}$ in terms of integrals of the mode fields; using $k \cdot p$ theory, for example, we can write $\omega_{m\bar{\mathbf{k}}}^{(i)} = v_{mm}^i(\mathbf{k})$, where the velocity vector $\mathbf{v}_{mm}(\mathbf{k})$ for band m at an arbitrary \mathbf{k} is

$$\mathbf{v}_{mm}(\mathbf{k}) = \frac{c}{\bar{n}} \int_{cell} \frac{d\mathbf{r}}{V_{cell}} \text{Re}[\mathcal{E}_{m\mathbf{k}}^*(\mathbf{r}) \times \mathcal{H}_{m\mathbf{k}}(\mathbf{r})], \quad (43)$$

where for notational convenience we have introduced dimensionless fields periodic over the unit cell that we associate with the electric field and magnetic displacement,

$$\begin{aligned} \mathcal{E}_{m\mathbf{k}}(\mathbf{r}) & \equiv \frac{\bar{n}^2}{n^2(\mathbf{r})} \mathcal{D}_{m\mathbf{k}}(\mathbf{r}), \\ \mathcal{H}_{m\mathbf{k}}(\mathbf{r}) & \equiv \mathcal{B}_{m\mathbf{k}}(\mathbf{r}). \end{aligned} \quad (44)$$

Equations such as Eq. (43) are of course exact, and are unrelated to approximations associated with a derivation of equations for effective fields. Whereas in older derivations [6,7] they had to be used in the course of such derivations, here they do not arise at all.

Having so easily disposed of the linear terms, we now move to the inclusion of the nonlinear effects. Here we must use our expression (36) for $\mathbf{D}(\mathbf{r}, t)$ in Eq. (31) for H_{NL} . We consider the standard example of a frequency spectrum such that at the $\bar{\mathbf{k}}$ of interest only one amplitude $g_m(\mathbf{r}, t)$ is significant, and we assume that we are sufficiently far from any phase-matching resonances to neglect third-harmonic generation into another band, although that could easily be included. Without pausing to make the multiple scales analysis rigorous, we will be interested in nonlinearities only sufficiently strong in their effects to be comparable to the $\omega_{m\bar{\mathbf{k}}}^{(ij)}$ term above Eq. (41), or at most, if that term is anomalously small, to the $\omega_{m\bar{\mathbf{k}}}^{(i)}$. Thus the fastest time behavior of $g_m(\mathbf{r}, t)$ will be $\exp(-i\omega_{m\bar{\mathbf{k}}} t)$, and the leading terms in H_{NL} with respect to the dynamics of $g_m(\mathbf{r}, t)$ will be those that involve two terms from the set $(g_m(\mathbf{r}, t), \partial g_m(\mathbf{r}, t)/\partial r_j)$ and two from the set $(g_m^\dagger(\mathbf{r}, t), \partial g_m^\dagger(\mathbf{r}, t)/\partial r_j)$. The kind of approximation where one keeps only these leading terms is sometimes called a ‘‘rotating wave approximation.’’ The other terms could also easily be kept, although it is easy to confirm that for $\bar{\mathbf{k}}$ at an arbitrary point in the Brillouin zone they will not in general survive the spacial integration in the expression (31) for \mathcal{H}_{NL} ; however, if they do survive their effects could easily be included by standard multiple scales techniques.

We keep only the leading terms and, since the $\partial g_m(\mathbf{r}, t)/\partial r_j$ terms in the expression (36) for $\mathbf{D}(\mathbf{r}, t)$ are assumed to be much smaller than the $g_m(\mathbf{r}, t)$ terms, we keep only contributions to H_{NL} involving one derivative term. Finally, we simplify those contributions following an approach used earlier in one-dimensional studies [13,14]. We note that the periodic functions $\mathbf{d}_{m'\bar{\mathbf{k}}}(\mathbf{r})$, $\gamma_{m\bar{\mathbf{k}}}^{(j)}(\mathbf{r})$, and $\Gamma_3^{ijnl}(\mathbf{r})$ can be expanded in terms of reciprocal lattice vectors. Thus their products that appear in H_{NL} can as well. And since by assumption the range of $|\mathbf{k}|$ appearing in $g_m(\mathbf{r}, t)$ is small, only the contribution from the zero reciprocal lattice vector of the product of periodic functions will survive. Employing all these considerations, we find

$$H_{NL} = -\frac{\hbar}{2} \alpha_{m\bar{\mathbf{k}}} \int d\mathbf{r} |g_m|^4 - \frac{\hbar}{2} \left(\tilde{\alpha}_{m\bar{\mathbf{k}}}^{(p)} \int d\mathbf{r} g_m^\dagger |g_m|^2 \frac{\partial g_m}{\partial r^p} + \text{c.c.} \right), \quad (45)$$

where

$$\begin{aligned} \alpha_{m\bar{\mathbf{k}}} & = \frac{3}{\hbar \epsilon_0} \int_{cell} \frac{d\mathbf{r}}{V_{cell}} \Gamma_3^{ijnl}(\mathbf{r}) \\ & \quad \times [d_{m\bar{\mathbf{k}}}^i(\mathbf{r})]^* [d_{m\bar{\mathbf{k}}}^j(\mathbf{r})]^* d_{m\bar{\mathbf{k}}}^n(\mathbf{r}) d_{m\bar{\mathbf{k}}}^l(\mathbf{r}), \\ \tilde{\alpha}_{m\bar{\mathbf{k}}}^{(p)} & = \frac{6}{\hbar \epsilon_0} \int_{cell} \frac{d\mathbf{r}}{V_{cell}} \Gamma_3^{ijnl}(\mathbf{r}) \\ & \quad \times [d_{m\bar{\mathbf{k}}}^i(\mathbf{r})]^* [d_{m\bar{\mathbf{k}}}^j(\mathbf{r})]^* d_{m\bar{\mathbf{k}}}^n(\mathbf{r}) \gamma_{m\bar{\mathbf{k}}}^{l(p)}(\mathbf{r}). \end{aligned}$$

Then, since we are keeping only one band in our calculation, with the inclusion of linear terms up to and including those involving $\omega_{m\bar{\mathbf{k}}}^{(ij)}$, our total Hamiltonian becomes

$$\begin{aligned}
 \mathbf{H}^{NLSE} = & \hbar \omega_{m\bar{\mathbf{k}}} \int d\mathbf{r} |g_m|^2 + \frac{i\hbar}{2} \omega_{m\bar{\mathbf{k}}}^{(i)} \int d\mathbf{r} \left(\frac{\partial g_m^\dagger}{\partial r^i} g_m - \text{c.c.} \right) \\
 & - \frac{\hbar}{4} \omega_{m\bar{\mathbf{k}}}^{(ij)} \int d\mathbf{r} \left(\frac{\partial g_m^\dagger}{\partial r^j} \frac{\partial g_m}{\partial r^i} + \text{c.c.} \right) - \frac{\hbar}{2} \alpha_{m\bar{\mathbf{k}}} \\
 & \times \int d\mathbf{r} |g_m|^4 - \frac{\hbar}{2} \left(\tilde{\alpha}_{m\bar{\mathbf{k}}}^{(p)} \int d\mathbf{r} g_m^\dagger |g_m|^2 \frac{\partial g_m}{\partial r^p} + \text{c.c.} \right).
 \end{aligned} \quad (46)$$

Using this in our equations of motion,

$$i\hbar \frac{\partial g_m}{\partial t} = [g_m, \mathbf{H}^{NLSE}],$$

the application of the commutation relations (35) for g_m and g_m^\dagger leads to

$$\begin{aligned}
 \frac{\partial g_m}{\partial t} = & -i\omega_{m\bar{\mathbf{k}}} g_m - \omega_{m\bar{\mathbf{k}}}^{(i)} \frac{\partial g_m}{\partial r^i} + \frac{i}{2} \omega_{m\bar{\mathbf{k}}}^{(ij)} \frac{\partial^2 g_m}{\partial r^i \partial r^j} \\
 & + i|g_m|^2 \left(\alpha_{m\bar{\mathbf{k}}} + 2i \text{Im}(\tilde{\alpha}_{m\bar{\mathbf{k}}}^{(p)}) \frac{\partial}{\partial r^p} \right) g_m.
 \end{aligned} \quad (47)$$

The first three terms on the right-hand side of this equation are linear, and describe the linear phase accumulation, group velocity, and group velocity dispersion experienced by the field. The first nonlinear term describes the familiar nonlinear self-phase modulation wherein the intensity of the pulse causes an effective correction in its own phase accumulation. The second nonlinear term is often called a ‘‘shock term,’’ and describes the nonlinear correction to the group velocity of an intense pulse. This intensity-dependent group velocity can lead to the formation of a shock front in the pulse envelope function. The form of this shock term is different from the usual shock term encountered in the literature; we return to this issue in Sec. VII. Note that it is only the imaginary part of $\tilde{\alpha}_{m\bar{\mathbf{k}}}^{(p)}$ that appears in Eq. (47); in fact, using a partial integration Eq. (46) can be rewritten to involve only the imaginary part of $\tilde{\alpha}_{m\bar{\mathbf{k}}}^{(p)}$ as well.

V. EFFECTIVE FIELDS: 1D STRUCTURES AND THE COUPLED MODE EQUATIONS

We now examine the situation where the medium of interest possesses periodicity in only one direction. Examples of such a system are fiber Bragg gratings, dielectric stacks or coupled microresonator structures [Fig. 1(a)], all of which possess periodicity only in the z direction. Also, the system shown in Fig. 1(b), which consists of a two-dimensional photonic crystal slab into which a line defect has been formed, is only truly periodic in the z direction. We label the period in the z direction by L_{cell} . The modes of interest are now indicated by a band index m and a continuous k that ranges over the first 1D Brillouin zone. We show in the Appendix that for this geometry the field expansions (20) are replaced by

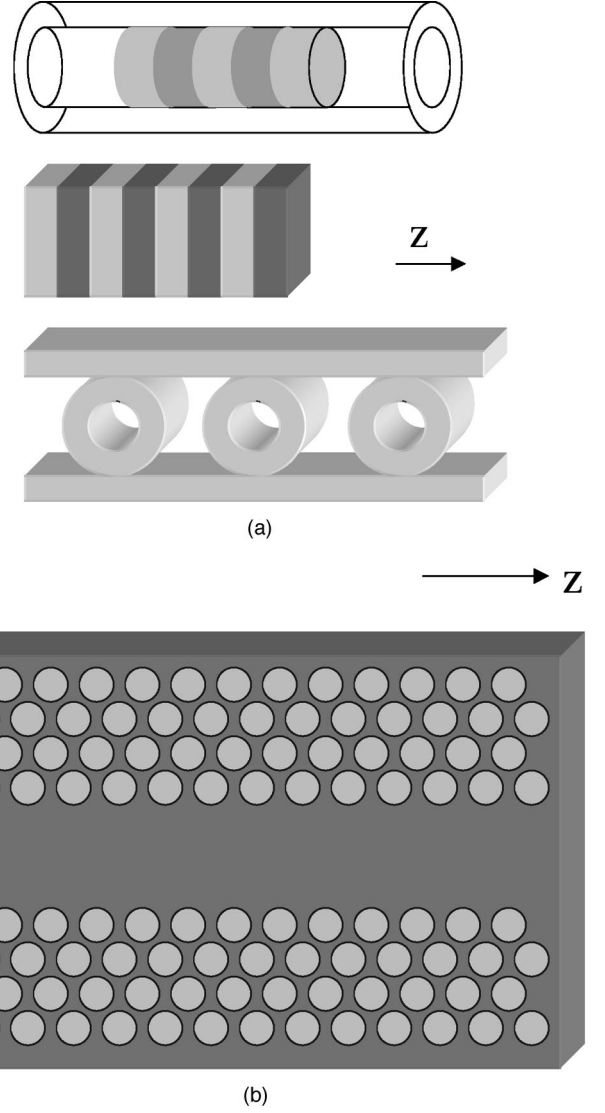


FIG. 1. (a) Three examples of optical systems of interest possessing periodicity in the z direction. From top to bottom, a fiber Bragg grating, a dielectric stack, and a coupled microresonator structure. The particular microresonator structure depicted here is a periodic two-channel side-coupled integrated spaced series of resonators, or periodic two-channel SCISSOR structure [27,28]. (b) A line defect waveguide in a 2D photonic crystal slab. The 2D photonic crystal slab is composed of a periodic lattice of cylinders of different refractive index from the background material. A number of missing rows of cylinders creates the defect waveguide. This structure has full periodicity only in the z direction.

$$\mathbf{D}(\mathbf{r}, t) = \sum_m \int dk [a_{mk}(t) \mathbf{D}_{mk}(\mathbf{r}) + a_{mk}^\dagger(t) \mathbf{D}_{mk}^*(\mathbf{r})],$$

$$\mathbf{B}(\mathbf{r}, t) = \sum_m \int dk [a_{mk}(t) \mathbf{B}_{mk}(\mathbf{r}) + a_{mk}^\dagger(t) \mathbf{B}_{mk}^*(\mathbf{r})], \quad (48)$$

our commutation relations (21) are replaced by

$$[a_{mk}, a_{m'k'}] = 0,$$

$$[a_{mk}, a_{m'k'}^\dagger] = \delta_{mm'} \delta(k - k'), \quad (49)$$

with mode functions ($\mathbf{D}_{mk}(\mathbf{r}), \mathbf{B}_{mk}(\mathbf{r})$) normalized according to

$$\int d\mathbf{r} \frac{\mathbf{D}_{mk}^*(\mathbf{r}) \cdot \mathbf{D}_{m'k'}(\mathbf{r})}{\varepsilon_0 n^2(\mathbf{r})} = \frac{\hbar \omega_{mk}}{2} \delta_{mm'} \delta(k - k'),$$

$$\int d\mathbf{r} \frac{\mathbf{B}_{mk}^*(\mathbf{r}) \cdot \mathbf{B}_{m'k'}(\mathbf{r})}{\mu_0} = \frac{\hbar \omega_{mk}}{2} \delta_{mm'} \delta(k - k'), \quad (50)$$

where the integrals range over all space, and we have used Bloch's theorem to write

$$\mathbf{D}_{mk}(\mathbf{r}) = \sqrt{\frac{\varepsilon_0 \bar{n}^2 \hbar \omega_{mk}}{4 \pi A}} \mathcal{D}_{mk}(\mathbf{r}) e^{ikz} \equiv \frac{\mathbf{d}_{mk}(\mathbf{r}) e^{ikz}}{\sqrt{2 \pi}},$$

$$\mathbf{B}_{mk}(\mathbf{r}) = \sqrt{\frac{\mu_0 \hbar \omega_{mk}}{4 \pi A}} \mathcal{B}_{mk}(\mathbf{r}) e^{ikz} \equiv \frac{\mathbf{b}_{mk}(\mathbf{r}) e^{ikz}}{\sqrt{2 \pi}}, \quad (51)$$

where A is a nominal area chosen for later convenience. The $\mathcal{D}_{mk}(\mathbf{r})$ and $\mathcal{B}_{mk}(\mathbf{r})$ have the periodicity of the structure,

$$\mathcal{D}_{mk}(\mathbf{r}) = \mathcal{D}_{mk}(\mathbf{r} + \mathbf{Z}),$$

$$\mathcal{B}_{mk}(\mathbf{r}) = \mathcal{B}_{mk}(\mathbf{r} + \mathbf{Z}), \quad (52)$$

where \mathbf{Z} is any integer times $L_{cell} \hat{\mathbf{z}}$. The constants preceding the periodic functions in Eq. (51) are here chosen so that the periodic functions are normalized according to

$$\int_{cell} \frac{dz}{L_{cell}} \int \frac{dxdy}{A} \mathcal{B}_{mk}^*(\mathbf{r}) \cdot \mathcal{B}_{m'k'}(\mathbf{r}) = \delta_{mm'},$$

$$\int_{cell} \frac{dz}{L_{cell}} \int \frac{dxdy}{A} \frac{\bar{n}^2}{n^2(\mathbf{r})} \mathcal{D}_{mk}^*(\mathbf{r}) \cdot \mathcal{D}_{m'k'}(\mathbf{r}) = \delta_{mm'}, \quad (53)$$

for each k ; here the integral over z only ranges over L_{cell} , but the integral over x and y is over the whole xy plane. The part of the Hamiltonian describing linear dynamics (10) takes the form

$$H_0 = \sum_m \int dk \hbar \omega_{mk} a_{mk}^\dagger a_{mk}, \quad (54)$$

and again we restrict ourselves to a Kerr nonlinearity (31), but with a $\Gamma_3^{ijmn}(\mathbf{r})$ that will only be periodic as z ranges over L_{cell} ,

$$\Gamma_3^{ijmn}(\mathbf{r}) = \Gamma_3^{ijmn}(\mathbf{r} + \mathbf{Z}).$$

Note that while the $\mathcal{D}_{mk}(\mathbf{r})$ and $\mathcal{B}_{mk}(\mathbf{r})$ introduced in this section are dimensionless, as are the corresponding quantities defined in the last section, other quantities, such as $\mathbf{D}_{mk}(\mathbf{r})$, $\mathbf{d}_{mk}(\mathbf{r})$, and a_{mk} have different units as defined in this section from those in the last, simply because of the one-dimensional nature of the band structure here.

Nonetheless, the approach identified in the last section can be implemented here. We can introduce effective fields associated with the different bands,

$$g_m(z, t) \equiv \int \frac{d\kappa}{\sqrt{2 \pi}} a_{m(\bar{k} + \kappa)}(t) e^{i\kappa z},$$

which satisfy the commutation relations

$$[g_m(z, t), g_{m'}(z', t)] = 0,$$

$$[g_m(z, t), g_{m'}^\dagger(z', t)] = \delta_{mm'} \delta(z - z'), \quad (55)$$

and if we consider an electromagnetic field that is characterized primarily by the effective field associated with one band we can repeat the derivation in the preceding section to lead immediately to a Hamiltonian

$$H^{NLSE} = \hbar \omega_{m\bar{k}} \int dz |g_m|^2 + \frac{i\hbar}{2} \left(\frac{\partial \omega_{mk}}{\partial k} \right)_{\bar{k}} \int dz \left(\frac{\partial g_m^\dagger}{\partial z} g_m - \text{c.c.} \right)$$

$$- \frac{\hbar}{4} \left(\frac{\partial^2 \omega_{mk}}{\partial k^2} \right)_{\bar{k}} \int dz \left(\frac{\partial g_m^\dagger}{\partial z} \frac{\partial g_m}{\partial z} + \text{c.c.} \right) - \frac{\hbar}{2} \alpha_{m\bar{k}}$$

$$\times \int dz |g_m|^4 - \frac{\hbar}{2} \left(\tilde{\alpha}_{m\bar{k}}^{(z)} \int dz g_m^\dagger |g_m|^2 \frac{\partial g_m}{\partial z} + \text{c.c.} \right), \quad (56)$$

where

$$\alpha_{m\bar{k}} = \frac{3}{\hbar \varepsilon_0} \int_{cell} \frac{dz}{L_{cell}} \int dxdy \Gamma_3^{ijnl}(\mathbf{r}) (d_{m\bar{k}}^i(\mathbf{r}))^* (d_{m\bar{k}}^j(\mathbf{r}))^*$$

$$\times d_{m\bar{k}}^n(\mathbf{r}) d_{m\bar{k}}^l(\mathbf{r}),$$

$$\tilde{\alpha}_{m\bar{k}}^{(z)} = \frac{6}{\hbar \varepsilon_0} \int_{cell} \frac{dz}{L_{cell}} \int dxdy \Gamma_3^{ijnl}(\mathbf{r}) (d_{m\bar{k}}^i(\mathbf{r}))^* (d_{m\bar{k}}^j(\mathbf{r}))^*$$

$$\times d_{m\bar{k}}^n(\mathbf{r}) \gamma_{m\bar{k}}^{l(z)}(\mathbf{r}), \quad (57)$$

and

$$\gamma_{m\bar{k}}^{(z)}(\mathbf{r}) \equiv -i \left(\frac{\partial}{\partial k} \mathbf{d}_{mk}(\mathbf{r}) \right)_{\bar{k}}. \quad (58)$$

The nonlinear Schrödinger equation that results, including the shock term, is then

$$\frac{\partial g_m}{\partial t} = -i \omega_{m\bar{k}} g_m - \left(\frac{\partial \omega_{mk}}{\partial k} \right)_{\bar{k}} \frac{\partial g_m}{\partial z} + \frac{i}{2} \left(\frac{\partial^2 \omega_{mk}}{\partial k^2} \right)_{\bar{k}} \frac{\partial^2 g_m}{\partial z^2}$$

$$+ i |g_m|^2 \left(\alpha_{m\bar{k}} + 2i \text{Im}(\tilde{\alpha}_{m\bar{k}}^{(z)}) \frac{\partial}{\partial z} \right) g_m. \quad (59)$$

But our primary concern here is when there are two bands sufficiently close in frequency that it is not sufficient to consider the effective field from only one band; effective fields from both must be included. This is the situation where one

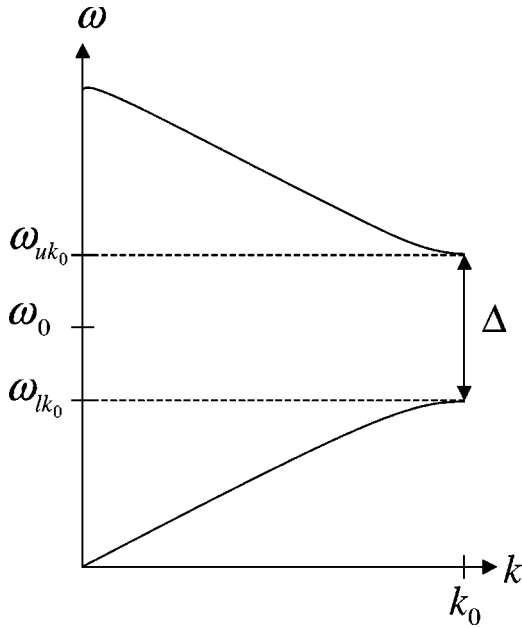


FIG. 2. A schematic diagram of the photonic band gap and first and second bands at the edge of the first Brillouin zone. Parameters relevant to the coupled mode theory are indicated.

expects coupled nonlinear mode equations to result. In earlier derivations those mode amplitudes were associated with slowly varying envelope functions modulating Bloch functions at the band edge [6,29]. In our approach, we will see that the amplitudes in the NLCME are associated with the effective field amplitudes of the two bands, but as combined by a Bogoliubov transformation.

Pulses of interest here are those whose frequency content is essentially contained in two bands $m=u,l$, where $m=u(l)$ refers to the band just above (below) the given photonic band gap. To characterize the band gap we define the gap width Δ and the Bragg frequency ω_0 ,

$$\begin{aligned}\Delta &\equiv (\omega_{uk_0} - \omega_{lk_0}), \\ \omega_0 &\equiv \frac{1}{2}(\omega_{uk_0} + \omega_{lk_0}),\end{aligned}\quad (60)$$

where ω_{uk_0} is the frequency at the upper edge of the band gap, ω_{lk_0} is the frequency at the lower edge of the band gap, and $|k_0|$ can take on the value 0 or π/L_{cell} , depending on the photonic band gap of interest. The quantities ω_0 , ω_{uk_0} , ω_{lk_0} , and Δ are indicated in Fig. 2. The photonic band gap shown in the figure is the lowest-order gap, so that $l=1$, $u=2$, and $|k_0|=\pi/L_{cell}$.

Because both the analysis of the length and time scales necessary to derive the equations, and the derivation itself, are very similar to those previously presented for a purely one-dimensional system [14], we here provide only a brief summary of the results. We start by introducing mode amplitudes s_{lk} and s_{uk} via

$$\begin{aligned}a_{uk} &= \gamma_k s_{uk} + i \eta_k s_{lk}, \\ a_{lk} &= \gamma_k s_{lk} + i \eta_k s_{uk},\end{aligned}\quad (61)$$

where γ_k and η_k are assumed to be real, and satisfy

$$\gamma_k^2 + \eta_k^2 = 1; \quad (62)$$

we set their values below. From the definitions (61) of the s_{lk} and s_{uk} , and the commutation relations (25) of the a_{ik} , we find that

$$[s_{lk}, s_{l'k'}^\dagger] = [s_{uk}, s_{u'k'}^\dagger] = \delta(k - k'), \quad (63)$$

with all other commutators vanishing. It is the s_{ik} , for $i=u,l$, that we will use to build our basic effective fields in this problem, writing

$$s_i(z, t) \equiv \int \frac{d\kappa}{\sqrt{2\pi}} s_{i(k_0+\kappa)}(t) e^{i\kappa z}. \quad (64)$$

Next we assume that to a good approximation the dispersion relation about the Bragg frequency can be considered symmetric; we can then write

$$\begin{aligned}\omega_{uk} &= \omega_0 + \frac{\Delta}{2} + \theta(\kappa), \\ \omega_{lk} &= \omega_0 - \frac{\Delta}{2} - \theta(\kappa),\end{aligned}\quad (65)$$

where we have introduced the wave number detuning

$$\kappa \equiv k - k_0. \quad (66)$$

In practice we assume that for wave numbers of importance we can take $\theta(\kappa)$ to be quadratic in κ , the coefficient of which then follows from $k \cdot p$ theory; a symmetric dispersion relation indeed then results if the far bands (i.e., those other than l and u) make a negligible contribution in the expression for the effective mass [14]. Within these approximations, we have

$$\theta(\kappa) = \frac{\kappa^2}{2} \left(\frac{\partial^2 \omega_{uk}}{\partial k^2} \right)_{k=k_0} = -\frac{\kappa^2}{2} \left(\frac{\partial^2 \omega_{ul}}{\partial k^2} \right)_{k=k_0} = \frac{|v_g|^2}{\Delta} \kappa^2, \quad (67)$$

where from a $k \cdot p$ expansion [14] we have

$$v_g = \frac{c}{\bar{n}} \int_{cell} \frac{dz}{L_{cell}} \int \frac{dx dy}{A} \hat{\mathbf{z}} \cdot \text{Re}[\mathcal{E}_{uk_0}^*(\mathbf{r}) \times \mathcal{H}_{lk_0}(\mathbf{r})], \quad (68)$$

which has the dimensions of velocity and plays the role that a ‘‘velocity matrix element’’ between the bands would in a theory of electrons in a periodic potential. We are now in a position to choose γ_k and η_k , which we do according to

$$\gamma_k = \sqrt{\frac{\Delta + \theta(\kappa)}{\Delta + 2\theta(\kappa)}}, \quad \eta_k = \text{sgn}(\kappa) \sqrt{\frac{\theta(\kappa)}{\Delta + 2\theta(\kappa)}}, \quad (69)$$

so as to guarantee

$$\omega_{uk} \gamma_k^2 + \omega_{lk} \eta_k^2 = \omega_{uk_0},$$

$$\omega_{lk}\gamma_k^2 + \omega_{uk}\eta_k^2 = \omega_{lk_0}. \quad (70)$$

Then, writing the portion of the Hamiltonian (54) that generates the linear dynamics in terms of the s_{ik} and s_{ik}^\dagger , we find

$$\begin{aligned} H_L^{CME} = & \hbar\omega_0 \int d\kappa (s_{u(k_0+\kappa)}^\dagger s_{u(k_0+\kappa)} + s_{l(k_0+\kappa)}^\dagger s_{l(k_0+\kappa)}) \\ & + \frac{\hbar\Delta}{2} \int d\kappa (s_{u(k_0+\kappa)}^\dagger s_{u(k_0+\kappa)} - s_{l(k_0+\kappa)}^\dagger s_{l(k_0+\kappa)}) \\ & - i\hbar|v_g| \int \kappa d\kappa (s_{l(k_0+\kappa)}^\dagger s_{u(k_0+\kappa)} - s_{u(k_0+\kappa)}^\dagger s_{l(k_0+\kappa)}), \end{aligned} \quad (71)$$

or

$$\begin{aligned} H_L^{CME} = & \hbar\omega_0 \int dz [s_u^\dagger(z)s_u(z) + s_l^\dagger(z)s_l(z)] \\ & + \frac{\hbar\Delta}{2} \int dz [s_u^\dagger(z)s_u(z) - s_l^\dagger(z)s_l(z)] \\ & - \frac{\hbar|v_g|}{2} \int dz \left(s_l^\dagger(z) \frac{\partial s_u(z)}{\partial z} - s_u^\dagger(z) \frac{\partial s_l(z)}{\partial z} + \text{c.c.} \right), \end{aligned} \quad (72)$$

where we keep only the contributions from band u and l , and we have assumed that for κ of importance we have $|\theta(\kappa)| \ll \Delta$.

This last inequality implies that $|\gamma_k| \gg |\eta_k|$ for k of importance, and thus to very lowest order in all our inequalities the displacement field (48) can be written as

$$\begin{aligned} \mathbf{D}(\mathbf{r}, t) \approx & \int d\kappa (s_{u(k_0+\kappa)}(t) \mathbf{D}_{uk_0}(\mathbf{r}) \\ & + s_{l(k_0+\kappa)}(t) \mathbf{D}_{lk_0}(\mathbf{r}) + \text{c.c.}) \\ = & [s_u(z, t) \mathbf{d}_{uk_0}(\mathbf{r}) + s_l(z, t) \mathbf{d}_{lk_0}(\mathbf{r})] e^{ik_0 z} + \text{c.c.} \end{aligned}$$

This is the only order we keep in evaluating the nonlinear term (31). Using the considerations discussed before Eq. (45), we find that here Eq. (31) reduces to

$$\begin{aligned} H_{NL}^{CME} = & -\frac{\hbar}{2} \alpha_{uuuu} \int |s_u(z)|^4 dz - \frac{\hbar}{2} \alpha_{llll} \int |s_l(z)|^4 dz \\ & - \frac{\hbar}{2} \alpha_{uull} \int ([s_l^\dagger(z)]^2 s_u^2(z) + [s_u^\dagger(z)]^2 s_l^2(z) \\ & + 4|s_u(z)|^2 |s_l(z)|^2) dz - \hbar \alpha_{ulll} \\ & \times \int [s_u^\dagger(z) |s_l(z)|^2 s_l(z) + s_l^\dagger(z) |s_l(z)|^2 s_u(z)] dz \\ & - \hbar \alpha_{luuu} \int [s_l^\dagger(z) |s_u(z)|^2 s_u(z) \\ & + s_u^\dagger(z) |s_u(z)|^2 s_l(z)] dz, \end{aligned} \quad (73)$$

where

$$\begin{aligned} \alpha_{mnpq} = & \frac{3}{\hbar \epsilon_0} \int_{\text{cell}} \frac{dz}{L_{\text{cell}}} dx dy \Gamma^{ijvs}(z) d_{mk_0}^i(\mathbf{r}) d_{nk_0}^j \\ & \times (\mathbf{r}) d_{pk_0}^v(\mathbf{r}) d_{qk_0}^s(\mathbf{r}), \end{aligned}$$

with m, n, p, q each equal to one of l and u , and we have used the fact that the $\mathbf{d}_{mk_0}(\mathbf{r})$ are real since k_0 is at a band edge. Because the Bloch functions there are standing waves, the coupled mode equations that the $s_m(z, t)$ satisfy are not the same as the coupled mode equations most often used in the literature. Therefore, instead of using the $s_m(z, t)$, we introduce new fields $S_\pm(z, t)$ that are associated with traveling waves:

$$S_\pm(z, t) = \frac{[s_l(z, t) \mp i s_u(z, t)]}{\sqrt{2}}. \quad (74)$$

Using the commutation relations (63) for the $s_m(z, t)$, it is straightforward to verify that the S_\pm satisfy

$$[S_\pm(z, t), S_\pm^\dagger(z', t)] = \delta(z - z'), \quad (75)$$

with all other commutation relations vanishing.

We now use the S_\pm to rewrite Eqs. (72) and (73); we find a total Hamiltonian

$$H^{CME} = H_L^{CME} + H_{NL}^{CME}, \quad (76)$$

with

$$\begin{aligned} H_L^{CME} = & \hbar\omega_0 \int dz [|S_+(z)|^2 + |S_-(z)|^2] - \frac{\hbar\Delta}{2} \\ & \times \int dz [S_-^\dagger(z) S_+(z) + S_+^\dagger(z) S_-(z)] - i \frac{\hbar|v_g|}{2} \\ & \times \int dz \left[\left(S_+^\dagger(z) \frac{\partial S_+(z)}{\partial z} - S_-^\dagger(z) \frac{\partial S_-(z)}{\partial z} \right) - \text{c.c.} \right], \end{aligned} \quad (77)$$

and

$$\begin{aligned} H_{NL}^{CME} = & -\frac{\hbar\alpha_0}{2} \int dz [|S_+(z)|^4 + |S_-(z)|^4 \\ & + 4|S_+(z)|^2 |S_-(z)|^2] - \hbar\alpha_1 \int dz [S_+^\dagger(z) S_+(z) \\ & + S_-^\dagger(z) S_-(z)] [S_-^\dagger(z) S_+(z) + S_+^\dagger(z) S_-(z)] \\ & - i\hbar\alpha_3 \int dz [S_+^\dagger(z) S_+(z) + S_-^\dagger(z) S_-(z)] \\ & \times [S_-^\dagger(z) S_+(z) - S_+^\dagger(z) S_-(z)] \\ & - \frac{\hbar\alpha_2}{2} \int dz \{ [S_-^\dagger(z)]^2 S_+^2(z) + [S_+^\dagger(z)]^2 S_-^2(z) \} \end{aligned}$$

$$-\frac{i\hbar\alpha_4}{2}\int dz\{[S_-^\dagger(z)]^2S_+^2(z)-[S_+^\dagger(z)]^2S_-^2(z)\}, \quad (78)$$

where

$$\begin{aligned} \alpha_0 &\equiv \frac{1}{4}(\alpha_{uuuu} + \alpha_{llll} + 2\alpha_{uull}), \\ \alpha_1 &\equiv \frac{1}{4}(\alpha_{llll} - \alpha_{uuuu}), \\ \alpha_2 &\equiv \frac{1}{4}(\alpha_{uuuu} + \alpha_{llll} - 6\alpha_{uull}), \\ \alpha_3 &\equiv \frac{1}{2}(\alpha_{ulll} + \alpha_{luuu}), \\ \alpha_4 &\equiv \alpha_{ulll} - \alpha_{luuu}. \end{aligned} \quad (79)$$

The field dynamics are recovered from the Heisenberg equations of motion,

$$i\hbar\frac{\partial S_\pm}{\partial t} = [S_\pm, H^{CME}], \quad (80)$$

which then yield the nonlinear coupled mode equations

$$\begin{aligned} 0 = & i\frac{\partial S_\pm}{\partial t} \pm i|v_g|\frac{\partial S_\pm}{\partial z} - \omega_0 S_\pm + \frac{\Delta}{2} S_\mp \\ & + \alpha_0(|S_\pm|^2 + 2|S_\mp|^2)S_\pm + \alpha_1(|S_+|^2 + |S_-|^2)S_\mp \\ & + \alpha_1(S_\mp^\dagger S_\pm + S_\pm^\dagger S_\mp)S_\pm \mp i\alpha_3(|S_+|^2 + |S_-|^2)S_\mp \\ & \pm i\alpha_3(S_\mp^\dagger S_\pm - S_\pm^\dagger S_\mp)S_\pm + (\alpha_2 \mp i\alpha_4)S_\pm^\dagger S_\mp^2. \end{aligned}$$

Early works [6,14] were restricted to unit cells that had center-of-inversion symmetry; in such a case the α_{ulll} and α_{luuu} terms vanish, leading to vanishing α_3 and α_4 . More recent work [30] has made use of unit cells where this is not the case.

VI. CONSERVED QUANTITIES

An advantage of a Hamiltonian formulation is that conserved quantities can be identified by looking at symmetries of the Hamiltonian. While this has been discussed earlier in Refs. [13,14], we can identify here an approach that holds for both the NLSE and the NLCME, and would hold as well for their generalizations to include higher order terms than we have done here. For definiteness we consider the three-dimensional NLSE presented in Sec. IV, and so the Hamiltonians we consider for the NLSE and NLCME are Eqs. (46) and (76), respectively.

We begin by noting that both these Hamiltonians are invariant under the infinitesimal transformation

$$\zeta_\kappa \rightarrow \zeta_\kappa e^{i\rho}, \quad (81)$$

where ζ_κ refers either to the $a_{m(\bar{\mathbf{k}}+\boldsymbol{\kappa})}$ that form the Fourier components that determine the effective field (34) that appear in the NLSE Hamiltonian (46), or one of the $s_{i(k_0+\kappa)}$, $i=u,l$, that form the Fourier components that determine the effective fields (64) that appear in the CME Hamiltonian

(76). For the NLSE, the infinitesimal quantity ρ can be taken to be either a fixed phase σ or $\nu\cdot\kappa$, where ν is a constant vector; for the CME $\rho=\sigma$ or $\nu\kappa$, where ν is a fixed number. These invariances lead to conserved quantities [13], as we now demonstrate. To do so, we define new coordinate and momentum variables, which are real

$$\begin{aligned} \phi_\kappa &= \sqrt{\frac{\hbar}{2\bar{\omega}}}(\zeta_\kappa^\dagger + \zeta_\kappa), \\ \pi_\kappa &= i\sqrt{\frac{\hbar\bar{\omega}}{2}}(\zeta_\kappa^\dagger - \zeta_\kappa), \end{aligned} \quad (82)$$

where $\bar{\omega} = \omega_{m\bar{\mathbf{k}}}(\omega_0)$ when $\zeta_\kappa = a_{m(\bar{\mathbf{k}}+\boldsymbol{\kappa})}(s_{i(k_0+\kappa)})$ for the NLSE (NLCME). In terms of these, the Heisenberg equations of motion become

$$\frac{d\phi_\kappa}{dt} = \frac{\partial H}{\partial \pi_\kappa}, \quad \frac{d\pi_\kappa}{dt} = -\frac{\partial H}{\partial \phi_\kappa}, \quad (83)$$

and the infinitesimal transformations (81) become

$$\begin{aligned} \phi_\kappa &\rightarrow \phi_\kappa - \rho \frac{1}{\bar{\omega}} \pi_\kappa, \\ \pi_\kappa &\rightarrow \pi_\kappa + \bar{\omega} \rho \phi_\kappa. \end{aligned} \quad (84)$$

Under these transformations the Hamiltonian becomes

$$H \rightarrow H + \delta H, \quad (85)$$

where, because the Hamiltonian is invariant under the transformation, $\delta H=0$. One can also determine an explicit expression for δH :

$$\begin{aligned} \delta H &= \sum_i \int d\kappa \left\{ \frac{\partial H}{\partial \phi_\kappa} \delta \phi_\kappa + \frac{\partial H}{\partial \pi_\kappa} \delta \pi_\kappa \right\} \\ &= \sum_i \int d\kappa \left\{ \frac{1}{\bar{\omega}} \frac{d\pi_\kappa}{dt} \pi_\kappa + \bar{\omega} \frac{d\phi_\kappa}{dt} \phi_\kappa \right\} \rho \\ &= \frac{d}{dt} \sum_i \int d\kappa \left\{ \frac{1}{\bar{\omega}} \pi_\kappa^2 + \bar{\omega} \phi_\kappa^2 \right\} \rho = \frac{d}{dt} \sum_i \int d\kappa \zeta_\kappa \zeta_\kappa^\dagger \rho, \end{aligned} \quad (86)$$

where we have used Eq. (82) to convert from the ϕ_κ, π_κ to the ζ_κ . Here we write the result specifically for the NLCME example, where the sum is over the fields for the different $i=u,l$. There is no sum in the example of the NLSE, and the integration involved is instead over $d\kappa$. In both cases the summation-integral on the last line is conserved, since its time derivative vanishes. This generates two conserved quantities: The first, associated with phase invariance ($\rho=\sigma$), we call the charge \mathbf{Q} ; the second, associated with translational invariance ($\rho=\nu\cdot\kappa$ or $\nu\kappa$) we call the momentum \mathbf{P} .

For the NLCME, the results are

$$\begin{aligned} Q &= \hbar \omega_0 \int_{-\infty}^{\infty} (|s_u|^2 + |s_l|^2) dz, \\ P &= \frac{\hbar}{2} \int_{-\infty}^{\infty} (s_u^\dagger \partial_z s_l - s_l^\dagger \partial_z s_u + \text{c.c.}) dz. \end{aligned} \quad (87)$$

In terms of the traveling fields (74), the quantities are

$$\begin{aligned} Q &= \hbar \omega_0 \int_{-\infty}^{\infty} (|S_+|^2 + |S_-|^2) dz, \\ P &= \frac{\hbar}{2i} \int_{-\infty}^{\infty} \left(S_+^\dagger \frac{\partial S_+}{\partial z} + S_-^\dagger \frac{\partial S_-}{\partial z} - \text{c.c.} \right) dz. \end{aligned} \quad (88)$$

For the NLSE we find

$$\begin{aligned} Q &= \hbar \omega_{m\bar{k}} \int_V d\mathbf{r} |g_m|^2, \\ P^j &= \frac{\hbar}{2i} \int_V d\mathbf{r} \left(g_m^\dagger \frac{\partial g_m}{\partial r^j} - g_m \frac{\partial g_m^\dagger}{\partial r^j} \right), \end{aligned}$$

where here the momentum is a vector quantity.

Of course, the Hamiltonian is itself a conserved quantity for both the NLSE and the NLCME as well. Including the Hamiltonian itself, we then have three conserved quantities so derived for both the NLSE and NLCME. Of these, H is straightforward to understand, since it represents conservation of energy. The quantity P represents a conserved momentum, which arises out of the translational invariance of the system. Of course, the underlying photonic crystal medium is not translationally invariant; it is only at the level of the effective equations, the NLSE and NLCME, that translational invariance obtains, and hence momentum is conserved. The quantity Q has often been referred to as the ‘‘energy’’ in the electromagnetic field, while $\bar{H} = H - Q$ has been called the ‘‘Hamiltonian’’ [9,31]. Certainly the quantity \bar{H} can be used (via Hamilton’s equations of motion) to derive the correct equations of motion for the effective fields once the carrier frequency $\bar{\omega}$ is factored out. However, unlike H , \bar{H} does not represent the total energy in the electromagnetic field. We have discussed this problem in detail elsewhere for the one-dimensional nonlinear Schrödinger equation [13], and now consider the more complicated situation that arises in the Hamiltonian formulation of the nonlinear Schrödinger equation with a shock term.

VII. DIFFERENT SHOCK TERMS

The nature of the shock term that appears in our nonlinear Schrödinger equations, for example, in the one-dimensional example described by Eq. (59), is different from the kind of shock term that often appears in the literature. In this section we address that difference and its physical meaning, which highlights the difference between our approach here and the more usual one of deriving slowly varying envelope functions. To focus on that we consider the simple limit of a

uniform (nondispersive) medium, with $n(\mathbf{r}) = \bar{n}$. Our one-dimensional structure equations from the start of Sec. V can be applied by simply taking the area A to be a normalization area in the xy plane; that is, in integrals such as those appearing in Eqs. (53) and (57) we take the integral over the plane to range only over an area A . The band index m can be dropped, and if we consider displacement fields polarized in the x direction we find from Eq. (53) the simple result that

$$\mathcal{D}_k(\mathbf{r}) = \hat{\mathbf{x}}, \quad (89)$$

and then from Eq. (57) that

$$\alpha_{\bar{k}} = \frac{3 \varepsilon_0 \bar{n}^2 c^2 \bar{k}^2 \hbar \Gamma_3^{xxxx}}{4A}$$

and

$$\bar{\alpha}_{\bar{k}}^{(z)} = -\frac{i}{\bar{k}} \alpha_{\bar{k}}, \quad (90)$$

the area A appearing in these expressions simply because $|g(z,t)|^2$ is (approximately) equal to the energy flux through that area. With these expressions the Hamiltonian (56) reduces to

$$\begin{aligned} H &= \hbar \bar{\omega} \int dz |g|^2 + \frac{i \hbar c}{2 \bar{n}} \int dz \left(\frac{\partial g^\dagger}{\partial z} g - \text{c.c.} \right) - \frac{\hbar}{2} \alpha_{\bar{k}} \int dz |g_m|^4 \\ &+ \frac{i \hbar}{2 \bar{k}} \left(\alpha_{\bar{k}} \int dz g_m^\dagger |g_m|^2 \frac{\partial g_m}{\partial z} - \text{c.c.} \right), \end{aligned} \quad (91)$$

where we have put $\bar{\omega} \equiv c \bar{k} / \bar{n}$, and our dynamical Eq. (59) becomes

$$\frac{\partial g}{\partial t} + \frac{c}{\bar{n}} \frac{\partial g}{\partial z} = -i \bar{\omega} g + i \alpha_{\bar{k}} |g|^2 g + \frac{2 \alpha_{\bar{k}}}{\bar{k}} |g|^2 \frac{\partial g}{\partial z}. \quad (92)$$

More usual equations in the literature given in Refs. [15,32,33], on the other hand, are of a different form,

$$\frac{\partial f}{\partial t} + \frac{c}{\bar{n}} \frac{\partial f}{\partial z} = i \alpha_{\bar{k}} |f|^2 f + \frac{\alpha_{\bar{k}}}{\bar{k}} \frac{\partial}{\partial z} (|f|^2 f), \quad (93)$$

in our notation. The rapidly varying term $(-i \bar{\omega} g)$ that appears in Eq. (92) but not Eq. (93) is of course a trivial difference; it can be removed from Eq. (92) or added to Eq. (93) by redefining the field in terms of a rapidly varying phase term: $g = g' \exp(-i \bar{\omega} t)$. The more serious difference is the shock term, where Eq. (92) seems to be missing one of the terms that would result from taking the derivative in Eq. (93).

In fact both equations are correct, if understood to be at the same level of approximation; the fields g and f are simply different. To see that we need to briefly review the derivation of Eq. (93), which is not completely trivial. While this is usually done in the literature by beginning with the electric field as the fundamental field, for comparison with our work

we do it here in terms of the displacement field. In the one-dimensional uniform medium we consider, the second-order equation that $D(z,t)$ satisfies follows directly from the equations at the start of Sec. II, and is

$$\frac{\bar{n}^2}{c^2} \frac{\partial^2 D}{\partial t^2} - \frac{\partial^2 D}{\partial z^2} = -\bar{n}^2 \Gamma_3^{\text{xxxx}} \frac{\partial^2 (D^3)}{\partial t^2}. \quad (94)$$

To get an equation similar to Eq. (93) one looks for a slowly varying amplitude function $f(z,t)$, writing

$$D(z,t) = \nu f(z,t) e^{i(\bar{k}z - \bar{\omega}t)} + \text{c.c.}, \quad (95)$$

where we have chosen an overall factor

$$\nu = \sqrt{\frac{\varepsilon_0 \bar{n}^2 \hbar \bar{\omega}}{2A}}$$

for convenience in comparisons below. Using the ansatz (95) in the differential equation (94) we find

$$\frac{\partial f}{\partial t} + \frac{c}{\bar{n}} \frac{\partial f}{\partial z} = i \alpha_{\bar{k}} |f|^2 f + \frac{2 \alpha_{\bar{k}}}{\bar{k}} \frac{\partial}{\partial z} (|f|^2 f) + T_{\text{corr}}, \quad (96)$$

where

$$T_{\text{corr}} = -\frac{i}{2\bar{k}} \left(\frac{\bar{n}}{c} \frac{\partial^2 f}{\partial t^2} - \frac{c}{\bar{n}} \frac{\partial^2 f}{\partial z^2} \right). \quad (97)$$

In going from Eqs. (94) and (95) to Eqs. (96) and (97) we have neglected the terms in D^3 that result in third harmonic generation, as well as a higher-order shock term of the form $\partial^2(|f|^2 f)/\partial z^2$. Often, of course, higher-order derivative terms of slowly varying envelope functions such as those appearing in T_{corr} Eq. (97), can also be neglected. However, here they must be kept, because in keeping the shock terms in our equations we keep terms of first order in both $\alpha_{\bar{k}}$ and $\alpha_{\bar{k}} \bar{k}^{-1} \partial/\partial z$. Nonetheless, at this level of approximation it does suffice, in evaluating T_{corr} in terms of f , to use only the first term on the right-hand side of Eq. (96), and then indeed even replace $\partial/\partial t$ simply by $c\bar{n}^{-1} \partial/\partial z$ when that derivative is premultiplied by $\alpha_{\bar{k}}$. When this is done and the terms are collected, we find Eq. (93).

The derivation makes clear the difference between the fields $f(z,t)$ and $g(z,t)$. From Eq. (95) and recalling Eqs. (89) and (51) we see that the ansatz (95) can be written in the form

$$\mathbf{D}(\mathbf{r},t) = \mathbf{d}_{\bar{k}}(\mathbf{r}) f(z,t) e^{i(\bar{k}z - \bar{\omega}t)} + \text{c.c.}, \quad (98)$$

simply the one-dimensional analog in this simple problem of the general form Eq. (33), while our derivation of the Eq. (92) makes use of the one-dimensional analog of Eq. (36). Comparing these, the relation between $f(z,t)$ and $g(z,t)$ is

$$f(z,t) = e^{i\bar{\omega}t} \left[g(z,t) - \frac{i}{2\bar{k}} \frac{\partial g(z,t)}{\partial z} + \dots \right], \quad (99)$$

and when this is used in Eq. (93) and terms are kept at the appropriate level of approximation, as discussed above, we recover Eq. (92).

We note, however, that while the effective field $g(z,t)$ satisfies canonical commutation relations (55), the field $f(z,t)$ does not; furthermore, while the Hamiltonian (56) could be written to the appropriate level of approximation in terms of $f(z,t)$, neither its derivation beginning from Eq. (98), nor its application with noncanonical commutation relations, would be as simple as the derivation and application of the Hamiltonian (91), and others in this paper similar to it.

Indeed, the way that terms such as ‘‘Hamiltonian’’, as well as others such as ‘‘momentum’’ and ‘‘energy’’, arise in the literature in equations such as Eq. (93) is rather different than in the kind of canonical approach we have taken here. To see this in some detail, we reinstate the dispersive term in our one-dimensional equation. Retaining the uniform medium approximation but otherwise taking $\omega = \omega(k)$, the relation analogous to Eq. (99) is

$$f(z,t) = e^{i\bar{\omega}t} \left[g(z,t) - i \frac{\bar{\omega}'}{2\bar{\omega}} \frac{\partial g(z,t)}{\partial z} + \dots \right], \quad (100)$$

where $\bar{\omega}' \equiv (\partial\omega/\partial k)_{\bar{k}}$; in what follows we will also use $\bar{\omega}'' \equiv (\partial^2\omega/\partial k^2)_{\bar{k}}$. Then we have, instead of Eq. (93), the equation

$$\frac{\partial f}{\partial t} + \bar{\omega}' \frac{\partial f}{\partial z} = \frac{i}{2} \bar{\omega}'' \frac{\partial^2 f}{\partial z^2} + i \alpha_{\bar{k}} |f|^2 f + i \bar{\alpha}_{\bar{k}}^{(z)} \frac{\partial}{\partial z} (|f|^2 f), \quad (101)$$

which follows from our Eq. (59) and the use of relation (100), keeping contributions to the appropriate order; we have reinstated the explicit appearance of the factor $\bar{\alpha}_{\bar{k}}^{(z)}$, which is seen to be purely imaginary from a relation analogous to Eq. (90). As Eq. (59) and Eq. (101) is integrable by means of an inverse scattering transform [34]. Thus an infinite set of conservation laws can be derived from a recursion formula. The first three such conserved quantities, which we have scaled by overall constants, are

$$\begin{aligned} \mathbf{C}_1 &= \int dz |f|^2, \\ \mathbf{C}_2 &= \int dz \left[i \left(f^\dagger \frac{\partial f}{\partial z} - f \frac{\partial f^\dagger}{\partial z} \right) + \frac{2i \bar{\alpha}_{\bar{k}}^{(z)}}{\bar{\omega}''} |f|^4 \right], \\ \mathbf{C}_3 &= \int dz \left[\bar{\omega}'' \frac{\partial f^\dagger}{\partial z} \frac{\partial f}{\partial z} - \alpha_{\bar{k}} |f|^4 + \frac{3}{2} i (\bar{\alpha}_{\bar{k}}^{(z)}) |f|^2 \right. \\ &\quad \left. \times \left(f^\dagger \frac{\partial f}{\partial z} - f \frac{\partial f^\dagger}{\partial z} \right) + \frac{2}{\bar{\omega}''} (i \bar{\alpha}_{\bar{k}}^{(z)})^2 |f|^6 \right], \end{aligned} \quad (102)$$

and these have been given varying interpretations in the literature. For example, they have been called the ‘‘energy’’, ‘‘momentum’’, and ‘‘Hamiltonian’’ respectively, [32]. In order to compare these conserved quantities of Eq. (101) with

those of Eq. (59), we first consider both equations in the limit $\bar{\alpha}_k^{(z)} \rightarrow 0$, where they share a common form apart from a trivial phase term, which we neglect below. Then the quantities (102) take the simple form

$$\begin{aligned} \mathbf{C}_1^{NLSE} &= \int dz |f|^2, \\ \mathbf{C}_2^{NLSE} &= \int dz \left(if^\dagger \frac{\partial f}{\partial z} - if \frac{\partial f^\dagger}{\partial z} \right), \\ \mathbf{C}_3^{NLSE} &= \int dz \left(\bar{\omega}'' \frac{\partial f^\dagger}{\partial z} \frac{\partial f}{\partial z} - \alpha_k |f|^4 \right). \end{aligned} \quad (103)$$

The conserved quantity \mathbf{C}_3^{NLSE} has been called a Hamiltonian [35], and rightly so, since the NLSE (101) with $\bar{\alpha}_k^{(z)} = 0$ can be written straightforwardly in canonical form—i.e., as Hamilton's equations for a pair of fields composed from a linear combination of f and f^\dagger , satisfying canonical commutation relations—with \mathbf{C}_3^{NLSE} as the Hamiltonian [36,13]. Furthermore, one can compose a canonical Hamiltonian, i.e., one that is numerically equal to the electromagnetic energy, by taking a particular linear combination of \mathbf{C}_1^{NLSE} , \mathbf{C}_2^{NLSE} , and \mathbf{C}_3^{NLSE} [13]. A problem arises, however, when the shock term is reinstated, since \mathbf{C}_3 has a term proportional to $|f|^6$. Certainly in this case one cannot form a pair of fields from a linear combination of f and f^\dagger , introduce canonical commutation relations for those fields, and recover an equation with nonlinear terms like those of Eq. (101) from Hamilton's equations. So although \mathbf{C}_3 is a conserved quantity associated with Eq. (101), it cannot be used as a Hamiltonian with canonical commutation relations to generate Eq. (101).

Furthermore, there is no straightforward way for Eq. (101) to be generated by *any* Hamiltonian, and to thus obtain a shock term of the form $\partial(|f|^2 f)/\partial z$ from a canonical Hamiltonian formulation, in the following sense. Assume we impose canonical commutation relations on a pair of fields ϕ and $\bar{\phi}$, which are linear combinations of f and f^\dagger . If we then write down any integral H composed of sums of products of f , f^\dagger , and their spatial derivatives, and write H in terms of ϕ and $\bar{\phi}$, then Hamilton's equations for ϕ and $\bar{\phi}$, with H as the Hamiltonian can only yield a shock term of the form we have presented in this paper. The relevant commutator, for equal times, is

$$\begin{aligned} & \left[f(z'), \int dz \left(\xi_1 f^\dagger(z) f^\dagger(z) f(z) \frac{\partial f(z)}{\partial z} \right. \right. \\ & \quad \left. \left. + \xi_2 f(z) f(z) f^\dagger(z) \frac{\partial f^\dagger(z)}{\partial z} \right) \right] \\ & = 2(\xi_1 - \xi_2) |f(z')|^2 \frac{\partial f(z')}{\partial z'}, \end{aligned}$$

where ξ_1 and ξ_2 are complex numbers.

We also note that the quantity \mathbf{C}_1 clearly does not correspond to the electromagnetic energy, as can be verified by

using Eq. (100) in Eq. (56). Instead, it is better interpreted as a “charge,” as we have done here, or a “particle number” [35].

The quantity \mathbf{C}_2^{NLSE} gives the familiar expression for the momentum of the NLSE in the absence of the shock term. In this limit, the expression for the momentum \mathbf{C}_2 of f has the same form as the momentum \mathbf{P} of the effective field g derived in the previous section. This similarity is lost, however, if the shock term is reinstated. In that case, \mathbf{C}_2 acquires a term proportional to $|f|^4$, while the expression for \mathbf{P} for the field g is unchanged. Since the integral over all z of $|f|^4$ is not itself conserved, it is clear that the expression for the conserved momentum of the NLSE must be modified if one augmented it with the conventional shock term. In fact, the shock term derived in this paper is the only possible shock term involving one spatial derivative and three factors of g or g^\dagger that can be added to the NLSE without changing the expression for the conserved momentum.

The simplicity with which the field equations can be derived by the canonical approach described here, together with the way we can truly identify quantities connected with symmetries and called “charge”, “momentum”, and “energy” as they are in the rest of physics, seems to us a cogent argument for our approach.

VIII. SHOCK TERM ENHANCEMENT IN PHOTONIC CRYSTALS

Concern with the nature and treatment of the shock term is not purely academic, for the shock term can be enhanced in photonic crystals over the value it would take in a uniform medium, and it—and perhaps even successive terms in the expansion that generated it—can be comparable in size to the usual self-phase modulation term in the nonlinear Schrödinger equation. To demonstrate this, we consider a photonic crystal structure composed of a square lattice of cylindrical rods of infinite length, from which three adjacent (100)-direction rows of rods have been removed, as indicated in the inset of Fig. 3. This structure is similar to the one depicted in Fig. 1(b); it differs in that it avoids the complications associated with cylinders of finite length, but is similar in supporting guided modes in the defect region. It is in these guided modes that we will examine shock term enhancement. This defect paradigm for photonic crystal waveguides has been the subject of intense fabrication efforts [37–41] and has also been studied numerically [42–47].

To consider guided modes of the waveguide structure, we find Bloch modes with wave vector $\mathbf{k}=(0,0,k)$, as indicated in the inset of Fig. 3. The calculations are accomplished by constructing a supercell in the direction in which the periodicity is broken by the defect, so we are formally considering a periodic array of adjacent waveguides separated by a supercell width. As long as the amplitude of the guided fields is low at the edge of the supercell, the results should provide a good approximation to the behavior of the guided fields of a single line defect waveguide. Since this supercell structure has three-dimensional periodicity, we can describe the guided modes of the structure by using the 3D structure formalism from Sec. IV for frequencies within a band, or not

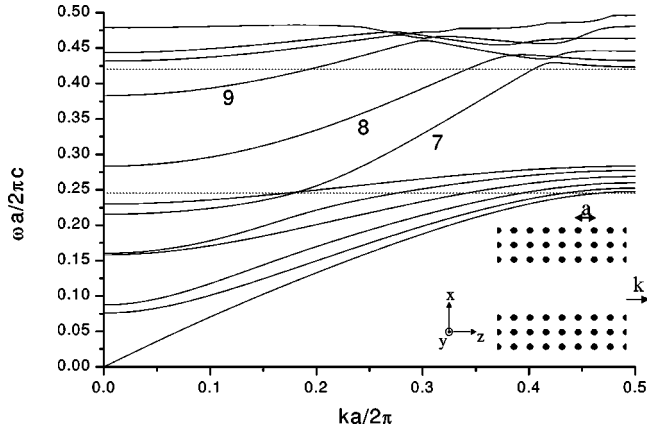


FIG. 3. Band structure of a 2D photonic crystal with a line defect waveguide. Three adjacent (100)-direction rows of rods have been removed from a bulk crystal of lattice constant a to form the waveguide. The dielectric function is depicted in the inset, which also indicates the direction of k . The region between the horizontal dotted lines corresponds to the in-plane photonic band gap of the bulk crystal, and indicates the location of the guided defect modes.

too far within a band gap [48].

Because the wave vector lies in the plane of the lattice, the Bloch modes can be separated by polarization, and we specifically consider TM modes, i.e., those with electric fields polarized parallel to the rods. The calculations are performed using a freely available package [49] which uses a polarized plane wave basis to solve the linear Maxwell eigenproblem using a conjugate gradient method. In units of the lattice constant a , the supercell consists of a 9×1 array of cylindrical rods of radius $r=0.2$, with three adjacent rods removed to form the defect. The rods are taken to have an index of refraction of 3.4, typical of a semiconductor material at optical or telecommunications wavelengths. The background is taken to be air. This supercell dielectric function is shown in the inset of Fig. 3.

In selecting a band labeling scheme, we favor smoothness of the bands in k , at the cost of having to forego global numbering by ascending order in frequency. Specifically, we choose to number the bands in order of ascending frequency, when smoothly followed to the X point, which is at $ka/2\pi = 0.5$ in Fig. 3. Thus $\partial\omega_{mk}/\partial k$ is continuous everywhere in k space, and following the discussion after Eq. (37), it is possible to have continuity in k of \mathbf{d}_{mk} . The band structure is plotted in Fig. 3. While most of the bands are bulk modes, each of the bands 7, 8, and 9 are guided modes for some region of the ΓX line in k space. These bands, respectively, correspond to bound modes with zero, one, and two nodal planes parallel to the yz plane. In what follows, we focus on band 8.

Since the TM mode has a linearly polarized displacement field, the following calculations are independent of the symmetry of the third-order nonlinear response. Since we will be interested in comparing the relative size of the shock term and the self-phase modulation term, we will not need definite values for $\Gamma_3^{ijmn}(\mathbf{r})$, and we scale all our results to the value of the one important response tensor component Γ_3^{yyyy} in the dielectric. From the Eqs. (57) for $\alpha_{m\bar{k}}$ and $\tilde{\alpha}_{m\bar{k}}^{(z)}$ we have

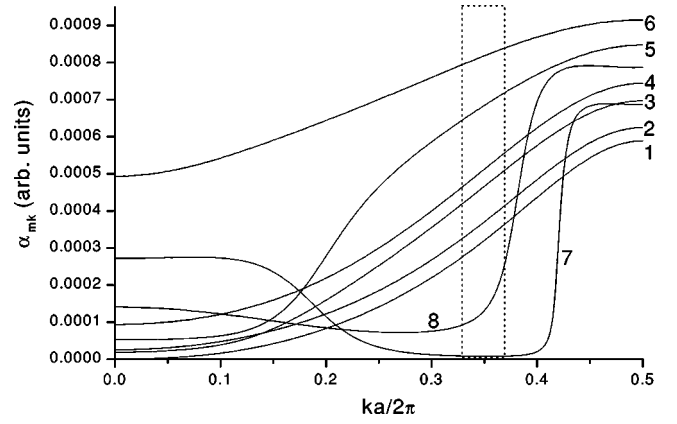


FIG. 4. The nonlinear coefficient α_{mk} for k up to the Brillouin zone edge in the z direction, for the lowest eight bands.

$$\text{Im } \tilde{\alpha}_{m\bar{k}}^{(z)} = -\frac{1}{2} \frac{\partial}{\partial k_z} (\alpha_{mk})_{\bar{k}}.$$

Figure 4 shows the coefficient α_{mk} for k up to the Brillouin zone edge in the z direction for the lowest eight bands. For this structure, we find that the bulk modes show no interesting features in terms of α_{mk} , but the guided modes can show both negative slopes and sharp rises.

The ratio of the shock term to the self-phase modulation term in the dynamical equation (59) is given by

$$R = -iR_c R_p,$$

where we have defined the dimensionless quantities

$$R_c \equiv (a\alpha_{mk})^{-1} \frac{\partial}{\partial k_z} (\alpha_{mk})_{\bar{k}},$$

$$R_p \equiv (g_m)^{-1} a \frac{\partial g_m}{\partial z}, \quad (104)$$

where a is the lattice constant. Here R_c contains the information about the photonic crystal, and R_p contains the information about the pulse. We note that while the ratios R , R_c , and R_p have arisen here within a formulation of the NLSE in terms of field amplitudes in Eq. (59), these ratios have numerical values common to formulations in terms of field amplitudes, power amplitudes, or intensity amplitudes. Now our whole expansion of the linear part of the dynamics requires that $R_p \ll 1$, and so for the shock term to be as large as the self-phase modulation term, in the regime where the kind of effective field description we are constructing here is applicable, we require $R_c \gg 1$, so that $|R| \approx 1$. For many typical points in the band structure, this condition is not met; in fact, we often find $R_c \lesssim 1$, so that it is reasonable to neglect the shock term in characterizing the dynamics, at least at the order considered in this paper. However, at certain points in the band structure, R_c can be enhanced by an order of magnitude, so that $R_c \gtrsim 1$ and $|R| \lesssim 1$. While not as large as the self-phase modulation term in this case, the shock term could not be dismissed out of hand, and indeed could make a significant contribution to the dynamics. In this work we only

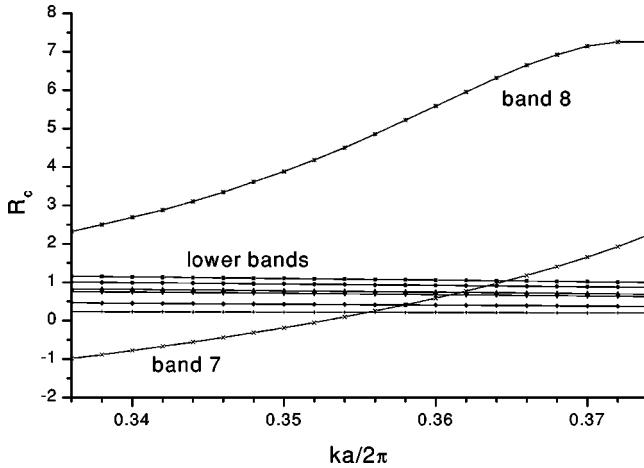


FIG. 5. The shock-enhancement factor R_c , calculated for the lowest eight bands of the photonic crystal for wave vector k in the z direction, over the domain corresponding to the boxed area in Fig. 4. This corresponds to the domain for which the upper bound mode, band 8, is near the upper band edge of the photonic band gap of the bulk crystal. Note the significant k dependence, and the range of values attained by the guided modes near the upper band edge.

concern ourselves with showing an order-of-magnitude enhancement of the shock term and arguing for the plausibility of a significant effect; we defer a more detailed analysis to later work.

Figure 5 shows R_c calculated for the lowest eight bands of the photonic crystal for wave vector k ranging over the domain corresponding to the boxed area in Fig. 4. This corresponds to the domain for which the upper bound mode, band 8, is near the upper band edge of the photonic band gap of the bulk crystal. While the lowest six bands show no significant k dependence of R_c over this range and have R_c less than or very close to unity, the guided modes show significant k -dependence, and take on positive or negative values. Band 8 shows a significant enhancement of R_c as the mode frequency approaches the upper band edge of the bulk crystal. For example, when $ka/(2\pi)=0.36$, band 8 is still a well-confined mode, and yet has $R_c=5.6$, an order of magnitude larger than that obtained for most of the lower bands. Band 4, in comparison, has $R_c=0.40$ at the same point.

This enhancement of the shock effect can be readily interpreted within the framework of this paper. The factor α_{mk} can be interpreted as the degree to which the Bloch mode samples the nonlinearity of the dielectric. As we traverse band 8 from the center of the bulk gap region towards the upper band edge, the mode profile remains relatively constant. However, in crossing the upper band edge and changing from a strongly confined mode to an unconfined bulk mode of a different profile, the mode undergoes a significant change. Although this only corresponds to a small change in the mode energy, it corresponds to a significant change in the quartic sampling of the nonlinearity by the Bloch mode. And since the change occurs over a relatively small range of k vectors near the band edge, the derivative is large, and thus $\text{Im } \alpha_{mk}^p$ is large. Furthermore, since the waveguide has an air core, the guided modes sample little of the dielectric, so α_{mk} is low. Thus R_c is large.

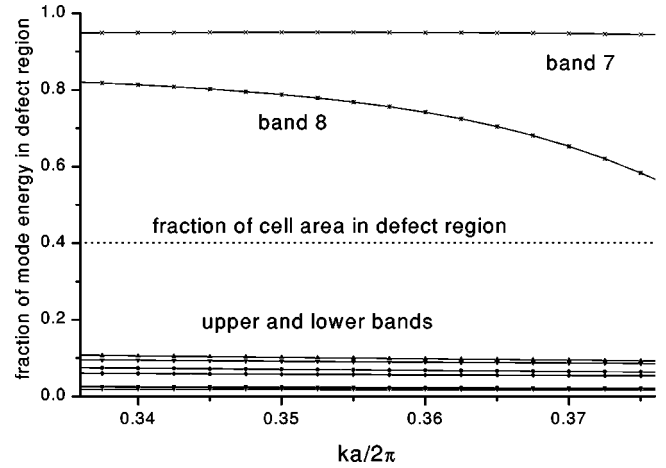


FIG. 6. Fraction of mode energy confined in the defect region. As a baseline for comparison, the defect region—which is taken to be the largest rectangular zone that can be inscribed in the cell without overlapping any of the cylinders—comprises 40% of the unit cell, and the nonguided lower supercell modes all have roughly 10% of their energy or less confined to the defect region.

This shock enhancement is significant even where the mode is still well confined. In the case of $ka/(2\pi)=0.36$ given above, 74% of the total mode energy of band 8 is in the defect region, compared with 85% when optimally confined. Beyond this, the dropoff in confined energy is shown in Fig. 6. As a baseline for comparison, the defect region—which is taken to be the largest rectangular zone that can be inscribed in the cell without overlapping any of the cylinders—comprises 40% of the unit cell, and each of the rest of the lowest ten bands have roughly 10% of their energy or less confined to it.

Of course, we have only shown here that in a specific case the shock term can get large enough in a photonic crystal to be of concern when considering nonlinear propagation. Whether or not such a term will remain significant as time evolves, and indeed whether or not the kind of expansion we have used in this paper will remain adequate as the field propagates are more complicated issues that we plan to address in a future paper.

IX. CONCLUSION

The goal of this paper has been to develop an approach to treat the nonlinear propagation of electromagnetic fields in photonic crystals based on the introduction of effective fields. While we began with $\mathbf{D}(\mathbf{r},t)$ and $\mathbf{B}(\mathbf{r},t)$ as our fundamental fields, rather than the more usual $\mathbf{E}(\mathbf{r},t)$ and $\mathbf{H}(\mathbf{r},t)$, this was only to facilitate the simple canonical formulation of the electromagnetic field. The fields that become our dynamical quantities in this approach are neither $\mathbf{D}(\mathbf{r},t)$ and $\mathbf{B}(\mathbf{r},t)$, nor $\mathbf{E}(\mathbf{r},t)$ and $\mathbf{H}(\mathbf{r},t)$, but rather effective fields that we construct in real space from the canonical amplitudes of the different Fourier components of the electromagnetic field. These scalar fields satisfy the canonical commutation relations exactly, so even when their dynamics are only described approximately they remain simple quantities with which to work. And, indeed, it is simpler to derive their

approximate dynamics than to derive the approximate dynamics of the slowly varying envelope functions associated with the electromagnetic field itself. Because this approach is based on a canonical formulation of the electromagnetic field, the Hamiltonian and its symmetries are available for the investigation and identification of conserved quantities, and the resulting theory is such that quantization can be easily undertaken.

We have used this approach to derive the usual nonlinear Schrödinger equation and nonlinear coupled mode equations that have formed the basis of much of the discussion of nonlinear propagation in one-dimensional structures. Through the approach developed here, they can be extended to higher dimensional structures with large variations in the linear properties of the photonic crystal. We have also shown how the approach easily allows for the extension of these usual equations to include higher-order terms, investigating the first “shock” type correction that appears in the nonlinear Schrödinger equation. We have argued that this term arises in our approach in a form that is more convenient than it does in other, more direct approaches based directly on envelope functions characterizing one of the Maxwell fields, in that a canonical Hamiltonian theory results. And we have argued that this term can indeed be important in nonlinear propagation in photonic crystals.

Throughout we have considered only a Kerr nonlinearity, investigated only third-order nonlinear processes associated with an intensity dependent refractive index, and restricted ourselves to wave packets centered at points in the band structure where there are no degeneracies. And the canonical formulation we have employed is restricted to material media that themselves are approximated as lossless and dispersionless. But extensions to more complicated nonlinearities, to nonlinear parametric processes involving frequency mixing, and to effective fields associated with points or lines of degeneracy can also be considered within this framework. And recent work that allows a canonical formulation of a dispersive and lossy material medium [50] can be generalized to treat photonic crystals and included in this framework. We plan to turn to these issues in future papers.

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APPENDIX: DISCRETE AND CONTINUOUS MODE NOTATION

In this Appendix we sketch how the various normalization factors that appear in Secs. IV and V arise in moving from the discrete labeling of modes used in Sec. III to the continu-

ous labeling used in those latter sections. That continuous labeling is of two types. In Sec. IV we are interested in a 3D photonic crystal, or in a region of the Brillouin zone of a lower dimensional photonic structure where the solutions of the linear Maxwell equations are characterized by band indices m and crystal wave vectors \mathbf{k} that range continuously in all directions about a given point in reciprocal space. In Sec. V we focus on lower dimensional structures and a region of the Brillouin zone where, for a given band index m or a given set of band indices, there is a family of solutions of the linear Maxwell equations characterized by a one dimensional crystal wave number k that varies continuously. We consider the mode notation for these two cases below. In this appendix, and only here, we use tildes to indicate the discrete mode functions and associated amplitudes introduced in Sec. III, such as $(\tilde{\mathbf{D}}_\alpha(\mathbf{r}), \tilde{\mathbf{B}}_\alpha(\mathbf{r}))$ and $\tilde{a}_\alpha(t)$ to distinguish between these discretely labeled mode functions and the continuously labeled mode functions we introduce here. While the discussion here is self-contained, rather than repeating equations we will refer back to those that already appear in the text.

We begin first with the mode structure of interest in Sec. IV, and consider first the use of Bloch’s theorem to label our modes by a band index m and a crystal wave vector \mathbf{k} that lies within the first Brillouin zone. Our index α then is replaced by the pair $m\mathbf{k}$, and we write our modes as

$$\begin{aligned}\tilde{\mathbf{D}}_{m\mathbf{k}}(\mathbf{r}) &= \sqrt{\frac{\epsilon_0 \bar{n}^2 \hbar \omega_{m\mathbf{k}}}{2V}} \mathcal{D}_{m\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}, \\ \tilde{\mathbf{B}}_{m\mathbf{k}}(\mathbf{r}) &= \sqrt{\frac{\mu_0 \hbar \omega_{m\mathbf{k}}}{2V}} \mathcal{B}_{m\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}},\end{aligned}\quad (\text{A1})$$

where \bar{n} is a reference refractive index, the value of which can be chosen for convenience; we assume a unit cell volume V_{cell} and a normalization volume of N unit cells, with volume $V = NV_{cell}$. We choose the factors in Eq. (A1) so that the periodic parts (28) of the Bloch functions are normalized according to Eq. (29) for any \mathbf{k} , as follows from Eq. (A1) and Eqs. (17) and (18). We do not use tildes on the functions $(\mathcal{D}_{m\mathbf{k}}(\mathbf{r}), \mathcal{B}_{m\mathbf{k}}(\mathbf{r}))$ because we will keep these functions as we move to continuous notation, which we now do.

We want to move from discrete mode amplitudes satisfying

$$[\tilde{a}_{m\mathbf{k}}, \tilde{a}_{m'\mathbf{k}'}^\dagger] = \delta_{mm'} \delta_{\mathbf{k}\mathbf{k}'},$$

to continuously labeled mode amplitudes satisfying

$$[a_{m\mathbf{k}}, a_{m'\mathbf{k}'}^\dagger] = \delta_{mm'} \delta(\mathbf{k} - \mathbf{k}').$$

From these follow

$$\begin{aligned}\sum_{m'\mathbf{k}'} [\tilde{a}_{m\mathbf{k}}, \tilde{a}_{m'\mathbf{k}'}^\dagger] &= 1, \\ \sum_{m'} \int [a_{m\mathbf{k}}, a_{m'\mathbf{k}'}^\dagger] d\mathbf{k}' &= 1,\end{aligned}\quad (\text{A2})$$

respectively, and using

$$\sum_{\mathbf{k}'} \rightarrow V \int \frac{d\mathbf{k}'}{8\pi^3} \quad (\text{A3})$$

as we move from discrete to continuous labeling of wave vectors, Eq. (A2) imply that

$$\tilde{a}_{m\mathbf{k}} \rightarrow \sqrt{\frac{8\pi^3}{V}} a_{m\mathbf{k}}. \quad (\text{A4})$$

The same approach, as we move from the normalization conditions (17) and (18) to Eq. (26) leads to

$$\begin{aligned} \tilde{\mathbf{D}}_{m\mathbf{k}}(\mathbf{r}) &\rightarrow \sqrt{\frac{8\pi^3}{V}} \mathbf{D}_{m\mathbf{k}}(\mathbf{r}), \\ \tilde{\mathbf{B}}_{m\mathbf{k}}(\mathbf{r}) &\rightarrow \sqrt{\frac{8\pi^3}{V}} \mathbf{B}_{m\mathbf{k}}(\mathbf{r}), \end{aligned} \quad (\text{A5})$$

and hence to Eq. (27). Using the relations (A4) and (A5) together with the summation-to-integration form Eq. (A3) we recover Eq. (24) from Eq. (20) and Eq. (30) from Eq. (22).

We now turn to the mode structure of interest in Sec. V, where we only have periodicity in one direction, which we take as z . Our general index α then now replaced by the pair mk , and we write our modes as

$$\begin{aligned} \tilde{\mathbf{D}}_{mk}(\mathbf{r}) &= \sqrt{\frac{\epsilon_0 \bar{n}^2 \hbar \omega_{mk}}{2LA}} \mathbf{D}_{mk}(\mathbf{r}) e^{ikz}, \\ \tilde{\mathbf{B}}_{mk}(\mathbf{r}) &= \sqrt{\frac{\mu_0 \hbar \omega_{mk}}{2LA}} \mathbf{B}_{mk}(\mathbf{r}) e^{ikz}. \end{aligned} \quad (\text{A6})$$

Here we assume a periodicity of L_{cell} in the z direction and a normalization length of N unit cells, with length $L = NL_{cell}$. Now integrals in Eqs. (17) and (18) range over L in the z direction but over all x and y ; nonetheless, we introduce a nominal area A in the xy plane that we use for convenience in our normalization constants. The factors in Eq. (A6) are such that the periodic parts (52) of the Bloch functions are normalized according to Eq. (53) for any k , following from Eqs. (A6), (17), and (18). Again we do not use

tildes on the functions ($\mathcal{D}_{m\mathbf{k}}(\mathbf{r}), \mathcal{B}_{m\mathbf{k}}(\mathbf{r})$) because we will keep these functions as we move to continuous notation.

Here our task is to move from discrete mode amplitudes satisfying

$$[\tilde{a}_{mk}, \tilde{a}_{m'k'}^\dagger] = \delta_{mm'} \delta_{kk'},$$

to continuously labeled mode amplitudes satisfying

$$[a_{mk}, a_{m'k'}^\dagger] = \delta_{mm'} \delta(k-k').$$

The procedure follows that above; from

$$\begin{aligned} \sum_{m'k'} [\tilde{a}_{mk}, \tilde{a}_{m'k'}^\dagger] &= 1, \\ \sum_{m'} \int [a_{mk}, a_{m'k'}^\dagger] dk' &= 1, \end{aligned} \quad (\text{A7})$$

and now

$$\sum_{k'} \rightarrow L \int \frac{dk'}{2\pi} \quad (\text{A8})$$

as we move from discrete to continuous labeling of wave vectors, Eq. (A7) imply that

$$\tilde{a}_{mk} \rightarrow \sqrt{\frac{2\pi}{L}} a_{mk}. \quad (\text{A9})$$

The same approach, as we move from the normalization conditions (17) and (18) to Eq. (50) leads to

$$\begin{aligned} \tilde{\mathbf{D}}_{mk}(\mathbf{r}) &\rightarrow \sqrt{\frac{2\pi}{L}} \mathbf{D}_{mk}(\mathbf{r}), \\ \tilde{\mathbf{B}}_{mk}(\mathbf{r}) &\rightarrow \sqrt{\frac{2\pi}{L}} \mathbf{B}_{mk}(\mathbf{r}), \end{aligned} \quad (\text{A10})$$

and hence to Eq. (51). Following the approach used in the three-dimensional case above, using the relations (A9) and (A10) together with the summation-to-integration form (A8) we recover Eq. (48) from Eq. (20) and Eq. (54) from Eq. (22).

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- [1] H. Kogelnik, AT&T Tech. J. **48**, 2909 (1969).
[2] A. Hasegawa and F. Tappert, Appl. Phys. Lett. **23**, 142 (1973).
[3] C.M. de Sterke and J.E. Sipe, Phys. Rev. A **38**, 5149 (1988).
[4] H.G. Winful and G.D. Cooperman, Appl. Phys. Lett. **40**, 298 (1982).
[5] C.M. de Sterke and J.E. Sipe, in *Progress in Optics*, edited by E. Wolf (North-Holland, Amsterdam, 1994), Vol. XXXIII, pp. 203–260.
[6] C.M. de Sterke, D.G. Salinas, and J.E. Sipe, Phys. Rev. E **54**, 1969 (1996).
[7] N.A.R. Bhat and J.E. Sipe, Phys. Rev. E **64**, 056604 (2001).
[8] W. Samir, S.J. Garth, and C. Pask, J. Opt. Soc. Am. B **11**, 64 (1994).
[9] C.M. de Sterke and J.E. Sipe, Phys. Rev. A **39**, 5163 (1989).
[10] C. Pask, D.R. Rowland, and W. Samir, J. Opt. Soc. Am. B **15**, 1871 (1998).
[11] V.V. Konotop, Phys. Rev. E **53**, 2843 (1996).
[12] J. Kevorkian and J.D. Cole, *Multiple Scale and Singular Perturbation Methods* (Springer-Verlag, New York, 1996), Chap. 4.
[13] S. Pereira and J.E. Sipe, Phys. Rev. E **65**, 046601 (2002).
[14] S. Pereira and J.E. Sipe, Phys. Rev. E **66**, 026606 (2002).
[15] G.P. Agrawal, *Nonlinear Fiber Optics* (Academic Press, San Diego, 2001).
[16] R.W. Boyd, *Nonlinear Optics* (Academic Press, Boston, 1992).

- [17] J.D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1999), Chap. 4.
- [18] G.B. Arfken and H.J. Weber, *Mathematical Methods for Physicists* (Academic Press, San Diego, 1995).
- [19] In the early 1D work, Ref. [3] it was the electric rather than the displacement field that was so treated, and in the 3D work, Ref. [7], it was the dual potential rather than the displacement field, but these matters are irrelevant to the issues considered here.
- [20] J.E. Sipe and H.G. Winful, *Opt. Lett.* **13**, 132 (1988).
- [21] In the final stages of preparation of this manuscript, we became aware of a paper in which a one-dimensional analog of $g_m(\mathbf{r}, t)$ is introduced in the context of a one-dimensional treatment of quantum gap solitons: Z. Cheng and G. Kurizki, *Phys. Rev. A* **54**, 3576 (1996).
- [22] M. Lax, *Symmetry Principles in Solid State and Molecular Physics* (Wiley, New York, 1974).
- [23] N.F. Johnson and P.M. Hui, *J. Phys.: Condens. Matter* **5**, L355 (1993).
- [24] P.M. Hui, W.M. Lee, and N.F. Johnson, *Solid State Commun.* **91**, 65 (1994).
- [25] N.F. Johnson, P.M. Hui, and K.H. Luk, *Solid State Commun.* **90**, 229 (1994).
- [26] J.E. Sipe, *Phys. Rev. E* **62**, 5672 (2000).
- [27] J.E. Heebner, R.W. Boyd, and Q-Han Park, *Phys. Rev. E* **65**, 036619 (2002).
- [28] P. Chak, J.E. Sipe, and S. Pereira, *Opt. Commun.* **213**, 163 (2002).
- [29] S. Pereira and J.E. Sipe, *Phys. Rev. E* **62**, 5745 (2000).
- [30] J. Poon, E. Istrate, M. Allard, and E.H. Sargent, *IEEE J. Quantum Electron.* **39**, 778 (2003).
- [31] C. Pask, D.R. Rowland, and W. Samir, *J. Opt. Soc. Am. B* **15**, 1871 (1998).
- [32] E.A. Golovchenko, E.M. Dianov, A.M. Prokhorov, and V.N. Serkin, *Sov. Phys. Dokl.* **31**, 494 (1986); we note here that there is an error in the expression for the Hamiltonian in this particular paper, and in the original Russian paper of which it is a translation, Ref. [51]. The corresponding variable in this paper is C_3 , which is expressed correctly here in our notation.
- We thank V. N. Serkin (private communication) for confirming this.
- [33] N. Tzoar and M. Jain, *Phys. Rev. A* **23**, 1266 (1981).
- [34] M. Wadati, K. Konno, and Y. Ichikawa, *J. Phys. Soc. Jpn.* **46**, 1965 (1979).
- [35] V.E. Zakharov and A.B. Shabat, *Sov. Phys. JETP* **34**, 62 (1972).
- [36] C. Sulem and P-L. Sulem, *The Nonlinear Schrödinger Equation: Self-Focusing and Wave Collapse* (Springer-Verlag, New York, 1999).
- [37] T. Zijlstra, E. van der Drift, M.J.A. de Dood, E. Snoeks, and A. Polman, *J. Vac. Sci. Technol. B* **17**, 2734 (1999).
- [38] V.V. Poborchii, T. Tada, and T. Kanayama, *J. Appl. Phys.* **91**, 3299 (2002).
- [39] B. Temelkuran and E. Ozbay, *Appl. Phys. Lett.* **74**, 486 (1999).
- [40] J. Zimmermann, M. Kamp, R. Schwertberger, J.P. Reithmaier, A. Forchel, and R. März, *Electron. Lett.* **38**, 178 (2002).
- [41] M. Notomi, A. Shinya, K. Yamada, J. Takahashi, C. Takahashi, and I. Yokohama, *IEEE J. Quantum Electron.* **38**, 736 (2002).
- [42] H. Benisty, *J. Appl. Phys.* **79**, 7483 (1996).
- [43] K. Sakoda, T. Ueta, and K. Ohtaka, *Phys. Rev. B* **56**, 14 905 (1997).
- [44] A. Mekis, S. Fan, and J.D. Joannopoulos, *Phys. Rev. B* **58**, 4809 (1998).
- [45] S.G. Johnson, P.R. Villeneuve, S. Fan, and J.D. Joannopoulos, *Phys. Rev. B* **62**, 8212 (2000).
- [46] S. Olivier, M. Rattier, H. Benisty, C. Weisbuch, C.J.M. Smith, R.M. De La Rue, T.F. Krauss, U. Oesterle, and R. Houdré, *Phys. Rev. B* **63**, 113311 (2001).
- [47] M. Lončar, D. Nedeljković, T.P. Pearsall, J. Vučković, A. Scherer, S. Kuchinsky, and D.C. Allan, *Appl. Phys. Lett.* **80**, 1689 (2002).
- [48] C.M. de Sterke and J.E. Sipe, *Opt. Lett.* **14**, 871 (1989).
- [49] MIT Photonic Bands Package, as described in S.G. Johnson and J.D. Joannopoulos, *Opt. Express* **8**, 173 (2001).
- [50] A. Tip, A. Moroz, and J.M. Combes, *J. Phys. A* **33**, 6223 (2000).
- [51] E.A. Golovchenko, E.M. Dianov, A.M. Prokhorov, and V.N. Serkin, *Dokl. Akad. Nauk SSSR* **288**, 851 (1986). See Ref. [32] for the English translation of this paper.