

# Canonical Hamiltonian formulation of the nonlinear Schrödinger equation in a one-dimensional, periodic Kerr medium

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A canonical Hamiltonian formulation of the nonlinear Schrödinger equation has been derived in this paper. This formulation governs the dynamics of pulse propagation in a one-dimensional, periodic Kerr medium when the frequency content of the pulse is sufficiently narrow relative to a carrier frequency, and sufficiently far removed from a photonic band gap of the medium. Our Hamiltonian is numerically equal to the energy, and our fields obey canonical commutation relations, so the theory can easily be quantized. We clarify the nature of the conserved quantities associated with simple symmetries.

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## I. INTRODUCTION

The investigation of optical pulse propagation in nonlinear Kerr media often proceeds *via* the slowly varying envelope function approximation [1–3], wherein the frequency content of an optical pulse is considered to be narrowly centered around a given carrier frequency  $\bar{\omega}$ . This approximation allows one to separate the pulse dynamics, contained in the slowly varying envelope functions, from the phase accumulation due to the carrier frequency. When applied to a homogenous, isotropic medium, this approach has been used to derive the familiar nonlinear Schrödinger equation (NLSE) [1] as the dynamical equations for the envelope function; when applied to a periodic structure, the approach has been used to derive both a NLSE [4,5] and a set of nonlinear coupled mode equations (CME) [2,5]. In the presence of birefringence, a set of coupled NLSEs have been derived for a homogeneous medium [3]; for a periodic medium, both a set of coupled NLSEs and a set of nonlinear CMEs have been derived [6]. The dynamics of these envelope-function equations have often been studied by constructing a Hamiltonian formulation of the dynamical equations [7–11]. From such a Hamiltonian two conserved quantities can easily be identified, one energylike, and one momentumlike. But the Hamiltonian itself is not equal to the energylike quantity, leading to a certain confusion in the literature [12,13]. One would naively expect that a nonlinear optical system would have two conserved quantities—energy and momentum. Since the Hamiltonian itself is also conserved, however, the optical system has *three* conserved quantities, and the interpretation of this third conserved quantity has presented some difficulties [7,8,12]. A correct understanding of these three conserved quantities is the goal of this paper.

In Sec. II of this paper we construct a canonical Hamiltonian formulation of Maxwell's equations in a one-dimensional, periodic medium with a Kerr nonlinearity, using a dual field first proposed by Hillery and Mlodinow [14]; see also [15,16]; although we here only consider classical fields we formally replace the canonical Poisson brackets with the associated commutators, with a view towards eventually quantizing the theory. By *canonical* we mean that our

Hamiltonian can be used to derive the exact equations of motion using the canonical commutation relations, *and* that it is numerically equal to the energy of the (nonlinear) electromagnetic field. In Sec. III we specialize our formulation to consider an effective field that varies slowly relative to the underlying Bloch functions of the periodic medium [17]. Use of these Bloch functions means that our resulting equations are valid in the presence of a strong periodic variation in the dielectric permittivity of the medium. We then generate a reduced canonical Hamiltonian in terms of this effective field. The dynamical equation governed by this reduced Hamiltonian is the familiar NLSE. In Sec. IV we discuss the relationship between our effective fields, and an alternate approach in which the fields of interest are considered slowly varying functions that modulate a given Bloch function. In Sec. V we use the reduced Hamiltonian, which, within our approximations, is conserved and equal to the energy, to identify two more conserved quantities: the momentum, associated with space-translation symmetry; and a conserved charge, associated with phase-translation symmetry.

In Sec. VI we discuss the use of the dual field and compare it with other fields used in the literature to derive the NLSE in periodic media. Although we have concentrated on deriving a NLSE, our method can be used to construct reduced canonical Hamiltonians associated with the nonlinear coupled mode equations in both isotropic and birefringent, periodic media. Furthermore, the dual field is generalizable to two and three dimensions [15], so it can likely be used to derive equations in higher-dimensional photonic band gap materials.

## II. CANONICAL FORMULATION OF MAXWELL'S EQUATIONS

We begin with Maxwell's equations in a one-dimensional, nonmagnetic medium

$$\partial_z E(z,t) = -\mu_0 \partial_t H(z,t), \quad (1)$$

$$\partial_z H(z,t) = -\partial_t D(z,t),$$

where

$$D = \epsilon_0 E + P, \quad (2)$$

$P$  is the full polarization,  $\varepsilon_0$  is the permittivity of free space, and  $\mu_0$  is the permeability of free space. To construct a canonical formulation of these dynamical equations, we introduce a dual field  $\Lambda$  [16], which satisfies

$$\partial_z \Lambda = D, \quad (3)$$

$$\partial_t \Lambda = -H.$$

The dual field will serve as the canonical coordinate field. We then define a Hamiltonian density [16]

$$\mathcal{H}(z, t) = \frac{1}{2\mu_0} p^2 + U(\Lambda_z), \quad (4)$$

where we have introduced the conjugate momentum field  $p(z, t)$ , and where

$$U(D) = \int_0^D E dD. \quad (5)$$

The canonical equations of motion that follow from this Hamiltonian density are

$$\partial_t p = -\frac{\partial \mathcal{H}}{\partial \Lambda} + \frac{\partial}{\partial z} \left[ \frac{\partial \mathcal{H}}{\partial \Lambda_z} \right], \quad (6)$$

$$\partial_t \Lambda = \frac{\partial \mathcal{H}}{\partial p},$$

which, using Eqs. (3) and (4) are found to be precisely Eq. (1). Alternately, one can recover (1) by using the equal-time commutators [16]

$$[\Lambda(z, t), p(z', t)] = i\hbar \delta(z - z') \quad (7)$$

with equations of motion [16]

$$i\hbar \frac{\partial p}{\partial t} = [p, H], \quad (8)$$

$$i\hbar \frac{\partial \Lambda}{\partial t} = [\Lambda, H],$$

where the associated Hamiltonian

$$H = \int_{-\infty}^{\infty} \mathcal{H}(z, t) dz \quad (9)$$

is numerically equal to [16,18]

$$\mathcal{E} = \int_{-\infty}^{\infty} \left[ \frac{\mu_0}{2} H^2 + \left( \int_0^D E dD \right) \right] dz, \quad (10)$$

the energy in the electromagnetic field.

### A. Linear, periodic medium

For a linear, periodic medium

$$H = H_L = \int_{-\infty}^{\infty} dz \left( \frac{1}{2\mu_0} p^2 + \frac{\Lambda_z^2}{2\varepsilon(z)} \right), \quad (11)$$

where  $\varepsilon(z) = \varepsilon(z + d)$  is the dielectric permittivity, with  $D(z, t) = \varepsilon(z)E(z, t)$ , and where  $d$  is the periodicity of the lattice. Using the equations of motion (6) we find a linear wave equation that  $\Lambda$  must satisfy

$$\mu_0 \varepsilon^2(z) \partial_{tt} \Lambda = \varepsilon(z) \partial_{zz} \Lambda - \partial_z \Lambda \partial_z \varepsilon(z). \quad (12)$$

To determine the Bloch functions of Eq. (12), we use the usual ansatz [19]

$$\Lambda(z, t) \propto \theta_\mu(z) e^{-i\omega_\mu t} + \text{c.c.}, \quad (13)$$

where c.c. stands for ‘‘complex conjugate.’’ Substitution of Eq. (13) in the wave equation (12) gives an equation for the Bloch functions  $\theta_\mu$

$$\left\{ \frac{1}{\varepsilon(z)} \partial_{zz} + \partial_z [1/\varepsilon(z)] \right\} \theta_\mu = -\mu_0 \omega_\mu^2 \theta_\mu. \quad (14)$$

Because the operator in the equation is self-adjoint, it admits real eigenvalues and orthogonal eigenfunctions.

From Bloch’s theorem [19], we can write our Bloch functions in terms of a discrete band index  $m$ , and a reduced wave number  $k$  ( $-\pi/d < k \leq \pi/d$ ), so that  $\theta_\mu \rightarrow \theta_{mk}$ , with

$$\theta_{mk}(z) = u_{mk}(z) e^{ikz}, \quad (15)$$

where the  $u_{mk}$  have the periodicity of the lattice,  $u_{mk}(z) = u_{mk}(z + d)$ . We note that  $\omega_{mk} = \omega_{m(-k)}$ , so we can choose our Bloch functions such that  $\theta_{mk}(z) = \theta_{m(-k)}^*$ . We normalize the Bloch functions *via*

$$\int_{-L/2}^{L/2} \theta_{mk}^*(z) \theta_{m'k'}(z) dz = N \delta_{mm'} \delta_{kk'}, \quad (16)$$

where  $L$  is a normalization length, and where we have chosen the normalization constant  $N = L/d$ , which is then identified as the number of unit cells in the normalization length. This choice of normalization means that our wave numbers take on only discrete values, and that the difference between two adjacent wave numbers is  $2\pi/L$ . The Bloch functions also satisfy

$$\int_{-L/2}^{L/2} \frac{\theta_{mk}^*(z) \theta'_{m'k'}(z)}{\varepsilon(z)} dz = \mu_0 \omega_{mk}^2 N \delta_{mm'} \delta_{kk'}, \quad (17)$$

where  $\theta'_{mk} = d\theta_{mk}/dz$ ; this follows by using Eqs. (16) and (14). A typical dispersion relation in this reduced-wave number scheme is sketched in Fig. 1; this dispersion relation is exactly equivalent to the dispersion relation associated with the more familiar electric field Bloch functions.

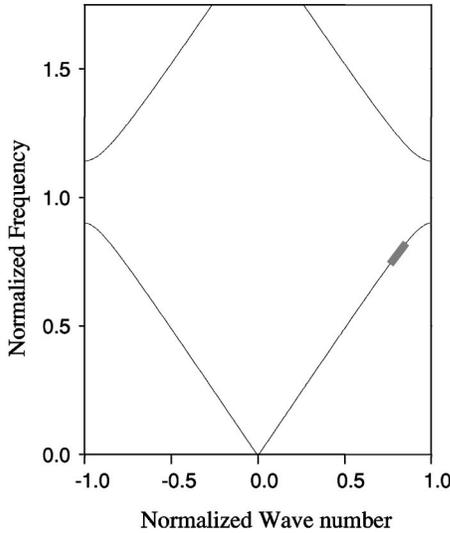


FIG. 1. Sketch of a dispersion relation for a one-dimensional, linear, periodic medium in the reduced wave number scheme. The wave numbers are normalized to  $\pi/d$ . The frequencies are normalized to the center frequency of the first photonic band gap. Note that the introduction of the normalization length  $L$  means that the wave numbers are discretized with adjacent wave numbers separated by  $2\pi/L$ . The solid band in the diagram represents the frequency content of a forward-propagating pulse whose dynamics are well described by the theory in this paper. The frequencies are confined to a narrow range so that third- and higher-order dispersion can be ignored. If the frequency content is brought closer to the photonic band gap, then the range of frequencies must be made more narrow, since near the gap the curvature of the dispersion relation is quite high.

### B. Periodic medium with a Kerr nonlinearity

We now turn to a periodic, Kerr nonlinear medium. At frequencies far below any resonances in the medium, for our one-dimensional geometry, the constitutive relation takes the form [1]

$$D = \varepsilon(z)E + \varepsilon_0\chi^{(3)}(z)E^3, \quad (18)$$

where we assume that the nonlinearity coefficient  $\chi^{(3)}(z)$  is periodic with period  $d$ ,  $\chi^{(3)}(z+d) = \chi^{(3)}(z)$ . To construct the Hamiltonian we first invert Eq. (18) to get

$$E \simeq \frac{D}{\varepsilon(z)} - \varepsilon_0\chi^{(3)}(z)\frac{D^3}{\varepsilon^4(z)}, \quad (19)$$

where we have assumed that  $\chi^{(3)}E^3 \ll E$ . This assumption of a weak nonlinearity is justified on physical grounds: we only want to discuss third-order nonlinear effects, but if the assumption of a weak  $\chi^{(3)}$  were not valid, then we would have no justification for not including fifth or higher order nonlinear effects in Eq. (18). Using Eq. (19) in Eq. (5) we find

$$H = H_L + H_{NL} = H_L - \int_{-L/2}^{L/2} dz \frac{\varepsilon_0\chi^{(3)}(z)\Lambda_z^4(z)}{4\varepsilon^4(z)}, \quad (20)$$

where  $H_L$  is defined above (11) and  $H_{NL}$  is the portion of the full Hamiltonian responsible for the nonlinearity in the dynamics of the electromagnetic field. The expression (20), when used as a Hamiltonian with equations of motion (6), leads to the correct equation of motion for  $\Lambda$  within the approximation (19) of a weak nonlinearity

$$\begin{aligned} \mu_0\varepsilon^2(z)\partial_{tt}\Lambda &= \varepsilon(z)\partial_{zz}\Lambda - [\partial_z\Lambda][\partial_z\varepsilon(z)] \\ &\quad - \varepsilon_0\frac{\partial}{\partial z}\left\{\frac{\chi^{(3)}(z)\Lambda_z^4}{\varepsilon^4(z)}\right\}. \end{aligned} \quad (21)$$

This expression can, of course, be verified by using  $\Lambda$  directly in Maxwell's equations.

It will be useful to express  $H$  in terms of the classical analog of the raising and lowering operators associated with the Bloch modes. To do so, we first expand  $\Lambda(z,t)$  and  $p(z,t)$  in terms of the Bloch modes of the periodic medium. We let

$$p(z,t) = \sum_{m=1}^{\infty} \sum_{k=-\pi/d}^{\pi/d} p_{mk}(t)\theta_{mk}(z), \quad (22)$$

$$\Lambda(z,t) = \sum_{m=1}^{\infty} \sum_{k=-\pi/d}^{\pi/d} \Lambda_{mk}(t)\theta_{mk}(z).$$

The reality of  $p$  and  $\Lambda$  requires that  $p_{mk}^* = p_{m(-k)}$  and  $\Lambda_{mk}^* = \Lambda_{m(-k)}$ , so we can express the four complex quantities  $p_{mk}$ ,  $\Lambda_{mk}$ ,  $p_{m(-k)}$ , and  $\Lambda_{m(-k)}$  in terms of two complex mode amplitudes  $a_{mk}(t)$  and  $a_{m(-k)}(t)$

$$\Lambda_{mk}(t) = \sqrt{\frac{\hbar}{2N\mu_0\omega_{mk}}}(a_{mk} + a_{m(-k)}^\dagger), \quad (23)$$

$$p_{mk}(t) = -i\sqrt{\frac{\hbar\mu_0\omega_{mk}}{2N}}(a_{mk} - a_{m(-k)}^\dagger),$$

and correspondingly for  $\Lambda_{m(-k)}$  and  $p_{m(-k)}$ . Using the  $a_{mk}(t)$ , the expansion (22) becomes

$$\Lambda(z,t) = \sum_{m=1}^{\infty} \sum_k \sqrt{\frac{\hbar}{2N\mu_0\omega_{mk}}}[a_{mk}(t)\theta_{mk}(z) + \text{c.c.}], \quad (24)$$

$$p(z,t) = -i\sum_{m=1}^{\infty} \sum_k \sqrt{\frac{\hbar\mu_0\omega_{mk}}{2N}}[a_{mk}(t)\theta_{mk}(z) - \text{c.c.}].$$

We note that since  $\Lambda(z,t)$  and  $p(z,t)$  are written in terms of Bloch functions that are normalized in the region  $-L/2 < z < L/2$ , they will become periodic with period  $L$ . This has no effect on the underlying physics, because we can always consider the limit where  $L \rightarrow \infty$ . However, it does mean that when evaluating the Hamiltonian (20) in terms of the  $\Lambda(z,t)$  and  $p(z,t)$  given by Eq. (24), we must restrict the integration to the region  $-L/2 < z < L/2$ ; and when evaluating the equal-time commutation relations (7) between  $\Lambda(z,t)$  and  $p(z',t)$  we must restrict both  $z$  and  $z'$  to be within  $\pm L/2$ . Adhering to these restrictions, we find that using Eq. (24) in Eq. (20),

and applying the orthogonality relations (16) to the portion of the Hamiltonian that generates the linear dynamics, the full Hamiltonian becomes

$$\begin{aligned} \mathbf{H} = & \sum_{mk} \hbar \omega_{mk} |a_{mk}|^2 \\ & - \frac{\hbar^2 \varepsilon_0}{16N^2 \mu_0^2} \int_{-L/2}^{L/2} dz \frac{\chi^{(3)}(z)}{\varepsilon^4(z)} \left[ \prod_{i=1}^4 \sum_{m_i k_i} \frac{(a_{m_i k_i} \theta'_{m_i k_i} + \text{c.c.})}{\sqrt{\omega_{m_i k_i}}} \right]. \end{aligned} \quad (25)$$

Adopting commutation relations

$$\begin{aligned} [a_{mk}(t), a_{m'k'}^\dagger(t)] &= \delta_{mm'} \delta_{kk'}, \\ [a_{mk}(t), a_{m'k'}(t)] &= 0 \end{aligned} \quad (26)$$

guarantees the commutation relations between  $\Lambda(z, t)$  and  $p(z', t)$  (7) for  $z$  and  $z'$  within the normalization length. In terms of the mode amplitudes, the canonical equations of motion (8) become [18,20]

$$i \frac{da_{mk}}{dt} = \frac{1}{\hbar} [a_{mk}, \mathbf{H}], \quad (27)$$

which, using Eq. (25) for  $\mathbf{H}$ , give

$$\begin{aligned} \frac{da_{mk}}{dt} = & -i \omega_{mk} a_{mk} + \frac{i \hbar \varepsilon_0}{4N^2 \mu_0^2} \int_{-L/2}^{L/2} dz \frac{\theta'_{mk} \chi^{(3)}}{\sqrt{\omega_{mk} \varepsilon^4}} \\ & \times \left[ \prod_{i=1}^3 \sum_{m_i k_i} \frac{(a_{m_i k_i} \theta'_{m_i k_i} + \text{c.c.})}{\sqrt{\omega_{m_i k_i}}} \right], \end{aligned} \quad (28)$$

where we have suppressed the  $z$  dependence of  $\theta'_{mk}(z)$ ,  $\chi^{(3)}(z)$  and  $\varepsilon(z)$ , and the time dependence of the  $a_{mk}(t)$ . This Eq. (28) is equivalent to Eqs. (1) and (2) with Eq. (19).

### III. REDUCED HAMILTONIAN AND THE NLSE

In this section we recast our Hamiltonian in a form more suitable to the study of pulse propagation. We build effective fields  $g_m(z, t)$ , as a Fourier superposition of the  $a_{mk}$ , and assume that the effective fields are centred at a given wave number  $\bar{k}$ , which corresponds to a frequency  $\omega_{m\bar{k}}$ . The  $g_m(z, t)$  can be used to rewrite the Hamiltonian (25) without any loss of generality.

This effective field approach is most valuable when the spread in the frequency content of the field is narrow relative to a central frequency  $\omega_{m\bar{k}}$  that lies in band  $m = \bar{m}$  with wave number  $\bar{k}$ . We assume that  $\omega_{m\bar{k}}$  is far from a photonic band gap, and that the frequency content of the pulse is entirely contained within band  $\bar{m}$ . Because the frequency content of our effective fields is narrowly centered around  $\omega_{m\bar{k}}$ , we can expand a frequency  $\omega_{m(\bar{k}+K)}$  in a Taylor series, which will involve the local group velocity and group velocity dispersion. We use a smallness parameter  $\eta$ , which we quantify below, to characterize the strength of the resulting terms in

our Hamiltonian. We examine the situation where the terms that are related to the group velocity of the pulse are  $O(\eta)$ , and the terms that are related to the Kerr nonlinearity and the group velocity dispersion of the pulse are both  $O(\eta^2)$  relative to the largest terms in the Hamiltonian. Higher-order nonlinear effects, and higher-order dispersion are not considered, because both are assumed to be  $O(\eta^3)$ . We denote the resulting Hamiltonian the ‘‘reduced Hamiltonian’’ since it is equal to the energy of the electromagnetic field to  $O(\eta^2)$ . Although our model formally includes third harmonic generation, we ignore its effects in the following. We are justified in doing so by physical considerations. We have assumed that the underlying material is nondispersive, and while this may be valid for frequencies near  $\omega_{m\bar{k}}$ , it will likely not be valid for frequency ranges extending to  $\omega \approx 3\omega_{m\bar{k}}$ ; furthermore, the assumption of no absorption at  $\omega \approx 3\omega_{m\bar{k}}$  will likely be in error. We expect, on physical grounds, that in many cases the actual material dispersion and absorption will make any buildup of the third harmonic unlikely, so that our model will be adequate.

We start by using the  $a_{mk}(t)$  to define an effective field  $g_m(z, t)$  that is centered around the wave number  $k = \bar{k}$ ,

$$\begin{aligned} g_m(z, t) &= \sqrt{\frac{1}{L}} \sum_k a_{mk}(t) e^{i(k-\bar{k})z}, \\ &= \sqrt{\frac{1}{L}} \sum_K g_{mK}(t) e^{iKz}, \end{aligned} \quad (29)$$

where we have introduced the detuning

$$K = k - \bar{k} \quad (30)$$

and the mode amplitudes

$$g_{mK}(t) = a_{m(\bar{k}+K)}(t). \quad (31)$$

Ultimately we seek to describe the evolution of our field  $\Lambda(z, t)$ , which we assume is a smoothly varying function of  $z$  as we move from a point in a unit cell to the corresponding point in a neighboring unit cell. The function  $g_m(z, t)$  will be one such smoothly varying function of  $z$  only if the  $a_{mk}(t)$  are smoothly varying functions of  $k$ . To ensure that the  $a_{mk}(t)$  vary smoothly in  $k$ , one must choose the Bloch functions to vary smoothly in  $k$ , which in practice can be done, for example, using a  $k \cdot p$  expansion [5,21] about  $\bar{k}$ .

Using Eq. (26), we find that the equal-time commutation relations for the  $g_m(z, t)$  are

$$[g_m(z, t), g_{m'}^\dagger(z', t)] = \delta_{mm'} \delta(z - z'), \quad (32)$$

for  $z$  and  $z'$  both in our normalization length  $L$ , where the Dirac delta function  $\delta(z - z')$  in Eq. (32) strictly appears only in the  $L \rightarrow \infty$  limit. By inverting Eq. (29) we find

$$a_{m(\bar{k}+K)}(t) = \frac{1}{\sqrt{L}} \int_{-L/2}^{L/2} dz g_m(z, t) e^{-iKz}. \quad (33)$$

Using Eq. (33), the Hamiltonian (25) can be written in terms of the  $g_m(z, t)$ .

In the following we restrict ourselves to consideration of electromagnetic fields for which at  $t=0$  the wave numbers of the pulse are contained entirely in band  $m=\bar{m}$ , and narrowly centered around  $\bar{k}$ , so that, replacing the  $a_{m(\bar{k}+K)}(t)$  with the  $g_{mK}(t)$ , and restricting the summation in the Hamiltonian (25) to one band, we find a reduced Hamiltonian

$$\begin{aligned} H^R = & \sum_K \hbar \omega_{\bar{m}(\bar{k}+K)} |g_{\bar{m}K}|^2 - \frac{\hbar^2 \epsilon_0}{16N^2 \mu_0^2} \int_{-L/2}^{L/2} dz \frac{\chi^{(3)}(z)}{\epsilon^4(z)} \\ & \times \left[ \prod_{i=1}^4 \sum_{K_i} \frac{(g_{\bar{m}K_i} \theta'_{\bar{m}(\bar{k}+K_i)} + \text{c.c.})}{\sqrt{\omega_{\bar{m}(\bar{k}+K_i)}}} \right], \end{aligned} \quad (34)$$

where the  $K_i$  are wave number detunings. Since we are considering only one band,  $m=\bar{m}$ , we drop the  $m$  subscript in the remainder of the paper. We stress that the Hamiltonian (34) is still exactly equal to the energy in the system at  $t=0$ . At later times the nonlinear interaction will generate new frequencies, but in the following we ignore third harmonic generation, as discussed, so that for reasonable propagation times and pulse intensities the new frequencies that are generated will still lie in band  $m=\bar{m}$ , and the reduced Hamiltonian will still represent the exact energy in the system. Furthermore, we assume that at  $t=0$  only forward-traveling waves are present, so that at later times there will be no interaction with any backward-traveling waves.

We first consider the linear portion of the reduced Hamiltonian (34). We expand the frequency  $\omega_{(\bar{k}+K)}$  as

$$\omega_{(\bar{k}+K)} = \bar{\omega} + K \bar{\omega}' + \frac{1}{2} K^2 \bar{\omega}'' + \dots, \quad (35)$$

where  $\bar{\omega} = \omega_{\bar{k}}$ ,  $\bar{\omega}' = \partial \omega_{(\bar{k}+K)} / \partial K|_{K=0}$  and  $\bar{\omega}'' = \partial^2 \omega_{(\bar{k}+K)} / \partial K^2|_{K=0}$ . Substituting this expression for  $\omega_{(\bar{k}+K)}$  and the expression for the effective fields (29) into the reduced Hamiltonian (34), we find that the portion of the reduced Hamiltonian associated with the linear dynamics of the field is

$$\begin{aligned} H_L^R = & \hbar \bar{\omega} \int_{-L/2}^{L/2} dz \left( |g|^2 + \frac{i}{2} \frac{\bar{\omega}'}{\bar{\omega}} (g \partial_z g^\dagger - \text{c.c.}) \right. \\ & \left. + \frac{1}{2} \frac{\bar{\omega}''}{\bar{\omega}} |\partial_z g|^2 \right). \end{aligned} \quad (36)$$

The exact Hamiltonian that generates the linear dynamics is given by

$$H_L = H_L^R + O(\eta^3),$$

where  $\eta$  is the smallness parameter used to characterize the relative strength of terms in the reduced Hamiltonian. We can quantify  $\eta$  by setting it to be the larger of

$$\eta = \frac{\bar{\omega}}{\bar{\omega}'} z_w, \quad \eta = 2 \frac{\bar{\omega}'}{\bar{\omega}''} z_w, \quad (37)$$

where  $z_w$  is an appropriate measure of the width of the pulse. As discussed, the third- and higher-order dispersion terms are considered to be  $O(\eta^3)$ . The values of  $\bar{\omega}'$  and  $\bar{\omega}''$  will depend on the dispersion relation itself; a variety of techniques exist to determine the dispersion relation of a one-dimensional, periodic system [19].

Turning to the portion of the reduced Hamiltonian (34) that generates the nonlinear dynamics of the fields, we first recall that we are dealing with a weak nonlinearity [see note following Eq. (19)]. We quantify the weakness of this nonlinearity by asserting that the ratio of the largest nonlinear term to the largest linear term is  $O(\eta^2)$ . Because we are only keeping terms in  $H^R$  to  $O(\eta^2)$ , this means that we can replace  $\theta'_{(\bar{k}+K)}$  with  $\theta'_k e^{iKz}$ , and the small error that it introduces will enter at the next level in the perturbation. Similarly, we replace  $\omega_{(\bar{k}+K)}$  with  $\bar{\omega}$ . The value of  $\eta$  set above determines the strength of the nonlinear term that can be accommodated by this theory. For a stronger nonlinear term (either through a larger  $\chi^{(3)}$ , or through a higher intensity in the pulse), more complicated nonlinear effects must be included. We find

$$\begin{aligned} H_{NL}^R = & - \frac{\hbar^2 \epsilon_0}{16N^2 \mu_0^2 \bar{\omega}^2} \int_{-L/2}^{L/2} dz \frac{\chi^{(3)}(z)}{\epsilon^4(z)} \\ & \times \left[ \prod_{i=1}^4 \sum_{K_i} \{g_{K_i} e^{iK_i z} \theta'_k(z) + \text{c.c.}\} \right]. \end{aligned} \quad (38)$$

An integral that will be important in  $H_{NL}^R$  is

$$\begin{aligned} I_{1234} = & \int_{-L/2}^{L/2} dz \exp\{i(K_1 - K_2 + K_3 - K_4)z\} \\ & \times \left[ \frac{\chi^{(3)}(z)}{\epsilon^4(z)} |\theta'_k(z)|^4 \right]. \end{aligned} \quad (39)$$

The portion in the square brackets contains only periodic quantities, with period  $d$ , and can be expanded as a Fourier series

$$\frac{\chi^{(3)}}{\epsilon^4} |\theta'_k|^4 = \sum_{n=0}^{\infty} \beta^{(n)} e^{i2n\pi z/d}, \quad (40)$$

with

$$\beta^{(n)} = \int_0^d dz \frac{\chi^{(3)}}{\epsilon^4} |\theta'_k|^4 e^{-i2n\pi z/d}, \quad (41)$$

where the integration proceeds over the length  $d$  of one unit cell. Using the expansion (40) in the integral (39) we find

$$I_{1234} = \sum_n \beta^{(n)} \int_{-L/2}^{L/2} dz \exp\{i(K_1 - K_2 + K_3 - K_4 + 2n\pi/d)z\}. \quad (42)$$

The integral will be zero unless  $(K_1 - K_2 + K_3 - K_4 + 2n\pi/d) = 0$ . But we have previously stipulated that all our detunings are  $\ll \pi/d$ , so  $I_{K_{1234}}$  only has a value for  $n=0$ . This means

$$I_{1234} = \beta^{(0)} \int_{-L/2}^{L/2} dz \exp\{i(K_1 - K_2 + K_3 - K_4)z\} \quad (43)$$

and

$$\sum_{K_1 K_2 K_3 K_4} g_{K_1} g_{K_2}^\dagger g_{K_3} g_{K_4}^\dagger I_{1234} = \beta^0 \int_{-L/2}^{L/2} dz |g(z,t)|^4. \quad (44)$$

In writing down  $I_{1234}$  we are only considering the integrals that will arise in Eq. (38) that contain terms with two complex conjugates. Terms with zero or four complex conjugates lead to third harmonic generation, which, as discussed, is ignored here. Terms with one or three complex conjugates vanish for the following reason. The expansion (40) could be made because the  $e^{ikz}$  portions of the Bloch function [see Eq. (15)] cancel out. If, on the other hand, we consider terms where either one or three of the Bloch functions are conjugated, then the expansion corresponding to Eq. (40) would be multiplied by a prefactor  $e^{\pm i2\bar{k}z}$ . The integral corresponding to Eq. (42) would then be nonzero only if  $(K_1 - K_2 + K_3 - K_4 + 2n\pi/d \pm 2\bar{k}) = 0$  which, since the detunings are all small, can never occur, which, since the detunings are all small, cannot occur unless  $k=0$  or  $k=\pi/d$ . We defer a discussion of these latter cases to a later paper.

From Eq. (38), there are six ways to generate terms involving two complex conjugates so including counting considerations we find

$$H_{NL}^R = -\frac{1}{2} \alpha \int_{-L/2}^{L/2} dz |g(z,t)|^4, \quad (45)$$

where, to simplify the expressions, we have defined the nonlinear coefficient

$$\alpha = \frac{3}{4} \frac{\hbar^2 \epsilon_0}{N^2 \mu_0^2 \omega^2} \int_0^d dz \frac{\chi^{(3)}(z)}{\epsilon^4(z)} |\theta_{\bar{k}}(z)|^4. \quad (46)$$

Collecting our results (36) and (45), we find a reduced Hamiltonian

$$H^R = \int_{-L/2}^{L/2} dz \mathcal{H}(z,t) \quad (47)$$

with a reduced Hamiltonian density

$$\begin{aligned} \mathcal{H}^R(z,t) = & \hbar \bar{\omega} |g|^2 + i \frac{\hbar \bar{\omega}'}{2} (g \partial_z g^\dagger - \text{c.c.}) + \frac{\hbar \bar{\omega}''}{2} |\partial_z g|^2 \\ & - \frac{\alpha}{2} |g|^4, \end{aligned} \quad (48)$$

where we have suppressed the  $z, t$  dependence of  $g(z, t)$ . The Heisenberg equations of motion follow from Eq. (27)

$$i \partial_t g(z,t) = \frac{1}{\hbar} [g(z,t), H^R(z,t)], \quad (49)$$

so that, using the commutation relations (32), the differential equation that governs the dynamics of the  $g(z, t)$  field is

$$\begin{aligned} i \partial_t g(z,t) = & \bar{\omega} g(z,t) - i \bar{\omega}' \partial_z g(z,t) - \frac{1}{2} \bar{\omega}'' \partial_z^2 g(z,t) \\ & - \alpha |g(z,t)|^2 g(z,t). \end{aligned} \quad (50)$$

#### IV. EFFECTIVE FIELDS AND ENVELOPE FUNCTIONS

In our treatment of the NLSE, we have constructed an effective field as a Fourier superposition of the mode amplitudes in the Hamiltonian. This differs from previous derivations of the NLSE in a periodic medium, in which the physical field of interest (often the electric field) was expanded as a slowly varying envelope function that modulated a Bloch function at a given wave number  $\bar{k}$  and band index  $\bar{m}$  [5,6]. The derived NLSE then gave the dynamics of the slowly varying envelope function. In this section we relate our effective fields to the envelope functions that would emerge if we used the dual field in the approach of previous derivations of the NLSE.

We start by noting that an arbitrary  $u_{mk}(z)$  can be written as

$$u_{mk}(z) = \sum_c \gamma_{m(\bar{k}+K)}^{c\bar{k}} u_{c\bar{k}}(z), \quad (51)$$

where the detunings are defined in Eq. (30), and where the value of the connections  $\gamma_{m(\bar{k}+K)}^{c\bar{k}}$  can be determined using “ $k \cdot p$ ” theory [5,21]. Using this expansion for the  $u_{mk}$  we find

$$\theta_{mk} = \sum_c \gamma_{m(\bar{k}+K)}^{c\bar{k}} \theta_{c\bar{k}} e^{iKz}, \quad (52)$$

and, using Eq. (52) in Eq. (24), we find

$$\Lambda(z,t) = \sum_c f_c(z,t) \theta_{c\bar{k}}(z) + \text{c.c.}, \quad (53)$$

where

$$f_c(z,t) = \left\{ \sum_{mK} \gamma_{m(\bar{k}+K)}^{c\bar{k}} a_{m(\bar{k}+K)}(t) e^{iKz} \right\}. \quad (54)$$

The  $f_c(z, t)$ , which are envelope functions that modulate Bloch functions at  $\bar{k}$ , are related to the  $a_{m(\bar{k}+K)} e^{iKz}$  via the

connections. Previous derivations of the NLSE would require the field  $\Lambda(z, t)$  to be separated as follows:

$$\Lambda(z, t) = f_{\bar{m}}^-(z, t) \theta_{\bar{m}\bar{k}}^-(z) + \sum_{c \neq \bar{m}} f_c(z, t) \theta_{c\bar{k}}^-(z) + \text{c.c.}, \quad (55)$$

where  $|f_c(z, t)| \ll |f_{\bar{m}}^-(z, t)|$ , since the frequency content of the field is assumed to be narrowly centered around  $\omega_{\bar{m}\bar{k}}$ . The  $f_{c \neq \bar{m}}(z, t)$  are typically called ‘‘companion’’ terms, while  $f_{\bar{m}}^-(z, t)$  is called the ‘‘principal’’ term. Using a method presented elsewhere [5] it can be shown that the principal term  $f_{\bar{m}}^-(z, t)$  obeys a dynamical equation analogous to Eq. (50). However, we have verified that the Hamiltonian from which the dynamical equation of the  $f_{\bar{m}}^-(z, t)$  can be derived is not equal to the energy in the electromagnetic field to the required order in perturbation theory.

We can use Eq. (54) to relate the envelope function  $f_{\bar{m}}^-(z, t)$  to the effective field  $g(z, t)$ . We start by recognizing that, using  $k$ - $p$  theory, the  $\gamma_{\bar{m}\bar{k}}^{\bar{m}\bar{k}}$  can be expanded as a Taylor series

$$\gamma_{\bar{m}(\bar{k}+K)}^{\bar{m}\bar{k}} = 1 + K(\gamma_{\bar{m}(\bar{k}+K)}^{\bar{m}\bar{k}})^{(1)} + \frac{1}{2}K^2(\gamma_{\bar{m}(\bar{k}+K)}^{\bar{m}\bar{k}})^{(2)} + \dots \quad (56)$$

Using this, and recalling that since the frequency content of the pulse is confined to the band  $\bar{m}$ , so that  $a_{p(\bar{k}+K)}(t) \approx 0$  if  $p \neq \bar{m}$ , we find

$$f_{\bar{m}}^-(z, t) = g(z, t) - i(\gamma_{\bar{m}(\bar{k}+K)}^{\bar{m}\bar{k}})^{(1)} \frac{\partial g(z, t)}{\partial z} - \frac{1}{2}(\gamma_{\bar{m}(\bar{k}+K)}^{\bar{m}\bar{k}})^{(2)} \frac{\partial^2 g(z, t)}{\partial z^2} + \dots, \quad (57)$$

where for envelope functions that vary slowly in space, the first term on the right-hand side of this equation will be much larger than the other terms.

Both the envelope function  $f_{\bar{m}}^-(z, t)$  and the effective field  $g(z, t)$  can be used to examine the evolution of the electromagnetic field in a periodic medium. However, a derivation of the propagation equation based on the effective field has the advantage that it extracts the linear pulse propagation parameters directly from the dispersion relation. The envelope-function technique generates complicated overlap integrals, which can subsequently be related to the linear pulse propagation parameters taken from the dispersion relation. We feel that this makes the effective field approach clearer and simpler to use.

We close this section with a brief discussion on how the Maxwell boundary conditions apply to our theory. The theory in this paper assumes an infinite periodic medium. Were the periodic medium not infinite, then one would have to apply the usual Maxwell boundary conditions, which, in a one-dimensional system, assert the continuity of  $E$  and  $H$  across the interface between the periodic medium and an adjacent medium. In the absence of nonlinearity, this is equivalent to asserting the continuity of  $\Lambda_z/(\epsilon_0 n^2)$  and  $\Lambda_t$ .

Because our effective fields are constructed as Fourier superpositions of mode amplitudes that modulate Bloch functions, the boundary conditions may appear difficult to apply, since they would have to be applied to each  $k$  point in a pulse. However, we have shown in this section that, to first order, the value of  $g(z, t)$  is equal to  $f_{\bar{m}}^-(z, t)$ , where the latter field modulates only the Bloch function  $\theta_{\bar{m}\bar{k}}^-(z)$ . Therefore, to first order, the boundary conditions can be applied as though  $g(z, t)$  modulated only  $\theta_{\bar{m}\bar{k}}^-(z)$ , which is a straightforward operation. We note that because we are considering a one-dimensional system, where the fields are transverse, the continuity conditions that concern the normal component of the  $D$  and  $B$  fields are not relevant.

## V. CONSERVED QUANTITIES OF THE HAMILTONIAN

We are now prepared to discuss the conserved quantities associated with the reduced Hamiltonian system described by Eq. (47). We first use Eq. (29) to exhibit the reduced Hamiltonian (47) in terms of the Fourier modes of the effective fields

$$\begin{aligned} H_L^R = \hbar \bar{\omega} \sum_K \left\{ g_K g_K^\dagger + \frac{1}{2} \frac{\bar{\omega}'}{\bar{\omega}} (K g_K g_K^\dagger + \text{c.c.}) \right. \\ \left. + \frac{1}{2} \frac{\bar{\omega}''}{\bar{\omega}} K^2 g_K g_K^\dagger \right\}, \quad (58) \end{aligned}$$

$$H_{NL}^R = -\frac{1}{2} \alpha \sum_{K_1 K_2 K_3} g_{K_1} g_{K_2}^\dagger g_{K_3} g_{(K_1 - K_2 + K_3 - K_4)}^\dagger.$$

We rewrite this reduced Hamiltonian in terms of the new coordinate and momentum variables, which in this problem are real and can be written in terms of the  $g$  and  $g^\dagger$  as

$$\begin{aligned} \phi_K &\equiv \sqrt{\frac{\hbar}{2\bar{\omega}}} (g_K^\dagger + g_K), \quad (59) \\ \pi_K &\equiv i \sqrt{\frac{\hbar \bar{\omega}}{2}} (g_K^\dagger - g_K). \end{aligned}$$

Substituting these into Eq. (47) the reduced Hamiltonian becomes

$$\begin{aligned} H^R = \frac{\bar{\omega}}{2} \sum_K \left( \bar{\omega} + \bar{\omega}' K + \frac{1}{2} \bar{\omega}'' K^2 \right) \left( \phi_K^2 + \frac{\pi_K^2}{\bar{\omega}} \right) \\ - \frac{\alpha \bar{\omega}^2}{8 \hbar^2} \sum_{K_1 K_2 K_3} \left( \phi_{K_1} + \frac{i \pi_{K_1}}{\bar{\omega}} \right) \left( \phi_{K_2} - \frac{i \pi_{K_2}}{\bar{\omega}} \right) \\ \times \left( \phi_{K_3} + \frac{i \pi_{K_3}}{\bar{\omega}} \right) \left( \phi_{(K_1 - K_2 + K_3)} - \frac{i \pi_{(K_1 - K_2 + K_3)}}{\bar{\omega}} \right), \quad (60) \end{aligned}$$

with equations of motion

$$\partial_t \phi_K = \frac{\partial H^R}{\partial \pi_K}, \quad \partial_t \pi_K = -\frac{\partial H^R}{\partial \phi_K}. \quad (61)$$

From Eq. (58) it is clear that the reduced Hamiltonian is invariant under the two infinitesimal transformations

$$\begin{aligned} g_K &\rightarrow g_K e^{i\sigma}, \\ g_K &\rightarrow g_K e^{i\nu K}, \end{aligned} \quad (62)$$

where it is assumed that  $\sigma$  and  $\nu K$  are infinitesimal quantities. If we convert back to real space, we can identify the first transformation as expressing the phase invariance of our reduced Hamiltonian, and the second expressing the translational invariance. We note that the system itself does not possess full translational invariance. However, at the level of the effective fields, the periodicity of the underlying structure has been captured in the dispersion relation, and the effective fields do possess translational invariance. In terms of the real coordinates  $\phi_K$  and  $\pi_K$ , the two infinitesimal transformations correspond to

$$\phi_K \rightarrow \phi_K - \rho \frac{1}{\omega} \pi_K, \quad (63)$$

$$\pi_K \rightarrow \pi_K + \bar{\omega} \rho \phi_K,$$

where  $\rho$  is either  $\sigma$  or  $\nu K$ . We use the invariance of the reduced Hamiltonian to construct the conserved quantities associated with these infinitesimal transformations. Under either transformation

$$\begin{aligned} H^R &\rightarrow H^R + \delta H^R, \\ \delta H^R &= \sum_K \left\{ \frac{\partial H^R}{\partial \phi_K} \delta \phi_K + \frac{\partial H^R}{\partial \pi_K} \delta \pi_K \right\} \\ &= \sum_K \rho \left\{ \frac{1}{\omega} \frac{\partial \pi_K}{\partial t} \pi_K + \bar{\omega} \frac{\partial \phi_K}{\partial t} \phi_K \right\} \\ &= \frac{\partial}{\partial t} \sum_K \rho \left\{ \frac{1}{\omega} \pi_K^2 + \bar{\omega} \phi_K^2 \right\} = 0, \end{aligned}$$

where we have used the equations of motion (61), and where we set  $\delta H^R = 0$  since the reduced Hamiltonian is invariant. We find two conserved quantities. The first, associated with phase invariance, we call the charge  $Q$ . The second, associated with translational invariance, we call the momentum  $P$ . In Fourier space, the two conserved quantities have the value

$$\begin{aligned} Q &= \hbar \bar{\omega} \sum_K \left\{ \frac{1}{\omega} \pi_K^2 + \bar{\omega} \phi_K^2 \right\} = \hbar \bar{\omega} \sum_K g_K g_K^\dagger, \\ P &= \hbar \frac{\bar{\omega}'}{c} \sum_K K \left\{ \frac{1}{\omega} \pi_K^2 + \bar{\omega} \phi_K^2 \right\} = \hbar \frac{\bar{\omega}'}{c} \sum_K K g_K g_K^\dagger. \end{aligned}$$

Converting back to real space we find

$$Q = \hbar \bar{\omega} \int_{-L/2}^{L/2} |g|^2 dz,$$

$$P = \frac{i}{2} \hbar \frac{\bar{\omega}'}{c} \int_{-L/2}^{L/2} (g \partial_z g^\dagger - g^\dagger \partial_z g) dz.$$

The reduced Hamiltonian can be written in terms of the conserved charge

$$H^R = Q + H' \quad (64)$$

with

$$\begin{aligned} H' &\equiv \int_{-L/2}^{L/2} dz \left( \frac{i \hbar \bar{\omega}'}{2} (g \partial_z g^\dagger - \text{c.c.}) \right. \\ &\quad \left. - \frac{1}{2} \hbar \bar{\omega}'' |g|^2 - \frac{1}{2} \alpha |g|^4 \right), \end{aligned} \quad (65)$$

where  $H'$  is obviously also conserved.

To understand the nature of these conserved quantities, we consider the differential equation satisfied by the  $g$  field (50). In the absence of group velocity, group velocity dispersion or nonlinearity ( $\bar{\omega}' = \bar{\omega}'' = \alpha = 0$ ), the solution to the differential equation (50) is  $g(z, t) = g(z, 0) e^{-i\bar{\omega}t}$ . When  $\bar{\omega}' = 0$ , it is clear that  $P = 0$ . Furthermore, the phase accumulation  $e^{-i\bar{\omega}t}$  is directly related to the increase in time  $t$  so that the accumulation of the time and phase are proportional. This means that the reduced Hamiltonian  $H^R$  is identical to the charge  $Q$ , and we effectively have only one independent conserved quantity. If we allow group velocity  $\bar{\omega}' \neq 0$ , but keep  $\bar{\omega}'' = \alpha = 0$ , then the equation of motion (50) describes a pulse that propagates at a speed  $\bar{\omega}'$ , and does not distort its shape. We can solve the equations of motion as  $g(z, t) = g(z - \bar{\omega}'t, 0) e^{-i\bar{\omega}t}$ , from which it is clear that an increase in the time variable is equivalent to a displacement in space plus an increase in the phase. That is, only two of the three displacements (time, space and phase) are independent and hence required to fully describe the effective field dynamics. Associated with this, one of the conserved quantities can be expressed in terms of the other two,  $H^R = Q + cP$ , which means that only two of our three conserved quantities are independent. Finally, if we place no restrictions on the coefficients in Eq. (50) then there are no simple solutions to the equation of motion, and we find that the time, space, and phase displacements must be treated independently; and the three conserved quantities  $H^R, Q, P$  are independent. The independence of these quantities is forced upon us by the introduction of either the group velocity dispersion or the Kerr nonlinearity, so the linear Schrödinger equation ( $\alpha = 0$ ) will also have three independent conserved quantities associated with time, space, and phase invariance.

To connect with the literature on nonlinear optical pulse propagation, we write our  $g$  field as the product of a new effective field  $r(z, t)$ , which varies slowly in time as well as space, and a carrier frequency,

$$g(z,t) = r(z,t)e^{-i\bar{\omega}t}, \quad (66)$$

then

$$\begin{aligned} \mathbf{H}' = \int_{-L/2}^{L/2} dz & \left( \frac{i\hbar\bar{\omega}'}{2} (r\partial_z r^\dagger - \text{c.c.}) \right. \\ & \left. - \frac{1}{2} \hbar\bar{\omega}'' |\partial_z r|^2 - \frac{1}{2} \alpha |r|^4 \right), \end{aligned} \quad (67)$$

and

$$[r(z,t), r^\dagger(z',t)] = \delta(z-z'), \quad (68)$$

which leads to

$$i\partial_t r = -i\bar{\omega}'\partial_z r - \frac{1}{2}\bar{\omega}''\partial_{zz}r - \alpha|r|^2r. \quad (69)$$

Although  $\mathbf{H}'$  correctly determines the dynamics of the  $r$  fields, it is clearly not equal to the energy in the electromagnetic field. In previous discussions, the nonlinear Schrödinger equation (69) has been derived directly from Maxwell's equations, and the  $r$  fields—effective fields that vary slowly in space *and* time—have been the primary fields of interest [1–3,5]. It was observed that the quantity  $\mathbf{H}'$  could be used in a Hamiltonian formulation, such that the correct equations of motion (69) were derived [8,12]; but the quantity  $\mathbf{H}'$  was clearly not equal to the energy of the system. However, to comprehensively compare the approach in this paper to the approach in the literature [8,12] would require a somewhat lengthy discussion about the relationship between the effective fields used in this paper, and the envelope functions used elsewhere [8,12]. We defer such a discussion to a future paper.

Although we have discussed these conserved quantities in the context of the NLSE, the concepts behind this extend to other nonlinear systems of interest. The coupled NLSEs relevant to birefringent systems are often derived from a Hamiltonian that is not equal to the energy [9,10], as are the nonlinear coupled mode equations that describe periodic, Kerr media (both isotropic and birefringent [7]). These equations can all be derived using the methodology in this paper; a Hamiltonian can be identified that is both equal to the energy in the system, and which can be used to derive the correct equations of motion.

## VI. ON THE USE OF THE DUAL FIELD

The reduced Hamiltonian (47), used in conjunction with the commutation relations (32) and the equations of motion (49), gives a NLSE that describes pulse propagation in a periodic medium, under the restriction pointed out at the beginning of Sec. III. A similar equation was derived by de Sterke *et al.* [5]. The advantage of the formulation in this paper is that the reduced Hamiltonian is presented in a form ready for quantization. However, since both papers arrived at the NLSE, it might be asked whether one could construct a canonical Hamiltonian using the formalism of de Sterke *et al.* rather than introducing the dual field  $\Lambda$ . In this section

we point out the difference between these two approaches, and show the advantages of using the dual field.

To construct their NLSE, de Sterke *et al.* introduced a formal vector field

$$\mathbf{A} = \begin{bmatrix} A^+ \\ A^- \end{bmatrix},$$

with

$$A^\pm(z,t) = \frac{1}{2}\sqrt{n(z)} \left[ E(z,t) \pm \frac{Z_0}{n(z)} H(z,t) \right],$$

where  $n(z)$  is the index of refraction and  $Z_0 = \sqrt{\mu_0/\epsilon_0}$  is the impedance of the free space. In a Kerr nonlinear, periodic medium, the field  $\mathbf{A}$  was shown to satisfy

$$\begin{aligned} n(z) \frac{\partial \mathbf{A}}{\partial t} = c & \begin{bmatrix} -\frac{\partial}{\partial z} & \frac{1}{2} \frac{n'}{n} \\ -\frac{1}{2} \frac{n'}{n} & \frac{\partial}{\partial z} \end{bmatrix} \cdot \mathbf{A} - \frac{1}{2} \frac{\chi^{(3)}(z)}{n^2(z)} \frac{\partial}{\partial t} \\ & \times \{ [A^+ + A^-]^3 \} \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \end{aligned} \quad (70)$$

where  $n'(z) = dn(z)/dz$ . One can readily construct a quantity  $E_A(A^+, A^-)$ , which is equal to the energy in the electromagnetic (e.m.) field. However, the construction of a canonical Hamiltonian in terms of the mode amplitudes of the  $A$  field appears impossible. To show this, we first imagine that one has constructed such a Hamiltonian  $\mathbf{H}_A(a_k)$ , where  $a_k$  are the appropriate mode amplitudes of the  $A$  field, with canonical commutation relations. One would then apply the Heisenberg equations of motion to find

$$i \frac{da_k}{dt} = \frac{1}{\hbar} [a_k, \mathbf{H}_A]. \quad (71)$$

The portion on the right-hand side will be some complicated combination of modes  $a_k$ . Unfortunately, the second term on the right-hand side of Eq. (70) makes clear that the time derivatives of the modes  $a_k$  must be expressed in terms of combinations of modes and their time derivatives. Thus, equations of motion of the form (71) cannot be exact, at least if there is the usual kind of linear expansion of the fields in terms of mode amplitudes. Nevertheless, if the nonlinearity itself is weak, then the nonlinear contribution to the time derivative,  $\partial \mathbf{A} / \partial t$  will also be weak. Then, in the spirit of perturbation, we could replace the time derivatives of the nonlinear portion of Eq. (70) by their linear value. This strategy allows the construction of a Hamiltonian formulation of Maxwell's equations in the presence of a weak nonlinearity. We have verified that such a Hamiltonian can, indeed, be constructed, but we do not present the results here.

The Hamiltonian generated by the use of the  $\mathbf{A}$  field is of as much practical value as that generated by the use of the dual field  $\Lambda$ . The advantage of the dual field formulation is that once a form of the function  $U(D)$  is chosen, no further approximations need to be made. Thus, for the investigation

of the formal properties of the Hamiltonian system the dual field approach is more useful, while for the calculation of experimental quantities either approach will work.

## VII. CONCLUSION

We have constructed a canonical Hamiltonian formulation for light in a nonlinear, periodic Kerr medium, with the appropriate frequency content such that the NLSE is the relevant equation of motion. To do so, we have introduced a reduced Hamiltonian that is equal to the energy in the electromagnetic field to the required order in perturbation theory. Using the reduced Hamiltonian we investigated the conserved quantities of the system. In addition to the familiar energy and momentum, we identified a conserved charge associated with phase invariance. In a future paper we will

explore the connection between this conserved charge and the “energy” given in other papers in the literature. A clarification of the energy of the system is necessary for the purpose of canonical quantization. To underscore the use of our Hamiltonian formulation in quantization of the fields, we have presented Hamilton’s equation of motion in terms of canonical commutation relations, although we stress that the results in this paper are purely classical. In a future work we will return to the quantization of the e.m. field in a periodic, Kerr-nonlinear medium.

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