Corrections to coupled mode theory for deep gratings

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We generalize the standard coupled mode equations describing interactions between forward and backward propagating waves in a nonlinear optical Bragg grating. Including the lowest order corrections of the grating depth, we obtain a Hamiltonian system that can be regarded as an extension of the usual coupled mode equations for shallow gratings. The results are consistent with existing results based on a Bloch wave expansion. We also obtain exact traveling solitary wave solutions, that can be regarded as a generalized gap soliton, modified by the grating's depth.

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I. INTRODUCTION

Wave propagation in nonlinear media with a periodic structure is of great current interest in linear and nonlinear physics. A striking aspect of the linear properties of such media is the drastic change in the linear dispersion, highlighted by the appearance of stop gaps. Coupled mode theory is the standard method to describe electromagnetic wave propagation in such structures [1,2]. A most remarkable result obtained using this method is the existence of gap solitons when the wave intensity is high enough for nonlinear effects to play a role [3]. This theoretical prediction was verified experimentally in an optical fiber geometry [4–6]. More recently, in an $Al_xGa_{1-x}As$ grating filter where the index modulations δn can be as great as 0.1, soliton propagations was also observed [7]. The general gap soliton solutions to the coupled mode equations were first obtained in a limiting case by Christodoulides and Joseph [8]. The full solutions were found by Aceves and Wabnitz [9], who also discussed aspects of their stability. Comprehensive analyses of Bragg solitons stability have also recently been reported [10,11].

Though the coupled mode equation are the usual governing equations for nonlinear gratings, their derivation from the Maxwell equations often requires the assumption that the grating is sufficiently *shallow*. This allows one to use the picture of coupling between forward and backward waves satisfying the Bragg condition. However, if the periodic variation of the refractive index $n(z)$ is comparable to the mean value, or, in other words, if the grating is *deep*, such as in a $Al_xGa_{1-x}As$ grating filter, then the shallow grating approximation is not justified.

One method to analyze deep gratings is by using Bloch wave solutions as the fundamental waves. Actually the modulation of a *single* Bloch wave is known to obey the nonlinear Schrödinger equation [12–15] in Kerr optical media, and its fundamental soliton corresponds to gap solitons in this geometry. To derive more general coupled mode equations it is necessary that the field can be written approximately as a superposition of *two* Bloch waves. Effects due to other Bloch waves can be treated perturbatively [14]. The Bloch wave approach can also be used to describe nonlinear effects in periodic $\chi^{(2)}$ media [16,17]. Note that the Bloch function formalism has the feature that the linear system needs to be solved first, and the nonlinearity is then considered as a perturbation which can be treated in a variety of approximations.

A different formalism to treat deep gratings was reported by Sipe *et al.* [18]. In this formalism, which was developed for linear gratings only, the properties of the linear system are determined within the method, and do not need to be calculated separately beforehand. The linear properties are therefore not obtained exactly, but in terms of an asymptotic series, only a few terms of which are retained. Nonetheless, the method leads naturally to low-order corrections to the coupled mode equations for shallow gratings. The aim of the present work to extend the analysis of Sipe *et al.* [18] to include nonlinear effects, particularly the Kerr effect. We also analyze how gap solitons are affected by the grating depth. The equations that are obtained are expected to have the forms

$$i\left(\frac{1}{v_g}\frac{\partial}{\partial t}+\frac{\partial}{\partial z}\right)E_+ +\delta(|E_+|^2+2|E_-|^2)E_+ +\overline{\kappa}E_- +\mathcal{C}=0,$$
$$i\left(\frac{1}{v_g}\frac{\partial}{\partial t}-\frac{\partial}{\partial z}\right)E_- +\delta(|E_-|^2+2|E_+|^2)E_- +\overline{\kappa}^*E_+ +\mathcal{C}=0. \quad (1)$$

As discussed in detail below, $E_\pm=E_\pm(z,t)$ are associated with envelopes of the forward$(+)$ and backward$(-)$ waves at the Nth Bragg wave numbers, and $\pm v_g$ are the group velocities in the absence of the grating. Parameters $\overline{\kappa}$ and δ are constants, representing the gap width and the strength of the nonlinearity, respectively. Without the terms indicated by $\mathcal{C}$, Eqs. (1) reduce to the conventional coupled mode equations for shallow gratings. Our main purpose here is to in-

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clude the effect of the grating depth up to $O(\eta^{\phi})$, where ϕ is less than 3 and parameter η represents the grating's depth. Therefore, we neglect $O(\eta^3)$ quantities, though larger terms should be collected. Note that in the conventional coupled mode theory only $O(\eta)$ are included.

In extracting the new terms, we must note three points. The first is that the dielectric function $\epsilon(z)$ is given by an infinite Fourier series [see Eq. (3)]. Thus, in addition to the forward and backward Bragg waves, we must consider an infinite number of plane waves $\exp[i(2m+N)kz]$ $(m=0,\pm 1, \pm 2 \ldots)$ [see Eq. (6)], where k is the lowest order Bragg wave number $k=\pi/d$, and d is the grating's period. The second point is that $\mathcal{E}^{(\pm 3N)}$, associated with $\exp[\pm 3iNkz]$, excited by the Bragg grating, affects the nonlinear terms, though other excited waves do not contribute to the order we consider. The last point is that we should also consider the periodicity of the Kerr coefficient $\chi^{(3)}$ [Eq. (4)]. In fact, the Fourier components $\chi_{\pm 1}$ and $\chi_{\pm 2}$, lead to additional nonlinear terms.

This paper is organized as follows. In Sec. II we introduce the perturbation expansion for the field. Neglecting nonlinear effects, we obtain a set of linear coupled mode equations, and we discuss how the dispersion relation and the photonic band gap are modified by the grating depth. In Sec. III we derive the nonlinear coupled mode equations, and we discuss some properties of these equations. In Sec. IV, analytic expressions for traveling solitary wave solutions, representing a generalization of gap solitons, are derived. Section V gives some concluding remarks and discussions.

II. FUNDAMENTAL EQUATION AND LINEAR ANALYSIS

We consider electromagnetic wave propagation in a grating in the z direction. We assume that the electric field is polarized in the x direction. The wave equation for the electric field $\mathbf{x}E(z,t)$ is

$$c^2 \frac{\partial^2 E}{\partial z^2} = \frac{\partial^2}{\partial t^2}[\epsilon(z)E + \chi^{(3)}(z)E^3], \tag{2}$$

which is derived directly from Maxwell's equations. Here c is the speed of light in vacuum, and the dielectric function ϵ, and the Kerr nonlinearity $\chi^{(3)} = \boldsymbol{\chi}^{(3)}_{xxxx}$ are periodic functions of z with period d, expressed by the Fourier expansions

$$\epsilon(z) = \sum_{l \in \mathbb{Z}} \epsilon_l e^{2ilkz}, \tag{3}$$

$$\chi^{(3)}(z) = \sum_{l \in \mathbb{Z}} \chi_l e^{2ilkz}, \tag{4}$$

Here $\epsilon_{-l} = \epsilon_l^*$ and $\chi_{-l} = \chi_l^*$. Further, $k = \pi/d$ is the Bragg wave number, and subscript $l \in [\mathbb{Z}]$ denotes summation over all integers $[\mathbb{Z}]$. Let us introduce a small but finite parameter η representing the grating's depth,

$$O(\eta) \sim e_l \equiv \frac{\epsilon_l}{\epsilon_0} \sim \frac{\chi_l}{\chi_0}, \tag{5}$$

for at least one $l \neq 0$. Since $\epsilon(z)$ and $\chi^{(3)}(z)$ are given by infinite Fourier series, we may choose nonanalytic functions such as piecewise constant ones. In this sense, the grating's *sharpness* is included in the analysis. We neglect the material dispersion which does not essentially change our results. We expand the electric field as

$$E = \left(\sum_{m \in \mathbb{Z}} \mathcal{E}^{(2m+N)} e^{i(2m+N)kz} \right) e^{-iN\omega t} + \text{c.c.}, \tag{6}$$

where $\mathcal{E}^{(2m+N)}$ are slowly changing envelopes and N is a natural number. In particular, $\mathcal{E}^{(N)}$ and $\mathcal{E}^{(-N)}$ are host waves which denote the amplitudes of the forward and backward waves at the Nth Bragg wave number Nk, respectively. Their amplitudes are assumed to be larger than the other envelopes. The fundamental frequency ω is related to the Bragg wave number k by the dispersion relation in the absence of the grating:

$$(ck)^2 = \epsilon_0 \omega^2. \tag{7}$$

Since we consider the Nth stop gap of the grating, the frequency of $E(z,t)$ is set to $N\omega$. We define a second dimensionless small parameter ε representing the nonlinearity and the gentleness of the modulation:

$$O(\varepsilon) \sim \chi_0 \sim \frac{\partial \mathcal{E}^{(\pm N)}}{\partial z} \sim \frac{\partial \mathcal{E}^{(\pm N)}}{\partial t}. \tag{8}$$

The relation between ε and η depends on the situation we consider. Here we assume $\mathcal{E}^{(\pm N)}$ and constants k, c, ω, and ϵ_0 to be normalized so as to be of $O(1)$.

First we consider the linear case $\chi^{(3)}(z) = 0$. Substitution of Eq. (6) into the wave equation (2), and a comparison of the coefficient of $\exp[i(2n+N)kz]\exp[-iN\omega t]$ give

$$-(2n+N)^2(ck)^2\mathcal{E}^{(2n+N)} + N^2\omega^2 \sum_{m \in \mathbb{Z}} \epsilon_{n-m}\mathcal{E}^{(2m+N)} + 2i(2n+N)c^2k\frac{\partial \mathcal{E}^{(2n+N)}}{\partial z} + 2i\omega N \times \sum_{m \in \mathbb{Z}} \epsilon_{n-m}\frac{\partial \mathcal{E}^{(2m+N)}}{\partial t} + c^2\frac{\partial^2 \mathcal{E}^{(2n+N)}}{\partial z^2} - \sum_{m \in \mathbb{Z}} \epsilon_{n-m}\frac{\partial^2 \mathcal{E}^{(2m+N)}}{\partial t^2} = 0. \tag{9}$$

For $n \neq 0, -N$ Eq. (9) reduces to

$$\frac{N^2 - (2n+N)^2}{N^2\omega^2}(ck)^2\mathcal{E}^{(2n+N)} + (\epsilon_n\mathcal{E}^{(N)} + \epsilon_{n+N}\mathcal{E}^{(-N)}) + \sum_{m \neq n, 0, -N} \epsilon_{n-m}\mathcal{E}^{(2m+N)} = O(\varepsilon\eta). \tag{10}$$

Since relation (10) suggests that $\mathcal{E}^{(2n+N)} \sim O(\eta)$ for $n \neq 0, -N$, the final term on the left-hand side is $O(\eta^2)$. We neglect it as we search for the lowest order correction due to the grating depth. The derivatives with respect to z and t were dropped since they are also smaller than $O(\varepsilon\eta)$. Thus

Eq. (10) yields an explicit form for the envelopes of the slave waves in term of the dominant waves $\mathcal{E}^{(\pm N)}$,

$$\mathcal{E}^{(2n+N)}=\frac{e_n\mathcal{E}^{(N)}+e_{n+N}\mathcal{E}^{(-N)}}{\left(\frac{2n+N}{N}\right)^2-1}\sim O(\eta)\quad (n\neq 0,-N), \tag{11}$$

where e_l were defined in Eq. (5). Substituting these into Eq. (9), we obtain a set of closed coupled equation for $\mathcal{E}^{(\pm N)}$ for $n=0,-N$ up to $O(\eta^2,\eta\varepsilon,\varepsilon^2)$:

$$i\left(\frac{1}{v_g}\frac{\partial}{\partial t}+\frac{\partial}{\partial z}\right)\mathcal{E}^{(N)}+\frac{Nk}{2}\kappa\mathcal{E}^{(-N)}+\frac{Nk}{2}\alpha\mathcal{E}^{(N)}+\frac{ie_N}{v_g}\frac{\partial\mathcal{E}^{(-N)}}{\partial t}+\frac{1}{2Nk}\left(\frac{\partial^2}{\partial z^2}-\frac{1}{v_g^2}\frac{\partial^2}{\partial t^2}\right)\mathcal{E}^{(N)}=0, \tag{12}$$

$$i\left(\frac{1}{v_g}\frac{\partial}{\partial t}-\frac{\partial}{\partial z}\right)\mathcal{E}^{(-N)}+\frac{Nk}{2}\kappa^*\mathcal{E}^{(N)}+\frac{Nk}{2}\alpha\mathcal{E}^{(-N)}+\frac{ie_{-N}}{v_g}\frac{\partial\mathcal{E}^{(N)}}{\partial t}+\frac{1}{2Nk}\left(\frac{\partial^2}{\partial z^2}-\frac{1}{v_g^2}\frac{\partial^2}{\partial t^2}\right)\mathcal{E}^{(-N)}=0, \tag{13}$$

where $v_g\equiv c\epsilon_0^{-1/2}>0$ is the group velocity at the Bragg wave number, and the dimensionless parameters κ, α, and β are defined by

$$\kappa=e_N+\beta, \tag{14}$$

$$\alpha=\sum_{j\neq -N,0}\frac{|e_j|^2}{\left(\frac{2j+N}{N}\right)^2-1}, \tag{15}$$

$$\beta=\sum_{j\neq -N,0}\frac{e_{-j}e_{j+N}}{\left(\frac{2j+N}{N}\right)^2-1}. \tag{16}$$

Recall that we dropped terms like $O(\eta^3)$ and $O(\eta^2\varepsilon)$ in deriving Eqs. (12) and (13). Now note the relation

$$\begin{aligned}\left(\frac{\partial^2}{\partial z^2}-\frac{1}{v_g^2}\frac{\partial^2}{\partial t^2}\right)\mathcal{E}^{(\pm N)}&=\left(\frac{\partial}{\partial z}\mp\frac{1}{v_g}\frac{\partial}{\partial t}\right)\left(\frac{\partial}{\partial z}\pm\frac{1}{v_g}\frac{\partial}{\partial t}\right)\mathcal{E}^{(\pm N)}\\&=\left(\frac{\partial}{\partial z}\mp\frac{1}{v_g}\frac{\partial}{\partial t}\right)(\pm i)\left(\frac{Nk}{2}\kappa_\pm\mathcal{E}^{(\mp N)}+O(\eta^2,\eta\varepsilon,\varepsilon^2)\right)\\&=\left(\frac{Nk}{2}\right)^2|\kappa|^2\mathcal{E}^{(\pm N)}+O(\varepsilon\eta^2,\eta\varepsilon^2,\varepsilon^3),\end{aligned} \tag{17}$$

where $\kappa_+=\kappa_-^*=\kappa$, and we used Eqs. (12) and (13) in the second and third lines. Now these equations become

$$i\left(\frac{1}{v_g}\frac{\partial}{\partial t}+\frac{\partial}{\partial z}\right)\mathcal{E}^{(N)}+\frac{Nk}{2}\kappa\mathcal{E}^{(-N)}+\frac{Nk}{2}\left(\alpha+\frac{1}{4}|\kappa|^2\right)\mathcal{E}^{(N)}+\frac{i}{v_g}e_N\frac{\partial\mathcal{E}^{(-N)}}{\partial t}=0, \tag{18}$$

$$i\left(\frac{1}{v_g}\frac{\partial}{\partial t}-\frac{\partial}{\partial z}\right)\mathcal{E}^{(-N)}+\frac{Nk}{2}\kappa^*\mathcal{E}^{(N)}+\frac{Nk}{2}\left(\alpha+\frac{1}{4}|\kappa|^2\right)\mathcal{E}^{(-N)}+\frac{i}{v_g}e_{-N}\frac{\partial\mathcal{E}^{(N)}}{\partial t}=0. \tag{19}$$

The first two terms in Eqs. (18) and (19) correspond to the conventional linear coupled mode equation, with κ given by Eq. (14), in which the second term is a correction to the shallow grating expression. The third and fourth terms are new, and are lowest order corrections due to the grating depth. The effect of the *sharpness* of the grating is included through α and β. Equations (18) and (19) correspond to Eqs. (39) of Sipe *et al.* [18], in which the explicit time dependence of the envelopes was dropped. In fact, if we take $N=1$ and change the notation by

$$z\to\xi, \tag{20}$$

$$\epsilon_0\to n_0^2\left(1+\eta^2\sum_{m\in\mathbb{Z}}\left|g_m\right|^2\right), \tag{21}$$

$$\frac{\epsilon_n}{\epsilon_0}\to 2\eta g_n+\eta^2\sum_{m\in\mathbb{Z}}g_{n-m}g_m\quad (n\neq 0), \tag{22}$$

$$\omega\to\omega\left(1-\frac{\eta^2}{2}\sum_{m\in\mathbb{Z}}|g_m|^2\right)\equiv\omega+\eta^2\Delta\omega, \tag{23}$$

$$\mathcal{E}^{(+1)}\to(u^{(0)}-\eta g_1v^{(0)})e^{i\eta^2\Delta\omega t}, \tag{24}$$

$$\mathcal{E}^{(-1)}\to(v^{(0)}-\eta g_{-1}u^{(0)})e^{i\eta^2\Delta\omega t}, \tag{25}$$

we confirm Eq. (39) of Sipe *et al.* [18] up to $O(\eta^2)$ in the uniform grating limit. The transformation for ϵ_n originates from $\epsilon(z)=(n(z))^2$, where $n(z)$ is the refractive index. The frequency difference $\eta^2\Delta\omega$ owes to the definition of ω; here $\omega\equiv ck/\sqrt{\epsilon_0}$, whereas in Ref. [18] $\omega\equiv ck/n_0$.

Setting $\mathcal{E}^{(\pm N)}(z,t)=\mathcal{E}_\pm\exp\{iNk2^{-1}(Kz-v_g\Omega t)\}$ and substituting into Eqs. (18) and (19), we find

$$\begin{pmatrix}\Omega-K+\left(\alpha+\frac{|\kappa|^2}{4}\right) & \kappa+e_N\Omega\\ \kappa^*+e_{-N}\Omega & \Omega+K+\left(\alpha+\frac{|\kappa|^2}{4}\right)\end{pmatrix}\cdot\vec{\mathcal{E}}=0, \tag{26}$$

where $\vec{\mathcal{E}}$ is the vector with elements $\mathcal{E}_\pm$. This leads to a dispersion relation between the dimensionless wave number K and dimensionless frequency Ω:

$$\left(\Omega+\alpha+\frac{|\kappa|^2}{4}\right)^2-K^2-|\kappa+e_N\Omega|^2=0. \tag{27}$$

In the conventional shallow grating case the corresponding relation is given by $\Omega^2-K^2=|e_N|^2$; indeed, this result is obtained when $O(\eta^3)$ quantities and smaller are omitted. Up to $O(\eta^4)$ Eq. (27) can be written

$$(1-|e_N|^2)(\Omega+\Delta\Omega)^2-K^2=|\kappa|^2+\frac{1}{2}|\kappa|^4+\alpha|\kappa|^2, \tag{28}$$

$$\Delta\Omega=(1+|e_N|^2)\left(\alpha-\frac{3}{4}|\kappa|^2\right)+\mathrm{Re}(\kappa\beta^*), \tag{29}$$

where Re indicates the real part. If $K=0$, the values $\Omega=\Omega_\pm$ give the upper $(+)$ and lower $(-)$ edges of the gap. From Eq. (28), neglecting $O(\eta^3)$ quantities, for the edges of the Nth gap we find

$$\Omega_\pm=-\Delta\Omega\pm|\kappa|. \tag{30}$$

Thus the center of the gap shifts by $-N\omega\Delta\Omega/2$ due to the depth of the grating; the width of the gap is $2|\kappa|$. Hereafter we refer to parameter κ defined in Eq. (14) as the *gap parameter*, as it plays a key role in our analysis.

Care should be taken with the *sharpness* parameters α and β, since they are given by infinite series [see Eqs. (15) and (16)]. If $\epsilon(z)$ is smooth enough, ϵ_j are close to zero for large j, and α and β are then expected to be small, of order η^2. Even for nonanalytic functions such as a piecewise constant function, e_j is at most approximated as j^{-1} for large j. Thus α and β converge for a large class of gratings, and remain at about $O(\eta^2)$.

We now consider the gap parameter κ, whose order is η, as seen from definition (14). Now for some gratings the upper and lower edges may be degenerate. However, even if the gap does not completely vanish, its width may become small compared to the grating depth: $|\kappa|\ll O(\eta)$. As seen in Eq. (14), such a case occurs when e_N is sufficiently small compared to η. Since in the fully deep case the gap width is $O(1)$, and in the shallow case it is $O(\eta)$ from Eq. (5), here, for convenience, we express its order by $\eta^{1/2}$. First, assume $e_N\sim O(\eta^2)$ or less. Then the gap width κ is also of order $O(\eta^2)$. Hereafter, we refer to such a case as the *narrow gap case*. In contrast to the *finite gap case*, e_N is about $O(\eta^{3/2})$, and, accordingly, the band width is of the same order. Finally, in the *wide gap case*, $e_N\sim O(\eta)$, and the grating depth is fully reflected in the gap width.

As seen from Eqs. (18) and (19), we must set the modulation parameter ε to be $O(\kappa)$, in order for a balance between the modulation terms and the Bragg grating resonance term. Then for narrow and finite gap cases, we assume

$$\varepsilon\sim\eta^2 \quad \text{(narrow gap case)}, \tag{31}$$

$$\varepsilon\sim\eta^{3/2} \quad \text{(finite gap case)}. \tag{32}$$

In formulating these criteria, the second lines in Eqs. (12) and (13) are neglected, though corrections related to the sharpness α in the third term remain. In Sec. III, we proceed with the nonlinear analysis for narrow and finite gaps only. A simple example of near degeneration of a gap is also discussed. In the wide gap case the modulation parameter should be set at $\varepsilon\sim\eta$, and the third and fourth terms in Eqs. (18) and (19) are to be regarded as the lowest order corrections. Nonlinear effects for such situation are discussed briefly in Sec. V.

III. NONLINEAR COUPLED MODE EQUATION

We now include the nonlinear Kerr effect, taking the Nth gap to be narrow or finite. Again, we substitute expansion (6) into wave equation (2) and extract the coefficients of $\exp[i(2n+N)kz-iN\omega t]$. If $n\neq 0,-N,N,-2N$, we again obtain Eq. (11) for the slave waves. For $n=N,-2N$ up to $O(\eta,\varepsilon)$ we have

$$\mathcal{E}^{(3N)}=\frac{1}{8}\left(e_{2N}\mathcal{E}^{(-N)}+3\frac{\chi_0}{\epsilon_0}(\mathcal{E}^{(N)})^2(\mathcal{E}^{(-N)})^*\right), \tag{33}$$

$$\mathcal{E}^{(-3N)}=\frac{1}{8}\left(e_{-2N}\mathcal{E}^{(N)}+3\frac{\chi_0}{\epsilon_0}(\mathcal{E}^{(-N)})^2(\mathcal{E}^{(N)})^*\right), \tag{34}$$

respectively, which include explicit nonlinear terms. We introduce a frequency shift to the host waves by the transformation

$$E_\pm\equiv\mathcal{E}^{(\pm N)}\exp(iv_gNk\alpha t/2), \tag{35}$$

corresponding to the gap center shift $-N\omega\Delta\Omega/2$ of the linear system up to $O(\eta^2)$ [see Eq. (29)]. For $n=0,-N$, we discuss the narrow gap and finite gap cases below.

A. Narrow gap case

For a narrow gap $(\varepsilon\sim\kappa\sim\eta^2)$, we find closed coupled equations for the modified host waves $E_\pm$:

$$i\left(\frac{1}{v_g}\frac{\partial}{\partial t}+\frac{\partial}{\partial z}\right)E_++\bar{\kappa}E_-+\delta(|E_+|^2+2|E_-|^2)E_+=0 \tag{36}$$

$$i\left(\frac{1}{v_g}\frac{\partial}{\partial t}-\frac{\partial}{\partial z}\right)E_-+\bar{\kappa}^*E_++\delta(|E_-|^2+2|E_+|^2)E_-=0, \tag{37}$$

where

$$\bar{\kappa}=\frac{Nk}{2}\kappa=\frac{Nk}{2}(e_N+\beta)\sim O(\eta^2), \tag{38}$$

$$\delta=\frac{3Nk}{2}\frac{\chi_0}{\epsilon_0}\sim O(\eta^2). \tag{39}$$

Here, $O(\eta^3)$ terms have been omitted. These coupled mode equations have the same forms as those for shallow gratings. However, the depth effects at $O(\eta^2)$ are included in $\bar{\kappa}$, and in the frequency shift (35) via the parameters β and α, respectively.

B. Finite gap case

For a finite gap ($\varepsilon \sim \kappa \sim \eta^{3/2}$), we have

$$i\left(\frac{1}{v_g}\frac{\partial}{\partial t}+\frac{\partial}{\partial z}\right)E_+ + \overline{\kappa}E_- + \delta(|E_+|^2+2|E_-|^2)E_+ + \mu(|E_-|^2+2|E_+|^2)E_- + \mu^* E_+^2 E_-^* + \nu E_-^2 E_+^* = 0, \quad (40)$$

$$i\left(\frac{1}{v_g}\frac{\partial}{\partial t}-\frac{\partial}{\partial z}\right)E_- + \overline{\kappa^*}E_+ + \delta(|E_-|^2+2|E_+|^2)E_- + \mu^*(|E_+|^2+2|E_-|^2)E_+ + \mu E_-^2 E_+^* + \nu^* E_+^2 E_-^* = 0, \quad (41)$$

where

$$\mu = \frac{3Nk}{2}\frac{\chi_N}{\epsilon_0} \sim O(\eta^{5/2}), \quad (42)$$

$$\nu = \frac{3Nk}{2}\left(\frac{\chi_{2N}}{\epsilon_0}+\frac{\chi_0}{2\epsilon_0}e_{2N}\right) \sim O(\eta^{5/2}), \quad (43)$$

where again $O(\eta^3)$ were dropped, and $\chi_j = (\chi_j/\chi_0)\chi_0 \sim O(\eta)\cdot O(\varepsilon) \sim O(\eta^{5/2})$ [see relations (3) and (5)]. We neglect nonlinear terms with derivatives because they are higher order quantities [$O(\eta^3)$ at most]. Coupled equations (40) and (41) are our main results and are generalization of the conventional results for shallow gratings. They are formally consistent with previous results of de Sterke *et al.* [14] [see Eq. (102) in this reference]. The first lines in Eqs. (40) and (41) correspond to the conventional nonlinear coupled mode equation; the remainder of $O(\eta^{5/2})$ are the lowest corrections arising form resonances with the linear and nonlinear grating.

Our results can be directly compared to those of de Sterke *et al.* [14] in the limit in which the linear grating is shallow, but the nonlinear coefficients are modulated strongly. In this limit the Bloch functions $\phi_u(z)$ and $\phi_l(z)$, at the upper (u) and lower (l) gap edges, are

$$\phi_u(z) = \sin(2k_B z) + O(\eta), \quad (44)$$

$$\phi_l(z) = \cos(2k_B z) + O(\eta). \quad (45)$$

Taking the nonlinear overlaps from Eq. (99) of Ref. [14] we find that δ, μ, and ν are proportional to χ_0, χ_1, and $-\chi_2$, consistent with result (106) from Ref. [14].

The difference between our analysis and that in Ref. [14], however, is that in the latter the nonlinear coefficients Γ_i are all deemed to be of the same order, whereas in our analysis μ and ν are regarded as lowest perturbation terms. Note further that the constants μ and ν can be complex, whereas Γ_1 and Γ_2, the corresponding parameters in the work of de Sterke *et al*. [14], are real. However, Γ_1 and Γ_2 are real because the Bloch functions from which they are calculated were chosen to be real. If this is not done, then they would come out to be complex as here. Complex nonlinear coefficients were earlier found by Broderick and de Sterke in the study of nonlinear effects in superstructure gratings [19]. We finally note that the fact that formally the same equations are obtained via different approaches suggests that the generalized coupled mode (GCM) equations (40) and (41) can be considered the appropriate model for deep gratings with small but finite gap.

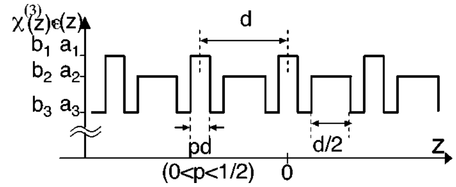

FIG. 1. Grating type used to illustrate the gap degeneracy. Each period consists of three kinds of materials. A particular choice of p leads to a narrow width for the Nth gap.

We expect the near degeneration of a gap $e_N \ll \eta$ for a large class of periodic functions $\epsilon(z)$, even though e_{2N}, χ_N, and χ_{2N} remain at $O(\eta)$. Here, using a simple grating model, we demonstrate gap degeneracy for $N=1$, and calculate e_2, χ_1, and χ_2, which give the correction terms μ and ν. We consider piecewise constant functions $\epsilon(z)$ and $\chi^{(3)}(z)$ with three distinct media in each period, as shown in Fig. 1. The Fourier expansion of $\epsilon(z)$ is

$$\epsilon(z) = pa_1 + \frac{1}{2}a_2 + \left(\frac{1}{2}-p\right)a_3 + \sum_{n\neq 0}\epsilon_n e^{2ikn\pi}, \quad (46)$$

$$\epsilon_n = \frac{a_1-a_3}{n\pi}\sin(n\pi p) - \frac{a_2-a_3}{n\pi}\sin\left(\frac{n\pi}{2}\right). \quad (47)$$

The Fourier expansion for $\chi^{(3)}(z)$ is identical, but with the a_i replaced by b_i. If p (with $0<p<1/2$) satisfies

$$\left|\sin(\pi p) - \frac{a_2-a_3}{a_1-a_3}\right| \leq O(\eta^{1/2}), \quad (48)$$

then ϵ_1 is obviously $O(\eta^{3/2})$ or less since $(a_1-a_3)\sim O(\eta)$, which corresponds to the narrow or finite gap cases. Nonetheless e_2, χ_1, and χ_2 generally remain at $O(\eta)$:

$$e_2 = \frac{a_1-a_3}{2\pi\epsilon_0}\sin(2\pi p), \quad (49)$$

$$\chi_1 = \frac{1}{\pi\chi_0}\left\{(b_1-b_3)\frac{a_2-a_3}{a_1-a_3} - (b_2-b_3)\right\}, \quad (50)$$

$$\chi_2 = \frac{1}{2\pi\chi_0}(b_1-b_3)\sin(2\pi p), \quad (51)$$

while μ and ν are $O(\eta^{5/2})$. We note that for gratings consisting of two media, if e_N is small then χ_N is also small. Then μ in the GCM equations can be neglected, though ν must be kept in general. The above example is an extreme and ideal model. Nonetheless, in real material, we expect that even if e_N happens to be smaller than η, other Fourier components e_{2N}, χ_N, and χ_{2N} are not always small and thus remain at $O(\eta)$.

It is well known that the GCM equations form a Hamiltonian system [14,19]. The Hamiltonian is given by

$$H=v_g\int_{-\infty}^{+\infty}dz\,\frac{i}{2}\left(E_+^*\frac{\partial E_+}{\partial z}-E_-^*\frac{\partial E_-}{\partial z}\right)$$
$$+\bar{\kappa}E_+^*E_-+\delta\left(\frac{|E_+|^4+|E_-|^4}{4}+|E_+E_-|^2\right)$$
$$+\mu(|E_+|^2+|E_-|^2)E_+^*E_-+\frac{\nu}{2}(E_+^*E_-)^2+\text{c.c.},\tag{52}$$

where the canonical equations are

$$\frac{\partial E_\pm}{\partial t}=i\frac{\delta H}{\delta E_\pm^*},\quad \frac{\partial E_\pm^*}{\partial t}=-i\frac{\delta H}{\delta E_\pm}.\tag{53}$$

The GCM have the conservation laws

$$0=\frac{\partial}{\partial t}(|E_+|^2+|E_-|^2)+\frac{\partial}{\partial z}v_g(|E_+|^2-|E_-|^2),\tag{54}$$

$$0=\frac{\partial}{\partial t}\frac{1}{i}\left(E_+\frac{\partial E_+^*}{\partial z}+E_-\frac{\partial E_-^*}{\partial z}\right)$$
$$+\frac{\partial}{\partial z}v_g\left\{\frac{1}{i}\left(E_+\frac{\partial E_+^*}{\partial z}-E_-\frac{\partial E_-^*}{\partial z}\right)\right.$$
$$+\delta(|E_+|^4+|E_-|^4+4|E_+E_-|^2)$$
$$+\mu(|E_+|^2+|E_-|^2)E_+^*E_-+\frac{\nu}{2}(E_+^*E_-)^2$$
$$\left.+\mu^*(|E_+|^2+|E_-|^2)E_+E_-^*+\frac{\nu^*}{2}(E_+E_-^*)^2\right\}.\tag{55}$$

In addition to the ''energy'' associated with Hamiltonian (52), the CGM equations have the two conserved quantities

$$N=\int_{-\infty}^{+\infty}dz\,(|E_+|^2+|E_-|^2),\tag{56}$$

$$P=\int_{-\infty}^{+\infty}dz\,\frac{1}{i}\left\{\left(E_+\frac{\partial E_+^*}{\partial z}+E_-\frac{\partial E_-^*}{\partial z}\right)\right\},\tag{57}$$

corresponding to the total ''photon number'' and ''momentum'' of the two waves, respectively.

IV. EXACT GAP SOLITON SOLUTIONS TO THE GENERALIZED COUPLED MODE EQUATION

Traveling solitary wave solutions of the GCM equations were obtained in Ref. [14] by means of numerical integration of the Stokes parameters. Here we choose another approach to obtain exact solution in the form of traveling waves. Let us look for solutions of the form

$$E_\pm=\Delta^{\mp 1/2}[F(\zeta)]^{1/2}e^{i[\theta_\pm(\zeta)-v_g\Omega t\pm g/2]},\tag{58}$$

where $\zeta=z-Vt$. Function $F(\zeta)$ and constant Δ are positive. Phases $\theta_\pm(\zeta)$, frequency Ω, and velocity V are taken to be real. Below we see that Ω and V characterize the solutions, just as in the Aceves-Wabnitz solutions for shallow gratings [9]. The real constant g is the argument of the parameter $\bar{\kappa}$, i.e., $\bar{\kappa}=|\bar{\kappa}|e^{ig}$. Substituting ansatz (58) into (40) and (41), we obtain equations for the real and imaginary parts, four in total. The consistency between the equations for the imaginary parts leads to

$$\Delta=\sqrt{\frac{v_g-V}{v_g+V}}.\tag{59}$$

Therefore, we must take $|V|\leq|v_g|$ for the speed V, consistent with the Aceves-Wabnitz solution of the standard coupled mode equations [9]. This leads to

$$\phi(\zeta)\equiv\theta_+-\theta_-,\tag{60}$$

$$\frac{dF}{d\zeta}=2\gamma|\bar{\kappa}|\sin(\phi)F+4\gamma^2|\mu|\sin(\phi-h)F^2$$
$$+2\gamma|\nu|\sin 2(\phi-c)F^2,\tag{61}$$

where γ is the Lorentz factor defined by

$$\gamma=\frac{1}{\sqrt{1-(V/v_g)^2}},\tag{62}$$

and $h=\arg(\mu)-g$ and $c=\arg(\nu)/2-g$. The relevant linear combination of the real parts of Eq. (40) and (41) gives

$$\frac{d\phi}{d\zeta}=2\gamma^2\Omega+2\gamma|\bar{\kappa}|\cos(\phi)+2(1+2\gamma^2)\gamma\delta F$$
$$+8\gamma^2|\mu|\cos(\phi-h)F+2\gamma|\nu|\cos 2(\phi-c)F.\tag{63}$$

The ordinary differential equations (61) and (63) have two degrees of freedom which determine the amplitude F and the phase difference $\phi=\theta_+-\theta_-$. Another combination gives an equation for $\theta_++\theta_-$,

$$\frac{d(\theta_++\theta_-)}{d\zeta}=2\gamma^2\frac{V}{v_g}\{\Omega+[2\gamma\delta+2|\mu|\cos(\phi-h)]F\}.\tag{64}$$

We return to this equation below. The system of equations (61) and (63) has an integral $I(F,\phi)$,

$$I=2\gamma^2\Omega F+2\gamma|\bar{\kappa}|F\cos(\phi)+\delta(1+2\gamma^2)\gamma F^2$$
$$+4\gamma^2|\mu|F^2\cos(\phi-h)+\gamma|\nu|F^2\cos 2(\phi-c),\tag{65}$$

which has the properties

$$\frac{d\phi}{d\zeta}=\frac{\partial I}{\partial F},\quad \frac{dF}{d\zeta}=-\frac{\partial I}{\partial\phi}.\tag{66}$$

Integral (65) leads to orbits in the $F-\phi$ plane (the phase space). Typical phase flows are shown for the ''in-gap case'' [20] ($|\bar{\kappa}|>\gamma|\Omega|$) in Fig. 2 for

$$c=h=0,\quad |\bar{\kappa}|=4\delta,\quad 1+2\gamma^2=4,\tag{67}$$

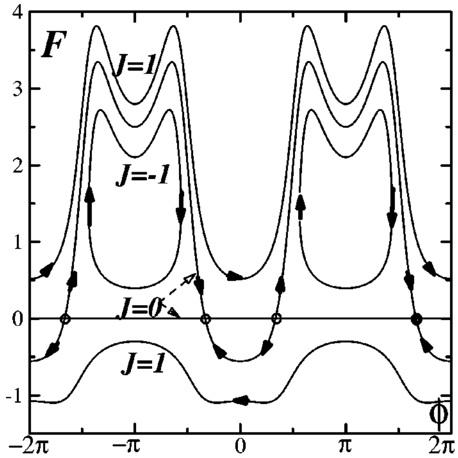

FIG. 2. Phase flows for the in-gap case. The circle dots at $F=0$ are fixed points, whereas orbits with $J \equiv I/(|\overline{\kappa}|\gamma)=0$ are separatrices. Orbits with $F<0$ are unphysical.

$$\gamma\Omega = -\frac{|\overline{\kappa}|}{2}, \quad 4\gamma|\mu| = 0.3|\overline{\kappa}|, \quad |\nu| = 0.5|\overline{\kappa}|,$$

with the normalized integral $J \equiv I/(|\overline{\kappa}|\gamma)$ chosen $J=0,\pm 1$.

Note that the separatrices for $J=0$ correspond to a localized wave. Further, flows in the lower half plane $F<0$ are not physical, because $F>0$ in Eq. (58). The flow diagram for the ''out-gap case'' ($|\overline{\kappa}|<\gamma|\Omega|$) is depicted in Fig. 3 for

$$\gamma\Omega = -2|\overline{\kappa}|, \tag{68}$$

and other values as in Eqs. (67). We further choose $J = I/(|\overline{\kappa}|\gamma) = 0$, -0.555, and ± 7. Note that the out-gap case does not allow for localized solutions, though the upper and lower separatrices ($J \simeq -0.555$) correspond to dark and bright solitons on a finite background, respectively. Here, we consider localized solutions, and we therefore limit ourselves to the in-gap case.

To find localized solution such that $F \to 0$ as $\zeta \to \pm\infty$, we set $I=0$. Then, except for the trivial solution, Eq. (65) gives

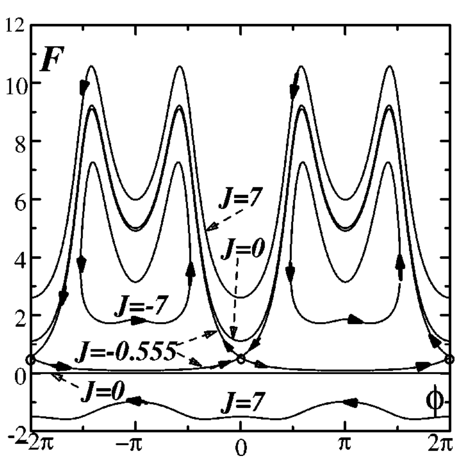

FIG. 3. Phase flow for the out-gap case. Separatrices occur at $J = I/(|\overline{\kappa}|\gamma) \simeq -0.555$. Orbits below the critical points (circles) represent dark solitons, whereas orbits above this points correspond to bright solitons on a finite background.

$$[(1+2\gamma^2)\gamma\delta + 4\gamma^2|\mu|\cos(\phi-h) + \gamma|\nu|\cos 2(\phi-c)]F + 2\gamma^2\Omega + 2\gamma|\overline{\kappa}|\cos(\phi) = 0 \tag{69}$$

which gives the separatrices. Substituting Eq. (69) into Eq. (63), we eliminate F and obtain an equation for $\phi(\zeta)$ only,

$$\frac{d\phi}{d\zeta} + 2\gamma^2\Omega + 2\gamma|\overline{\kappa}|\cos(\phi) = 0, \tag{70}$$

which is directly integrated into

$$\phi(\zeta) = -2\arctan\left[\sqrt{\frac{|\overline{\kappa}|+\gamma\Omega}{|\overline{\kappa}|-\gamma\Omega}}\tanh^{\mp 1}(\xi/2)\right], \tag{71}$$

$$\xi \equiv 2\{\sqrt{\overline{\kappa}^2-\gamma^2\Omega^2}\,\gamma(\zeta-\zeta_0)\}, \tag{72}$$

where ζ_0 is an arbitrary constant. Upper and lower signs correspond to the two solutions in the flow diagrams. Note that Eq. (70) for $\phi(\zeta)$ does not include μ or ν. Thus solution (71) is the same as for the conventional coupled mode equations. Indeed, careful analysis shows that it agrees with the result of Aceves and Wabnitz [9]. In contrast, the amplitude F differs from the conventional case. It is obtained from Eqs. (69) and (71) as

$$F(\zeta) = \frac{F_0(\zeta)}{1 + A\cos(\phi-h) + B\cos 2(\phi-c)}, \tag{73}$$

$$F_0(\zeta) = \frac{\pm 2(|\overline{\kappa}|^2 - \gamma^2\Omega^2)}{\delta(1+2\gamma^2)(|\overline{\kappa}|\cosh(\xi) \pm \gamma\Omega)}, \tag{74}$$

where the constants A and B are given by

$$A = \frac{4\gamma|\mu|}{\delta(1+2\gamma^2)} \sim O(\eta), \tag{75}$$

$$B = \frac{|\nu|}{\delta(1+2\gamma^2)} \sim O(\eta). \tag{76}$$

Since F should be positive, the upper and lower signs in Eq. (74) stand for $\delta>0$ (or $\chi_0>0$) and $\delta<0$ (or $\chi_0<0$), respectively. The denominator of Eq. (73) is determined using

$$\cos\phi(\zeta) = \mp\frac{|\overline{\kappa}| \pm \gamma\Omega\cosh\xi}{|\overline{\kappa}|\cosh\xi \pm \gamma\Omega}, \tag{77}$$

$$\sin\phi(\zeta) = \mp\frac{\sqrt{\overline{\kappa}^2-\gamma^2\Omega^2}\sinh\xi}{|\overline{\kappa}|\cosh\xi \pm \gamma\Omega}, \tag{78}$$

where we used Eq. (71). Quantity F_0 defined in Eq. (74) corresponds to the gap soliton amplitude for the standard coupled mode equation ($|\mu|=|\nu|=0$), the solutions of which were found by Aceves and Wabnitz [9]. Equation (73) explicitly shows the deformation of the gap soliton shape due to the grating depth. An example of a new gap soliton, with parameters as in Eqs. (67), is shown in Fig. 4. Note that the solution has a double peak. Such phenomena were discussed

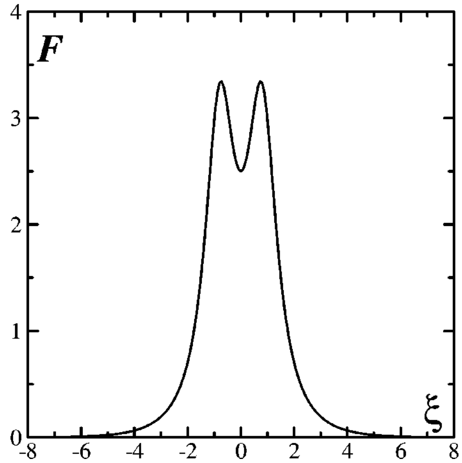

FIG. 4. Double hump traveling gap soliton with parameters as in Eqs. (67).

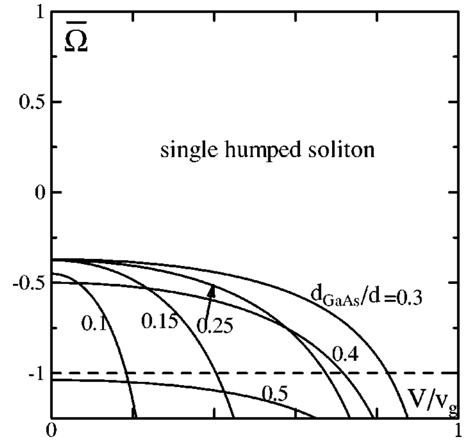

FIG. 5. Parameter regions for the existence of single and double humped gap solitons, for a GaAs-polymer grating with $d_{\text{GaAs}}/d = 0.1$, 0.15, 0.25, 0.3, 0.4, and 0.5. Parameter $\bar{\Omega}$ is the normalized detuning from Eq. (82), and V is the soliton velocity. The soliton are double humped below the curves.

before [14], though not fully analytically. The soliton velocity V and frequency Ω are found from Eq. (62) and (67) to be

$$V = v_g/\sqrt{3}, \quad \Omega = -|\bar{\kappa}|/\sqrt{6}. \tag{79}$$

It is interesting to derive the condition for a double humped soliton solution to the GCM equations (40) and (41) to exist. Considering the phase flow diagram in $F-\phi$ space, we find that the condition is

$$\frac{d^2F}{d\phi^2} > 0 \begin{cases} \text{at} \quad \phi = \pi \quad \text{for} \quad \delta > 0 \\ \text{at} \quad \phi = 0 \quad \text{for} \quad \delta < 0. \end{cases} \tag{80}$$

Using Eq. (69), we have

$$1 + 2\gamma^2 - 4\gamma\bar{\Omega}\,\text{Re}[\mu/\delta] + (\pm 4\bar{\Omega} - 3)\,\text{Re}[\nu/\delta] < 0, \tag{81}$$

where Re[ ] indicates the real part and

$$\bar{\Omega} \equiv \gamma\Omega/|\bar{\kappa}|, \tag{82}$$

is the normalized detuning parameter. Note that $|\bar{\Omega}| < 1$ for the ''in-gap'' case. The $\pm$ signs indicate positive and negative δ, respectively. The soliton parameters in Fig. 4 satisfy inequality (81), as required. It is obvious that if μ/δ and ν/δ are very small, the soliton is always single peaked. However, for deep gratings, μ and ν can be as large as δ, and double humped soliton solution can then be found. As an example, we consider the GaAs-polymer structure discussed in Ref. [14]. From Fig. 7 in that paper, we see that if the GaAs volume fraction is given, we know that Γ_0, Γ_1, and Γ_2 correspond to δ, μ, and ν, respectively. Then condition (81) can be evaluated explicitly. This result is shown in $\bar{\Omega} - V/v_g$ space in Fig. 5, for six values of the GaAs volume fraction d_{GaAs}/d. The curves give the boundaries below which the solitons are double humped. Since the results depend on $|V|$, only the results for $V > 0$ are shown. Figure 5 shows that double humped solitons exist only for negative detunings, corresponding to high intensities. In the limit $d_{\text{GaAs}}/d \to 0$, the boundary curve coincides with the $\bar{\Omega}$ axis, and no double humped solitons can then be found. This is not surprising since in this limit the grating is shallow.

Now we have obtained both the amplitude $F(\zeta)$ and the phase difference $\phi(\zeta)$, we can obtain total phase $\theta_+ + \theta_-$ by direct integration of Eq. (64). In fact, using Eq. (69) and (70), it can be explicitly written as

$$\theta_+ + \theta_- = 2\gamma^2 \frac{V}{v_g}\left(\Omega\zeta + \int \frac{[2\gamma\delta + 2|\mu|\cos(\phi - h)]\,d\phi}{s[1 + A\cos(\phi - h) + B\cos 2(\phi - c)]}\right), \tag{83}$$

where $s \equiv (1 + 2\gamma^2)\gamma\delta$.

V. CONCLUDING REMARKS

Corrections to conventional coupled mode theory in a $\chi^{(3)}$ optical system due to the depth of the grating have been discussed. In the linear case, this results in a deformation of the local dispersion relation, leading to changes in the position and width of the photonic band gap. Assuming a harmonic time dependence, our results reduce to those obtained by Sipe *et al.* [18]. Depending on the gap parameter κ, we analyze both the narrow gap case and the finite gap case in the nonlinear stage. The coupled equations in the former case reduce to the conventional equations, though the values of the coefficients differ at $O(\eta^2)$. These corrections are related to the sharpness parameters α and β, which originate from coupling with an infinite number of plane waves.

For a finite gap, we derived the GCM equations (40) and

(41), which include the lowest order corrections due to the grating depth and grating sharpness. We found that the periodicity of $\chi^{(3)}$ also contributes to the correction terms. The GCM equations constitute a Hamiltonian system and have at least three invariants: energy [Eq. (52)], photon number [Eq. (56)], and momentum [Eq. (57)]. The nonlinear part of the GCM equations has the same form as that of fully deep grating theory [14].

We also obtained the exact form of a two-parameter set of moving soliton solutions to the GCM equations. These solutions are generalizations of the well known gap solitons, deformed due to the grating depth. A typical double peaked solution was presented, illustrating a qualitative difference with conventional coupled mode theory for shallow gratings. Recent analyses of the conventional gap soliton stability [10,11] suggest that for a shallow Bragg grating with $\chi^{(3)}$ nonlinearity, the solitary wave solutions are stable for $\Omega > 0$ in gap, while for $\Omega < \Omega_c < 0$ a vibrational instability occurs. The critical detuning Ω_c depends on the soliton velocity V. If μ and ν in the GCM equations are small, $\sim O(\eta)$, the generalized gap solitons are expected to be stable for $\Omega > 0$. The stability of the humped solitons is still an open question. The double humped solutions occur for deep gratings, i.e. when μ, ν are comparable to δ. As discussed in Sec. IV, the realistic example of a deep grating allows double humped solutions only for negative detunings (see Fig. 5). Therefore, based on the results for shallow gratings mentioned above, it is likely that the double humped solutions are vibrationally unstable. However, the stability analysis of the solutions to the GCM equations remains to be done.

If the gap is wide enough, $e_N \sim \kappa \sim \eta$, we should set the modulation and nonlinear parameter ε equal to η. In this case we cannot neglect terms like $\chi_0 |E_\pm|^2 \partial(E_\pm)/\partial z$ and $\chi_0^2 |E_\pm|^4 E_\pm$, which are of $O(\eta^2)$, as they are comparable with the correction terms in the GCM equations. The nonlinear equation up to $O(\eta^2)$ thus obtained is very complex, though it can be reduced to a Hamiltonian form. We leave the analysis of wide gap case for future work.

In the present work, we have neglected polarization effects as usually done in this field, though it was considered explicitly in a recent shallow grating analysis by Pereira and Sipe [21]. While, to our knowledge, polarization effects have not been reported, they are most likely to be observable in corrugated guided wave structures.

In conclusion we have generalized conventional coupled mode theory for Bragg gratings by including the effects of the grating depth. Deriving a generalized coupled mode equation, we obtain expressions for traveling soliton solutions. We show how the grating depth affects gap solitons propagation, resulting in changes to their shape.

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