COHERENT STRUCTURES AND CARRIER SHOCKS IN THE 
NONLINEAR PERIODIC MAXWELL EQUATIONS*

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Abstract. We consider the one-dimensional propagation of electromagnetic waves in a weakly nonlinear and low-contrast spatially inhomogeneous medium with no energy dissipation. We focus on the case of a periodic medium, in which dispersion enters only through the (Floquet–Bloch) spectral band dispersion associated with the periodic structure; chromatic dispersion (time-nonlocality of the polarization) is neglected. Numerical simulations show that, for initial conditions of wave packet type (a plane wave of fixed carrier frequency multiplied by a slow varying, spatially localized function), a coherent multiscale structure emerges that persists for the lifetime of the simulation. This state features (i) a broad, spatially localized, and slowly evolving envelope and (ii) a train of shocks, approximately on the scale of the initial carrier wave. We loosely call this structure an envelope carrier-shock train. The structure of the solution violates the often assumed nearly monochromatic wave packet structure, whose envelope is governed by the nonlinear coupled mode equations (NLCME). The inconsistency and inaccuracy of NLCME lies in the neglect of all (infinitely many) resonances but the principle resonance induced by the initial carrier frequency. We derive, via a nonlinear geometrical optics expansion, a system of nonlocal integrodifferential equations governing the coupled evolution of backward and forward propagating waves. These equations incorporate all resonances. In a periodic medium, these equations may be expressed as a system of infinitely many coupled mode equations, which we call the extended nonlinear coupled mode system (xNLCME). Truncating xNLCME to include only the principle resonances leads to the classical NLCME. Numerical simulations of xNLCME demonstrate that it captures both large scale features, related to third harmonic generation, and the fine scale carrier shocks of the nonlinear periodic Maxwell equations.

Key words. nonlinear geometrical optics, shocks, solitons

AMS subject classifications. 74J35, 74J40, 35L65, 78A60

DOI. 10.1137/100810046

1. Overview. Realized and potential applications of microstructured dielectric media motivate a thorough mathematical study of wave propagation governed by nonlinear hyperbolic equations, e.g., Maxwell’s equations with periodic and nonlinear constitutive laws. This paper explores a class of nonlinear hyperbolic equations with a spatially periodic flux function:

\[ \begin{align*}
\partial_t v + \partial_x f(x, v) &= 0, \\
\partial_x f(x, 0) &= 0, \\
f(x + 2\pi, v) &= f(x, v).
\end{align*} \]

In particular, we shall assume that periodic variations are weak (a low-contrast structure) and study solutions whose amplitude is sufficiently small that the effects of periodicity-induced dispersion and nonlinearity are in balance.

Indeed, a nontrivial spatially periodic structure is dispersive. This can be seen by linearizing (1.1) about the state \( v = 0 \), giving the linear system

\[ \partial_t v + \partial_x f(x, v) = 0. \]

\[ \begin{align*}
\partial_x f(x, 0) &= 0, \\
f(x + 2\pi, v) &= f(x, v).
\end{align*} \]

*Received by the editors September 28, 2010; accepted for publication (in revised form) March 21, 2011; published electronically July 19, 2011.

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\[ \partial_t \mathbf{V} + \partial_x (D_x f(x, 0) \mathbf{V}) = 0, \]

which retains periodicity. Floquet–Bloch theory (see [8] and [37]) implies that associated to the PDE (1.2) is a family of band dispersion functions \( k \mapsto \omega_j(k), k \in (-\frac{1}{2}, \frac{1}{2}] \). Wave propagation is dispersive since the group velocities, \( \omega'_j(k) \), are typically nonzero. Thus, waves of different wavelengths travel with different speeds.

Dispersive properties, encoded in the functions \( \omega_j(\cdot) \) and the associated Floquet–Bloch states, can be manipulated by tuning the periodic structure through, for example, modification of the periodic lattice, the maximum and minimum variations of \( D_x f(x, 0) \) (material contrast), etc.

It is well known that, for general initial conditions, solutions of hyperbolic systems of conservation laws with spatially homogeneous nonlinear fluxes,

\[ \partial_t v + \partial_x f(v) = 0, \]

develop singularities (shocks) in finite time (see [21] and [25]).

**Question 1. Is spectral band dispersion, due to a periodic structure, sufficient to arrest shock formation?**

The ability to control or inhibit the formation of singularities in nonlinear wave propagation could have significant impact in, for example, electromagnetics and elasticity. Strictly speaking, the answer to Question 1 is no. Indeed, for a system of the form (1.1), let us suppose that the flux function was periodically piecewise constant. Finite propagation speed considerations imply that, for appropriate initial data, localized within a uniform region, a shock will form. The dispersive character of the periodic structure is manifested only on sufficiently large spatial and temporal scales. Thus, the problem of controlling shock formation should be posed relative to some class of initial conditions.

A second motivation is the study and design of media which support the propagation of stable soliton-like pulses. These have applications to optical devices which transfer, store, or, in general, process information which is encoded as light pulses. Associated with dispersive wave propagation at wavenumber \( k_\star \) is a dispersion length \( \sim (\omega''(k_\star))^{-1} \).

Soliton formation is possible on length scales where the dispersion length and the characteristic length on which nonlinear effects act are comparable. Technological advances have made it possible to fabricate microstructured media with specified dispersion lengths at specified wavelengths. For a given dispersion length, a balance between dispersion and nonlinearity is achieved by tuning the strength of the nonlinear effects through adjusting the field intensity (by an amount which is material dependent). An example of this balance at work is gap soliton formation in periodic structures. These are experiments in optical fiber periodic structures (gratings) involving highly intense (nonlinear) light with carrier wavelength satisfying the Bragg (resonance) condition. The length scale of such solitons is \( 10^{-2} \) meters [9].

Theory predicts the existence of gap solitons traveling at any speed, \( v \), between zero and the speed of light, \( c \) (see [1] and [4]). Experiments [9] demonstrate speeds as low as \( 0.3c \) to \( 0.5c \). Potential applications of gap solitons, based on the design of appropriate localized defects in a periodic structure, are all-optical storage devices [11]. The term gap

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1For example, though the solution of the inviscid Burgers equation, \( \partial_t u + u \partial_x u = 0 \), for typical smooth initial data, develops a shock in finite time, the corresponding solutions of the Korteweg–de Vries equation, \( \partial_t u + u \partial_x u + \partial^3_x u = 0 \), a dispersive perturbation, remain smooth for all time. This dispersive regularization is reflected in the generation of an oscillatory train of solitons behind a steepening, but smooth, front for initial data, which, for inviscid Burgers, evolves into a shock.

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soliton is used due to the frequency of the gap soliton envelope lying in the spectral gap of the linearized system.

Physical predictions of gap solitons are based on explicit solutions of the nonlinear coupled mode equations (NLCME) given below in (2.9). NLCME has been formally derived in, for example, [6] from (1.4); see also the discussion in section 2. Rigorous derivations of NLCME, from models with appropriate dispersion, have been presented for the anharmonic Maxwell–Lorentz equations [12] and other nonlinear dispersive equations; see, e.g., [13], [33], [34], [39], and [40].

Within the approximation of a small amplitude wave field as a wave packet with slowly varying envelope and single carrier frequency, propagating through a low-contrast periodic structure near the Bragg resonance (see the scaling in Figure 1), NLCME is argued to govern the principle forward and backward slowly varying envelopes of carrier waves; see [6] and references therein.

As discussed in [12] and in section 2, if the only source of dispersion for weakly nonlinear waves in low-contrast media is the spatial dispersion of the periodic medium (e.g., negligible chromatic dispersion), all nonlinearity-generated harmonics are resonant and therefore all mode amplitudes are coupled at leading order. The correct mathematical description would appear to require infinitely many interacting modes. Thus, the classical NLCME is not a mathematically consistent approximation. However, NLCME may be a satisfactory physical description for some purposes. Indeed, the soliton wave form prediction based on NLCME appears to describe some features of experiments.

\(^3\)Physicists argue in two ways that the coupling to higher harmonics is negligible: (i) The material systems considered are dissipative at higher wavenumbers. Higher wavenumbers are damped, and therefore these mode amplitudes can be ignored. (ii) Chromatic dispersion (arising due to the finite time response of the medium to the field) causes nonlinearly generated harmonics to be off-resonance. Therefore, an initial condition exciting the principle modes will not appreciably excite higher harmonics. These rationales are somewhat ad hoc since the precise damping mechanisms are not well understood and chromatic dispersion is a much weaker effect than photonic band dispersion for weak periodic structures.
QUESTION 2. Do nonlinear periodic hyperbolic systems have stable coherent structures, and can one develop a mathematical theory? How are the classical NLCME related to this theory? See the discussion in section 6.

In this article we report progress on Questions 1 and 2 in the context of the one-dimensional, nonlinear Maxwell equations governing the electric ($E$) and magnetic ($B$) fields

\begin{align}
\partial_t D &= \partial_z B, \quad \text{(1.4a)} \\
\partial_t B &= \partial_z E \quad \text{(1.4b)}
\end{align}

with constitutive law

\begin{align}
D &= \epsilon(z, E)E \equiv (n^2(z) + \chi E^2)E, \quad \text{(1.5)} \\
n(z) &= n_0 + \epsilon N(z). \quad \text{(1.6)}
\end{align}

$n(z)$ is a linear refractive index, consisting of a nonzero background average part, $n_0$, and a fluctuating (e.g., periodic) part $\epsilon N(z)$. The nonlinear term $\chi E^2$ is the nonlinear refractive index, arising from the Kerr effect; in regions of high intensity, the refractive index is higher. The constitutive law (1.5) prescribes $D$ as a local function of $E$. Thus, chromatic dispersion, which arises due to a time-nonlocal relation between $D$ and $E$, has been neglected. For simplicity, we assume $n_0 = 1$, which can be arranged by a simple scaling.

1.1. Summary of results.

1. In section 3 we present numerical simulations of the nonlinear periodic Maxwell equations (1.4) for initial data obtained from the explicit NLCME soliton. Under this time-evolution there is robust spatially localized structure on the scale of the NLCME soliton envelope. The persistence of a localized structure and speed of propagation are consistent with that of the NLCME soliton. There is, however, a deviation from the NLCME soliton related to third harmonic generation; these are the two accessory pulses around the principle wave in Figure 2(a).

![Figure 2](image_url)

**Fig. 2.** (a) A simulation of the Maxwell equations. (b) The simulation of a truncated asymptotic system, resolving the first and third harmonics. Both simulations were initiated with the same initial conditions. The two side pulses about the main wave appear to be the result of third harmonic generation.
2. On the microscopic scale of the carrier wave there is nonlinear steepening and shock formation. Therefore, the solution does not evolve as a slowly varying envelope of a single frequency carrier wave. The long-lived and spatially localized coherent structure which emerges has the character of a slowly varying envelope of a train of shocks. We call this an envelope carrier-shock train. Figure 3 illustrates the shock-like small spatial scale behavior under slowly varying envelope.

3. Numerical solution of the nonlinear Maxwell equation (1.4) is nontrivial due to the cubic nonlinearity. As a hyperbolic system, it is neither genuinely nonlinear nor linearly degenerate (see [26], [29], and [43]). To solve by finite volume methods, as we do, an appropriate solution of the Riemann problem must be constructed. Details of this are given in Appendix B. The appropriate entropy condition could, in principle, be derived from physical regularization mechanisms, which play the role of viscosity in gas dynamics. These mechanisms are not well understood. However, such mechanisms and the appropriate notion of weak solutions would respect thermodynamic principles, which are built into our numerical scheme.

4. Using a nonlinear geometric optics expansion (see [7], [14], [15], [16], [17], [22], and [30]), systematically keeping all resonances, we obtain nonlocal equations governing the interaction of all forward and backward propagating modes. Our asymptotic nonlocal system captures the slowly varying envelope of carrier-shock structures described above; see below. Specifically we introduce the general wave form (much more general than a slowly varying envelope of a nearly monochromatic carrier plane wave), which includes all harmonics

\[ E(z, t) = e^{1/2}(E^+(z - t, \epsilon z, \epsilon t) + E^-(z + t, \epsilon z, \epsilon t) + \mathcal{O}(\epsilon)). \]

Let

\[ \phi_\pm = z \mp t, \quad \epsilon t = T, \quad \text{and} \quad \epsilon z = Z. \]

At leading order, the slow evolution of backward and forward components is governed by the coupled integrodifferential equations for \( E^\pm(\phi_\pm, Z, T) \):

Fig. 3. (a) A simulation of the Maxwell equations. (b) The simulation of a truncated asymptotic system. Both simulations were initiated with the same initial conditions. There is an indication of shock formation in (a). In (b), we see that once sufficiently many harmonics are included, the Gibbs effect appears, confirming shock formation.
\[ \frac{\partial}{\partial T} E^+ + \frac{\partial}{\partial Z} E^+ = \partial_\phi \langle N(\phi + s) E^- (\phi + 2s, Z, T) \rangle_{\phi=\phi_+} \]
\[ + \Gamma \partial_\phi \left[ \frac{1}{3} (E^+)^3 + E^+ \langle (E^-)^2 \rangle \right]_{\phi=\phi_+}. \]  
(1.8a)

\[ \frac{\partial}{\partial T} E^- - \frac{\partial}{\partial Z} E^- = - \partial_\phi \langle N(\phi - s) E^+ (\phi - 2s, Z, T) \rangle_{\phi=\phi_-} \]
\[ - \Gamma \partial_\phi \left[ \langle (E^+)^2 \rangle E^- + \frac{1}{3} (E^-)^3 \right]_{\phi=\phi_-}. \]  
(1.8b)

Here \( \langle \cdot \rangle \) is an averaging operation in the \( \phi \) argument:
\[ \langle f \rangle \equiv \lim_{L \to \infty} \frac{1}{L} \int_0^L f(s) \, ds; \]
(1.9)

see also section 4. We note that in the first equation, the independent variables are \( Z, T \), and \( \phi_+ \), while in the second they are \( Z, T \), and \( \phi_- \). Equations (1.8a) and (1.8b) arise as constraints on \( E^\pm (\phi_\pm, Z, T) \), ensuring that the \( O(\epsilon) \) error term in (1.7) remains small on large time scales: \( T = O(1) \) or equivalently \( t = O(\epsilon^{-1}) \).

Spatial variations in the refractive index, \( N(z) \), give rise to a coupling of backward and forward waves. Indeed, if \( N(z) \equiv 0 \) and one specifies data for the system (1.8) at \( t = 0 \) with nonzero forward components \( (E^+ \neq 0) \) and no backward components \( (E^- = 0) \), then, formally, \( E^- \) remains zero for all time, i.e., no backward waves are generated. Continuing with this assumption of \( N = 0 \) and \( E^- = 0 \), if we let \( V(\phi, T) = E^+(\phi, Z_0 - T, T) \), with \( Z_0 \) arbitrary, then \( V \) satisfies
\[ \frac{\partial}{\partial T} V = \frac{\Gamma}{3} \partial_\phi (V^3), \]
whose solutions develop shock-type singularities in finite time.

5. The nonlocal equations may also be written as an infinite system of coupled mode equations. In the case where \( E^\pm \) is \( 2\pi \) periodic in \( \phi_\pm \), the integrodifferential equation (1.8) reduces to an infinite system of coupled mode equations for the Fourier coefficients \( \{ E^\pm_p(Z, T) ; p \neq 0 \} \):
\[ \frac{\partial}{\partial T} E^+_p + \frac{\partial}{\partial Z} E^+_p = ip N_{2p} E^-_p + \frac{\Gamma}{3} \left[ \sum_{q,r} E^+_q E^+_r E^+_p - q - r + 3 \left( \sum_q |E^-_q|^2 \right) E^+_p \right]. \]  
(1.10a)

\[ \frac{\partial}{\partial T} E^-_p - \frac{\partial}{\partial Z} E^-_p = ip \tilde{N}_{2p} E^+_p + \frac{\Gamma}{3} \left[ \sum_{q,r} E^-_q E^-_r E^-_p - q - r + 3 \left( \sum_q |E^+_q|^2 \right) E^-_p \right]. \]  
(1.10b)

We call this system the extended nonlinear coupled mode equations (xNLCME). xNLCME reduces to the classical NLCME if we neglect higher harmonics.
6. Simulations of successively higher-dimensional mode truncations of (1.10) show improved resolution of the carrier shocks under a slowly varying envelope, whose scale is captured by a comparatively low order truncation. Indeed, Figure 2(b) shows that inclusion of the third harmonic in the asymptotic system resolves the large scale feature, while inclusion of additional harmonics in Figure 3(b) shows the Gibbs effect, expected for a finite Fourier representation of a discontinuous function. This demonstrates that our asymptotic analysis leads to equations capturing the essential features of nonlinear Maxwell. However, if we consider how energy, initially only in the first harmonic, is redistributed in time, we see in Figure 4 that most of the energy persists in the first harmonic. This reflects the partial success of NLCME as a model for periodic nonlinear Maxwell.

**Relation to previous work.** Some of the earliest examinations on optical shocks can be found in Rosen [38] and DeMartini et al. [5]. In these works, the authors applied the method of characteristics to a unidirectional model. Kinsler [19] and Kinsler et al. [20] have continued to examine this problem and have developed an algorithm for detecting the onset of shock formation. Carrier shocks were also examined by Flesch, Pushkarev, and Moloney [10]. These works consider a spatially homogeneous Maxwell system with chromatic dispersion, arising from the time-nonlocal dependence of the polarization on the field. Ranka, Windeler, and Stentz [36] have found experimental evidence of optical shocks. In their work, a monochromatic pulse with sufficient power steepened and generated a broadband optical continuum.

Coherent structures in nonlinear and periodic media have also been studied by LeVeque [24], Yong and LeVeque [50], and Ketcheson [18] in a model for heterogeneous nonlinear elastic media. They considered solutions in high-contrast, rapidly varying, periodic structures. Their simulations yielded localized structures on the scale of many periods with oscillations on the scale of the period. For piecewise constant (discontinuous) periodic structures, they have a discontinuous carrier shock-like character on the scale of the period. This is due to discontinuities in the medium; the fluxes remain continuous. A two-scale (homogenization) expansion yields a nonlinear dispersive
equation, with solitary waves, similar to the computed solution envelope. In their physical regime, the variations in the properties of the media and the nonlinearity are $O(1)$. In contrast, we consider an asymptotic regime where the contrast of the periodic structure and nonlinearity are of the same order, $O(\epsilon)$. Furthermore, the initial condition has two scales (envelope and carrier scales), where the carrier wavelength is of the same order as (indeed, in resonance with) the periodic structure. These different scalings lead to different asymptotic descriptions. An early example of the interactions between nonlinearity and a periodic structure was in atmospheric science, studied by Majda et al. [31]. In this work, a model of the interaction of equatorial waves with topography gives rise to nonsmooth profiles (in this case, solitary waves with corner singularities).

A system similar to (1.8) has also been derived in a cubically nonlinear elastic medium in Anile et al. [2]. There the authors obtained integrodifferential terms, though they did not include slow spatial variations, corresponding to our $\partial_Z$ terms, or periodic variations of the medium.

Finally, systems of coupled modes have also been examined in prior works, though the work is typically limited to only two harmonics, such as a first and second harmonic system or a first and third harmonic system. Such a model was studied by Tasgal, Band, and Malomed [45], who found stable polychromatic solitons in a first and third harmonic system.

An outline of this paper is as follows. In section 2, we review how NLCME arises as a formal approximation of nonlinear Maxwell and the assumptions under which this approximation is valid. Results of nonlinear Maxwell simulations, showing the coherent structures and shocks, appear in section 3. In view of the nonvalidity of NLCME in the current setting, in section 4 we present a derivation of nonlocal/nonlinear geometric optics equations for the field. In the case of a periodic fast phase variable, this nonlocal system reduces to the infinite extended coupled mode system, xNLCME. In section 5 we present computer simulations of truncations of xNLCME of increasing dimension, showing behavior consistent with full nonlinear Maxwell simulations. A discussion of our results is in section 6.

2. Nonlinear Maxwell and NLCME. In this section we briefly review how NLCME arises from nonlinear Maxwell with a periodically varying index of refraction. We also identify the mathematical inconsistency of NLCME as a description of the wave envelope.

First, we write the nonlinear Maxwell equation (1.4) as

$$\partial_t^2(n(z)^2 E + \chi E^3) = \partial_z^2 E$$

with index of refraction

$$n(z) = 1 + \epsilon N(z), \quad 0 < \epsilon \ll 1,$$

where $N(z)$ is $2\pi$ periodic with mean zero and Fourier series

$$N(z) = \sum_{p \in \mathbb{Z}} N_p e^{ipz}.$$

We shall seek solutions which incorporate (i) slow variations in time and space due to the weak modulation about a constant refractive index, and (ii) a scaling of the wave field which seeks solutions in which the effects of dispersion and nonlinearity are in balance:
Formally expanding $\mathcal{E}^\varepsilon$ as

$$
\mathcal{E}^\varepsilon(z, t, Z, T) = \mathcal{E}_0(z, t, Z, T) + \varepsilon \mathcal{E}_1(z, t, Z, T) + \cdots,
$$

we obtain a hierarchy for $\mathcal{E}_j(z, t, Z, T)$, $j \geq 0$:

\begin{align*}
\mathcal{O}(\varepsilon^0) & (\partial_t^2 - \partial_z^2) \mathcal{E}_0 = 0, \\
\mathcal{O}(\varepsilon^1) & (\partial_t^2 - \partial_z^2) \mathcal{E}_1 = -2\partial_t \mathcal{E}_0 + 2\partial_z \mathcal{E}_0 - 2N(z)\mathcal{E}_0 - \chi(\mathcal{E}_0)^3, \\
& \vdots \\
\mathcal{O}(\varepsilon^j) & (\partial_t^2 - \partial_z^2) \mathcal{E}_j = \text{expressions in terms of } \mathcal{E}_i, \quad 0 \leq l \leq j - 1,
\end{align*}

Solving the $\mathcal{O}(\varepsilon^0)$ equation yields

$$
\mathcal{E}_0(z, t, Z, T) = \mathcal{E}^+(Z, T)e^{i(z-t)} + \mathcal{E}^-(Z, T)e^{-i(z+t)} + \text{c.c.},
$$

where c.c. is the complex conjugate. Thus, the leading order consists of backward and forward propagating waves, modulated by the slow envelope amplitude functions $\mathcal{E}^\pm(Z, T)$, which are to be determined.

Substitution of (2.6) into the $\mathcal{O}(\varepsilon^1)$ equation for $\mathcal{E}_1$ yields

\begin{align*}
(\partial_t^2 - \partial_z^2) \mathcal{E}_1 &= [2\partial_t \mathcal{E}^+ - 2i\partial_z \mathcal{E}^+ - 2N_2 \mathcal{E}^- - 3\chi(|\mathcal{E}^+|^2 + 2|\mathcal{E}^-|^2)\mathcal{E}^+]e^{i(z-t)} \\
&+ [2\partial_t \mathcal{E}^- - 2i\partial_z \mathcal{E}^- - 2\bar{N}_2 \mathcal{E}^+ - 3\chi(|\mathcal{E}^-|^2 + 2|\mathcal{E}^+|^2)\mathcal{E}^-]e^{-i(z+t)} \\
&+ (\mathcal{E}^+)^3 \mathcal{E}^3(z-t) + (\mathcal{E}^-)^3 e^{-3i(z+t)} + \text{c.c.} + \text{nonresonant terms}.
\end{align*}

We have used that $N_0 = 0$ and

\begin{align*}
N(z)(\mathcal{E}^+ e^{i(z-t)} + \mathcal{E}^- e^{-i(z+t)}) &= N_{-2} \mathcal{E}^+ e^{-i(z+t)} + N_2 \mathcal{E}^- e^{i(z-t)} + \text{c.c.} + \text{nonresonant terms}.
\end{align*}

Each term, explicitly written on the right-hand side of (2.7), is resonant with the kernel of $(\partial_t^2 - \partial_z^2)$. It follows that the coefficients of all harmonic plane waves, $e^{\pm iq(z-t)}$ and $e^{\pm iq(z+t)}$, $q \in \mathbb{Z}$, must vanish for $\mathcal{E}_1$ to be bounded in $t$.

The vanishing of the coefficients of $e^{i(z-t)}$ and $e^{-i(z+t)}$ yields the nonlinear coupled mode equations (NLCME):

\begin{align*}
\partial_t \mathcal{E}^+ + \partial_z \mathcal{E}^+ &= iN_2 \mathcal{E}^- + i\Gamma(|\mathcal{E}^+|^2 + 2|\mathcal{E}^-|^2)\mathcal{E}^+ , \\
\partial_t \mathcal{E}^- - \partial_z \mathcal{E}^- &= i\bar{N}_2 \mathcal{E}^+ + i\Gamma(|\mathcal{E}^-|^2 + 2|\mathcal{E}^+|^2)\mathcal{E}^- ,
\end{align*}

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where $\Gamma \equiv \frac{1}{2} \chi$ and $\tilde{N}_2 = N_{-2}$. The initial value problem for (2.9) is well-posed [12]. NLCME also has an explicit family of *gap soliton* solutions; see Appendix A.

Requiring $E^\pm$ to satisfy (2.9) removes only the lowest harmonic resonances. This is the approximation invoked in the physics literature; see the survey [6] and references cited therein for details. However, the remaining explicitly displayed terms on the right-hand side of (2.7) are resonant as well and induce linear-in-time growth. Even if we were to remove the resonant terms proportional to $e^{3i(z-t)}$ and $e^{-3i(z+t)}$ by including slow modulations of these plane waves, nonlinearity and parametric forcing through $N(z)$ would generate yet more resonant harmonics.

*A leading order solution which does not generate resonant terms at higher order must contain all harmonics.* Thus, NLCME is mathematically inconsistent. In section 4 we derive an integrodifferential system of equations, which consistently incorporates all resonances. As seen from our numerical and asymptotic studies, the nonlocal, nonlinear geometrical optics system more accurately captures features on both small and large spatial scales, e.g., changes in the envelope due to higher harmonic generation, as well as carrier shock formation.

**3. Simulations of nonlinear periodic Maxwell.** In this section we discuss the results of numerical simulations, based on the algorithms of Appendix B, of the nonlinear and periodic Maxwell equations.

- In section 3.1 we show that, for initial data derived from the classical NLCME soliton, spatially localized soliton-like states persist on long time scales. We discuss aspects of the large scale (envelope) structure of such states, which are consistent with the NLCME soliton, as well as significant deviations.

- In section 3.2 we show that smoothness breaks down in finite time. In particular, we observe shock formation on the fast spatial scale of the carrier wave.

We begin by expressing (2.1) as a first order system:

$$
(3.1) \quad \partial_t \left( \frac{n(z)^2 E + \chi E^3}{B} \right) + \partial_z \left( -\frac{B}{E} \right) = 0.
$$

We introduce the scaling $(E, B, D)^T = e^{1/2}(\tilde{E}, \tilde{B}, \tilde{D})$ and express the equations in terms of the $(\tilde{D}, \tilde{B})$ coordinates. Dropping tildes, this is

$$
(3.2) \quad \partial_t \left( \frac{D}{B} \right) + \partial_z \left( \frac{B}{-E(D, z)} \right) = 0,
$$

where $E(D, z)$ is the unique real solution of

$$
(3.3) \quad D = n(z)^2 E + \epsilon \chi E^3.
$$

**3.1. Soliton-like coherent structures.** As is well known [1], [4], NLCME has spatially localized gap soliton solutions. We use the analytical expression for the gap soliton to generate Cauchy data, $E(z, 0), \partial_t E(z, 0)$ for (2.1) and numerically simulate the evolution.

Using (2.6) and the leading order approximation for the magnetic field $B_1^\pm = \mp E_1^\pm$, NLCME soliton data (see (A.1) in Appendix A) can be seeded into Maxwell using

$$
(3.4a) \quad E = E^+(\epsilon z, ct) e^{i(z-t)} + E^-(\epsilon z, ct) e^{-i(z+t)} + c.c.,
$$

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We obtain $D$ via (3.3) and evaluate at $t = 0$ to get the initial condition.

For a spatially varying index of refraction, we take

\[
N(z) = \frac{4}{\pi} \cos(2z), \quad \text{i.e.,} \quad N_2 = N_{-2} = \frac{2}{\pi}, \quad N_p = 0, \quad |p| \neq 2,
\]

where $\epsilon = 0.0625$ and $\chi = 1$ ($\Gamma = \frac{3}{2}$). The results of our simulations appear in parts (a) through (d) of Figures 5 and 6. While there is attenuation in amplitude and some dispersive spreading of energy, the solutions remain spatially localized over long time intervals. Not only is there a persistence of the localization (with the periodic medium), but there is also good pointwise agreement with the NLCME approximation; see Figure 7.

Parts (e) through (h) of Figures 5 and 6 display the corresponding results in the absence of a periodic structure, i.e., $N(z) \equiv 0$. The delocalization, dispersive spreading, and attenuation of the wave amplitude is greatly enhanced. To understand this heuristically, note that a gap soliton is a localized state whose carrier frequency lies in the spectral gap of the linearized PDE at the zero solution. A focusing nonlinearity adds a (self-consistent) potential well, creating a (nonlinear) defect mode with frequency lying in this spectral gap. If $N(z) \equiv 0$, then the linearization at the zero state has no spectral gap. Thus, a wave oscillating with the gap soliton frequency would couple to radiation modes and dispersively spread and attenuate. This mechanism is discussed, for example, in [44].

We note that it is also essential that the data be properly prepared to see a persistence of localization. For the initial condition

\[
(3.6a) \quad D = 0.5 \cos(z) \text{sech}(\epsilon z),
\]

\[
(3.6b) \quad B = -D,
\]

we see in Figure 8 substantial spreading. These data mimic the gap soliton’s amplitude, slowly varying envelope, and carrier wave but are apparently too far outside the basin of attraction to converge to a localized state. Similar results were observed with Gaussian wave packet initial conditions.

**3.2. Envelope carrier-shock trains.** Although the slowly varying NLCME envelope shape is robust for the nonlinear Maxwell time-evolution, there is evidence of nonlinear steepening and shock formation on the short (carrier) microstructure spatial scale. Thus, the nearly monochromatic slowly varying envelope approximation of NLCME is violated.

Figure 9 displays the time-evolution for (a) moving and (b) stationary NLCME gap soliton data. For each initial condition, the nonlinear Maxwell evolution is simulated for different grid spacings. As we increase the number of grid points, sharp features are better resolved by the shock capturing algorithm. One can also examine the Fourier transform of the output to see that we obtain an algebraically decaying solution in wavenumber, with peaks at the integer wavenumber values.

In summary, our observations support the emergence of a persistent, slowly varying, wave envelope and shock formation on the carrier scale. We loosely call this structure an envelope carrier-shock train.

**4. Resonant nonlinear geometrical optics and nonlinear spatially inhomogeneous Maxwell equations.** In this section we derive a system of equations which
Simulations with varying refractive index, $(3.5)$:

(3.5)

Simulations with constant refractive index, $N(z) = 0$:

FIG. 5. Solution of the rescaled nonlinear periodic Maxwell equation (3.2) for data generated by the NLCME soliton with parameters $v = 0.9$ and $\theta = 0.9$; see (A.1). The solutions are computed with 20000 grid points on the domain $[-500, 500]$. 

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FIG. 6. Solution of the rescaled nonlinear periodic Maxwell equation (3.2) for initial data generated by the NLCME soliton with parameters $v = 0$ and $b = \pi/2$; see (A.1). The solutions are computed with 20000 grid points on the domain $[-500, 500]$. Simulations with varying refractive index, $N(z) = 0$:

Simulations with constant refractive index, $N(z) = 0$:
Fig. 7 Comparison of the solution appearing in Figures 5(a) through 5(d) with the exact NLCME soliton.

Fig. 8. Solution of rescaled nonlinear periodic Maxwell equation (3.2) with periodic refractive index (3.5) for initial data (3.6). In contrast to the NLCME soliton data, the shape of the solution does not persist. The solution is computed with 20000 grid points on the domain $[-500, 500]$. 

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incorporates all resonances and which our numerical simulations show captures the key features of the nonlinear Maxwell time-evolution, in particular, the presence of robust envelope carrier-shock train solutions. This is derived for general nonhomogeneous media using a nonlinear geometrical optics expansion; see, for example, [14], [15], and [30]. The equations obtained are the general integrodifferential equations (1.8). In the case of a periodic medium, they reduce to an infinite set of local equations, which we call the extended nonlinear coupled mode equations (xNLCME). If, in xNLCME, we neglect all but the principle resonances, xNLCME reduces to NLCME.

As we shall see, in our numerical simulations of successively higher dimensional truncations of xNLCME (section 5), this theory appears to accommodate the observed carrier shocks and large scale coherent structures.

4.1. Nonlinear geometric optics expansion. In contrast to the ansatz of section 2, we assume the more general form

\[
\mathbf{u}(z, t) = \mathbf{u}^{(0)}(z, t, Z, T) + \epsilon \mathbf{u}^{(1)}(z, t, Z, T) + \epsilon^2 \mathbf{u}^{(2)}(z, t, Z, T) + \cdots
\]

where \( \mathbf{u} = (E, B)^T \), \( Z = \epsilon z \), and \( T = \epsilon t \). Inserting (4.1) into (3.2) and (3.3), we expand the first order system

\[
\partial_t \left( \frac{n(z)^2 E + \epsilon \chi E^3}{B} \right) + \partial_z \left( -
\right)
\]

to get

\[
(\partial_t + B^{(0)} \partial_z) \mathbf{u}^{(0)} + \epsilon (\partial_t + B^{(0)} \partial_z) \mathbf{u}^{(1)} + (\partial_T + B^{(0)} \partial_Z) \mathbf{u}^{(0)} + A^{(1)}(z, \mathbf{u}) \partial_t \mathbf{u}^{(0)} = \mathcal{O}(\epsilon^2)
\]

with matrices

\[
B^{(0)} = \begin{pmatrix}
0 & -1 \\
-1 & 0
\end{pmatrix}, \quad A^{(1)} = \begin{pmatrix}
2N(z) + 3\chi E^2 & 0 \\
0 & 0
\end{pmatrix}.
\]

At \( \mathcal{O}(\epsilon^0) \),

\[
(\partial_t + B^{(0)} \partial_z) \mathbf{u}^{(0)} = 0.
\]
Solving the eigenvalue problem \( (B^0 - \lambda I) \mathbf{r} = 0 \), the solutions are

\[
\lambda_{\pm} = \pm 1, \quad r_{\pm} = \left( \frac{1}{\mp 1} \right).
\]

The corresponding left eigenvectors are

\[
l_{\pm} = \frac{1}{2}(1 \mp 1).
\]

With this normalization, \( l_i \cdot r_j = \delta_{i,j} \). The leading order fields are then

\[
u(0) = E^+(\phi_+, Z, T) r_+ + E^-(\phi_-, Z, T) r_-.
\]
\[
E(0) = E^+(\phi_+, Z, T) + E^-(\phi_-, Z, T),
\]
\[
\phi_{\pm} = z \mp t.
\]

This expression is much more general than (2.6) used in the derivation of NLCME. At \( \mathcal{O}(\varepsilon) \), the equation is

\[
(\partial_t + B(0) \partial_z) \mathbf{u}^{(1)} = -(\partial_T + B(0) \partial_Z) \mathbf{u}^{(0)} - A^{(1)}(z, \mathbf{u}^{(0)}) \partial_z \mathbf{u}^{(0)}.
\]

If we assume

\[
\mathbf{u}^{(1)}(z, t) = m^+(z, t) r_+ + m^-(z, t) r_-
\]

and substitute into (4.7), then left multiply by \( l_+ \) and then by \( l_- \), we get

\[
-(\partial_t m^+ + \partial_z m^+) = \partial_T E^+ + \partial_Z E^+ + l_+ A^{(1)}(\mathbf{u}^{(0)})
\]
\[
\times (-\partial_{\phi_+} E^+ r_+ + \partial_{\phi_+} E^- r_-),
\]

\[
-(\partial_t m^- - \partial_z m^-) = \partial_T E^- - \partial_Z E^- + l_- A^{(1)}(\mathbf{u}^{(0)})
\]
\[
\times (-\partial_{\phi_-} E^+ r_+ + \partial_{\phi_-} E^- r_-).
\]

The last term is the same in both equations,

\[
l_{\pm} A^{(1)}(u^{(0)})(-\partial_{\phi_{\pm}} E^+ r_{\pm} + \partial_{\phi_{\pm}} E^- r_{\mp})
\]
\[
= \frac{1}{2} (2 N(z) + 3 \chi E^{(0)2})(-\partial_{\phi_+} E^+ + \partial_{\phi_-} E^-)
\]
\[
= N(z)(-\partial_{\phi_+} E^+ + \partial_{\phi_-} E^-)
\]
\[
+ \frac{3}{2} \chi (E^+ + E^-)^2(-\partial_{\phi_+} E^+ + \partial_{\phi_-} E^-).
\]

Integration of (4.9) along the characteristic \( \partial_t z_+ = 1 \) from \( t = 0 \) to \( t = L \) yields
\[ -(m^+(z_+(L), L) - m^+(z_+(0), 0)) \]
\[ = \int_0^L \partial_T E^+(Z, T, z_+(0)) + \partial_Z E^+(Z, T, z_+(0)) \, ds \]
\[ - \int_0^L N(z_+(s)) \partial_{\phi^+} E^+(Z, T, z_+(0)) \, ds \]
\[ + \int_0^L N(z_+(s)) \partial_{\phi^-} E^-(Z, T, z_+(s)) \, ds \]
\[ - \int_0^L \left[ \frac{3}{2} \chi(E^+(Z, T, z_+(0)) - E^-(Z, T, z_+(s)) \right] \]
\[ \times \partial_{\phi^+} E^+(Z, T, z_+(0)) \, ds \]
\[ + \int_0^L \left[ \frac{3}{2} \chi(E^+(Z, T, z_+(0)) - E^-(Z, T, z_+(s)) \right] \]
\[ \times \partial_{\phi^-} E^-(Z, T, z_+(s)) \, ds. \]

(4.12)

Similarly, integration of (4.10) along the characteristic \( \partial_t z_- = -1 \) yields

\[ -(m^- (z_-(L), L) - m^- (z_-(0), 0)) \]
\[ = \int_0^L \partial_T E^-(Z, T, z_+(0)) - \partial_Z E^-(Z, T, z_+(0)) \, ds \]
\[ - \int_0^L N(z_-(s)) \partial_{\phi^+} E^+(Z, T, z_-(s) - s) \, ds \]
\[ + \int_0^L N(z_-(s)) \partial_{\phi^-} E^-(Z, T, z_-(0)) \, ds \]
\[ - \int_0^L \left[ \frac{3}{2} \chi(E^+(Z, T, z_-(s) - s) - E^-(Z, T, z_-(0)) \right] \]
\[ \times \partial_{\phi^+} E^+(Z, T, z_-(s) - s) \, ds \]
\[ + \int_0^L \left[ \frac{3}{2} \chi(E^+(Z, T, z_-(s) - s) - E^-(Z, T, z_-(0)) \right] \]
\[ \times \partial_{\phi^-} E^-(Z, T, z_-(s) - s) - E^-(Z, T, z_-(0)) \, ds \]

(4.13)

Necessary conditions for \( m_\pm \) to grow sublinearly in \( t \) as \( t \to \infty \) are the solvability conditions

\[ \partial_T E^+(Z, T, z_+(0)) + \partial_Z E^+(Z, T, z_+(0)) \]
\[ = - \lim_{L \to \infty} \frac{1}{L} \int_0^L N(z_+(s)) \partial_{\phi^+} E^+(Z, T, z_+(s) + s) \, ds \]
\[ + \lim_{L \to \infty} \frac{1}{L} \int_0^L \left[ \frac{3}{2} \chi(E^+(Z, T, z_+(0)) - E^-(Z, T, z_+(s) + s) \right] \]
\[ \times \partial_{\phi^+} E^+(Z, T, z_+(s)) \, ds. \]

(4.14a)
\[
\partial_t E^-(Z, T, z_-(0)) - \partial_x E^-(Z, T, z_-(0)) = \lim_{L \to \infty} \frac{1}{L} \int_0^L N(z_-(s)) \partial_{\phi_+} E^+(Z, T, z_-(s) - s) \, ds
\]
\[
- \lim_{L \to \infty} \frac{1}{L} \int_0^L \frac{3}{2} \chi(E^+(Z, T, z_-(s) - s) - E^-(Z, T, z_-(0)))^2 \times \partial_{\phi_+} E^-(Z, T, z_-(0)) \, ds.
\]
(4.14b)

Given \((z, t)\), we set \(z_+(0) = z - t = \phi_+\) and \(z_-(0) = z + t = \phi_-\). Defining

\[
\langle f \rangle = \lim_{L \to \infty} \frac{1}{L} \int_0^L f(s) \, ds
\]

the equations may be compactly expressed as

\[
\partial_T E^+ + \partial_x E^+ = -\langle N(\phi_+ + s) \partial_{\phi_+} E^-(\phi + 2s) \rangle_{s=\phi_+}.
\]
(4.16a)

\[
+ \frac{3}{2} \chi((E^+)^2 + 2E^+\langle E^- \rangle + \langle (E^-)^2 \rangle) \partial_{\phi_+} E^+|_{\phi_+},
\]

\[
\partial_T E^- - \partial_x E^- = \langle N(\phi_- - s) \partial_{\phi_-} E^+(\phi - 2s) \rangle_{s=\phi_-},
\]
(4.16b)

\[
- \frac{3}{2} \chi((E^-)^2 + 2E^-\langle E^+ \rangle + \langle (E^+)^2 \rangle) \partial_{\phi_-} E^-|_{\phi_-}.
\]

It is important to recognize that the arguments of the fields in (4.16a) are \(\phi_+ = z - t, Z,\) and \(T\), while in (4.16b), they are \(\phi_- = z + t, Z,\) and \(T\). This remark is critical if one wishes to return to the primitive variables.

As in our derivation of NLCME in section 2, \(\Gamma \equiv \frac{3}{2} \chi.\) With this notation, (4.16) can be rewritten, after an integration by parts, in conservation law form,

\[
\partial_T E^+ + \partial_x E^+ = \partial_{\phi_+} \langle N(\phi + s) E^-(\phi + 2s) \rangle_{s=\phi_+}.
\]
(4.17a)

\[
+ \Gamma \partial_{\phi_+} \left[ \frac{1}{3} (E^+)^3 + (E^+)^2 \langle E^- \rangle + E^+ \langle (E^-)^2 \rangle \right]_{\phi_+}.
\]

\[
\partial_T E^- - \partial_x E^- = -\partial_{\phi_-} \langle N(\phi - s) E^+(\phi - 2s) \rangle_{s=\phi_-}.
\]
(4.17b)

\[
- \Gamma \partial_{\phi_-} \left[ \langle (E^-)^2 \rangle E^- + \langle E^+ \rangle (E^-)^2 + \frac{1}{3} (E^-)^3 \right]_{\phi_-}.
\]

(4.17) correspond to the integrodifferential equations of section 1 if we omit the \(\langle E^\pm \rangle\) terms. Since \(\langle E^\pm \rangle\) is time-invariant (see section 4.3) by choosing initial conditions for which \(\langle E^\pm \rangle(T = 0) = 0\), these terms can be dropped from (4.17). Finally we note that (4.16) are applicable to a general heterogeneous dielectric material with the appropriate scalings.

**4.2. Periodic media and xNLCME.** We now specialize to the periodic case. Assume now that \(N(z + 2\pi) = N(z)\). Then (4.17) is invariant under the discrete translation \(\phi \mapsto \phi + 2\pi\), i.e.,
We denote the fast argument as $\phi$ and substitute in $\phi \pm C_6$ as appropriate.

Thus, under the assumption of existence and uniqueness of solutions to (4.17), if the initial data are $2\pi$ periodic in the $\phi \pm C_6$ arguments, then the solutions remain $2\pi$ periodic in $\phi$. The averaging operator (4.15) simplifies to

$$
\langle f \rangle = \frac{1}{2\pi} \int_0^{2\pi} f(s) ds.
$$

We now expand $N(z)$ and $E^\pm$ in Fourier series

$$
N(z) = \sum_{p \in \mathbb{Z}} \tilde{N}_p e^{ipz},
$$

$$
E^\pm(\phi, Z, T) = \sum_p E^\pm_p(Z, T) e^{\pm ip\phi},
$$

where $\tilde{N}_p = N_{-p}$ and $\tilde{E}^\pm_p = E^\pm_{-p}$ since $N$ and $E^\pm$ are real valued. In this case, the system of Fourier coefficients $\{E^\pm_p(Z, T) : p \in \mathbb{Z}\}$ satisfies the infinite system of xNLCME:

$$
\frac{\partial}{\partial T} E^+_p + \frac{\partial}{\partial Z} E^+_p = ip\tilde{N}_p E^-_p + \frac{\Gamma}{3} \left[ \sum_{q,r} E^+_q E^-_{p-q} E^+_r E^-_{p-q-r} \right],
$$

$$
\frac{\partial}{\partial T} E^-_p - \frac{\partial}{\partial Z} E^-_p = ip\tilde{N}_p E^+_p + \frac{\Gamma}{3} \left[ \sum_{q,r} E^-_q E^+_{p-q} E^-_{p-q} E^+_{p-q-r} \right] + 3 E^+_p \sum_{q} E^-_q E^-_{p-q} + 3 \left( \sum_{q} |E^-_q|^2 \right) E^-_p.
$$

### 4.3. Conservation laws and Hamiltonian structure

Equation (4.17), and alternatively (4.21), have several conservation laws.

**Proposition 4.1.** Assume that $E^\pm$ is a sufficiently smooth and sufficiently rapidly decaying in $Z$ solution of (4.17). Furthermore, assume that $\{E^\pm_p(Z, T) : p \in \mathbb{Z}\}$ is the corresponding solution of xNLCME. Then

$$
\frac{d}{dT} \int \langle E^+(\cdot, T) \rangle dZ = \frac{d}{dT} \int E^+_0(\cdot, T) dZ = 0,
$$

$$
\frac{d}{dT} \int \langle E^-(\cdot, T) \rangle dZ = \frac{d}{dT} \int E^-_0(\cdot, T) dZ = 0,
$$

$$
\frac{d}{dT} \int \langle |E^+(\cdot, T)|^2 \rangle + \langle |E^-(\cdot, T)|^2 \rangle dZ = \frac{d}{dT} \sum_p \int |E^+_p(\cdot, T)|^2 + |E^-_p(\cdot, T)|^2 dZ = 0.
$$
Proof. Setting \( p = 0 \) in (4.21),

\[
\begin{align*}
\partial_T E_0^+ + \partial_Z E_0^+ &= 0, \\
\partial_T E_0^- - \partial_Z E_0^- &= 0.
\end{align*}
\]

Integrating in \( Z \) establishes the first two conservation laws in terms of the Fourier modes. Integrating (4.20) in \( \phi \) over \([0, 2\pi)\) relates \( E^\pm \) to \( E_0^\pm \).

Multiplying (4.21a) by \( \bar{E}_p^+ \), summing over \( p \), and adding its complex conjugate,

\[
\sum_p \partial_T |E_p^+|^2 + \partial_Z |E_p^+|^2 = \sum_p i p N_{2p} E_p^+ \bar{E}_p^+ + \frac{\Gamma}{3} \sum_p i p \left[ \sum_{q, r} E_q^+ E_r^+ E_{-p}^+ E_{-p-q-r}^+ \right] + 3E_0^- \sum_q E_q^+ E_{p-q}^+ E_{-p}^+ + 3 \left( \sum_q |E_q^-|^2 \right) |E_p^+|^2 + \text{c.c.}
\]

The quartic terms will all vanish. Consider the first quartic term, and note that

\[
\sum_{p, q, r} p E_q^+ E_r^+ E_{-p}^+ E_{-p-q-r}^+ = \sum_{k_1 + k_2 + k_3 + k_4 = 0} k_1 E_{k_1}^+ E_{k_2}^+ E_{k_3}^+ E_{k_4}^+ = \sum_{k_1 + k_2 + k_3 + k_4 = 0} k_2 E_{k_1}^+ E_{k_2}^+ E_{k_3}^+ E_{k_4}^+ = \sum_{k_1 + k_2 + k_3 + k_4 = 0} k_3 E_{k_1}^+ E_{k_2}^+ E_{k_3}^+ E_{k_4}^+ = \sum_{k_1 + k_2 + k_3 + k_4 = 0} k_4 E_{k_1}^+ E_{k_2}^+ E_{k_3}^+ E_{k_4}^+.
\]

Hence

\[
\sum_{p, q, r} p E_q^+ E_r^+ E_{-p}^+ E_{-p-q-r}^+ = \frac{1}{4} \sum_{k_1 + k_2 + k_3 + k_4 = 0} (k_1 + k_2 + k_3 + k_4) E_{k_1}^+ E_{k_2}^+ E_{k_3}^+ E_{k_4}^+ = 0.
\]

The second quartic term vanishes using similar analysis. The last quartic term,

\[
\sum_p p \left( \sum_q |E_q^-|^2 \right) |E_p^+|^2,
\]

will vanish because the \( p \) and \(-p\) terms will cancel one another. Similar analysis holds for (4.21b), leaving us with the two equations

\[
(4.23a) \quad \sum_p \partial_T |E_p^+|^2 + \partial_Z |E_p^+|^2 = \sum_p i p N_{2p} E_p^+ \bar{E}_p^+ - i p N_{2p} E_p^+ \bar{E}_p^+,
\]

\[
(4.23b) \quad \sum_p \partial_T |E_p^-|^2 - \partial_Z |E_p^-|^2 = \sum_p i p N_{2p} E_p^- \bar{E}_p^- - i p N_{2p} E_p^- \bar{E}_p^-.
\]

Summing these two and integrating in \( Z \) gives the \( L^2 \) conservation law. \( \Box \)
To simplify our analysis we assume $E_0^\pm$ are initially zero from here on. The equations reduce to

$$\partial_T E^+ + \partial_Z E^+ = \partial_\phi \langle N(\phi_+ + s)E^-(\phi_+ + 2s) \rangle_s + \Gamma \partial_\phi \left[ \frac{1}{3} (E^+)^3 + E^+ \langle (E^-)^2 \rangle \right]_{\phi=\phi_+},$$

(4.24a)

$$\partial_T E^- - \partial_Z E^- = -\partial_\phi \langle N(\phi_- + s)E^+(\phi_- - 2s) \rangle_s |_{\phi=\phi_-} - \Gamma \partial_\phi \left[ \langle (E^-)^2 \rangle E^- + \frac{1}{3} (E^-)^3 \right]_{\phi=\phi_-},$$

(4.24b)

and

$$\partial_T E^+_p + \partial_Z E^+_p = ip N_{2p} E^-_p + ip \frac{\Gamma}{3} \left[ \sum_{q,r} E^+_{r} E^+_{p-r} E^+_q E^+_p - \frac{1}{3} \sum_q |E^-_q|^2 \right] E^+_p,$$

(4.25a)

$$\partial_T E^-_p - \partial_Z E^-_p = ip N_{2p} E^+_p + ip \frac{\Gamma}{3} \left[ \sum_{q,r} E^-_{r} E^-_{p-r} E^-_q E^-_p - \frac{1}{3} \sum_q |E^+_q|^2 \right] E^-_p.$$  

(4.25b)

These are (1.8) and (1.10) from section 1. Truncating (4.25) to just mode $E_{\pm 1}^\pm$ recovers the NLCME, subject to the identification of $E^\pm$ with $E_{\pm 1}^\pm$.

Another time-invariant functional is a consequence of the Hamiltonian structure given in the following result, which is straightforward to verify.

Proposition 4.2. The system (4.25) is a Hamiltonian system,

$$\partial_T E_p^+ = -ip \frac{\delta H}{\delta E_p^+}, \quad \partial_T E_p^- = -ip \frac{\delta H}{\delta E_p^-},$$

with time-invariant Hamiltonian

$$H[E^\pm_p, \bar{E}_p^\pm] = \int \mathcal{H} dZ$$

and Hamiltonian density

$$\mathcal{H} = \frac{i}{2} \sum_{p_1=1}^{\infty} \sum_{p_1=1}^{\infty} \left[ E^+_{p_1} \partial_\phi \bar{E}^+_{p_1} + E^-_{p_1} \partial_\phi \bar{E}^-_{p_1} \right] - \sum_{p_1=1}^{\infty} N_{2p_1} \bar{E}^+_{p_1} E^-_{p_1}$$

$$- \frac{\Gamma}{3} \left[ \sum_{p_1+p_2+p_3+p_4=0} E^+_{p_1} E^+_{p_2} E^+_{p_3} E^+_{p_4} + E^-_{p_1} E^-_{p_2} E^-_{p_3} E^-_{p_4} \right]$$

$$- \frac{\Gamma}{2} \sum_{p_1} \left( \sum_{p_1} |E^+_{p_1}|^2 \right) \left( \sum_{p_1} |E^-_{p_1}|^2 \right) + \text{c.c.}$$

(4.27)

5. Simulations of the truncated xNLCME. In this section we simulate truncations of the infinite dimensional xNLCME system, performed pseudospectrally with fourth order Runge–Kutta time stepping. These simulations suggest that

- xNLCME has its own localized soliton-like structures which better capture the dynamics of the nonlinear periodic Maxwell equation for our class of initial conditions than NLCME, and
NLCME has singular solutions \( \{ E_p^\pm (Z, T) \} \) which induce a cascade of energy to higher wavenumbers \( p \). The physical electric field

\[
E(z, t) \approx e^{1/2} \left( E^+(z - t, \epsilon z, \epsilon t) + E^-(z + t, \epsilon z, \epsilon t) \right)
\]

\[
= e^{1/2} \sum_{p \in \mathbb{Z} \setminus 0} \left( E_p^+(Z, T) e^{ip(Z - T)/\epsilon} + E_p^-(Z, T) e^{-ip(Z + T)/\epsilon} \right) + \text{c.c.}
\]

develops a carrier-shock train structure.

As we saw in section 3.1, particularly Figure 6, though the NLCME soliton data appeared robust, there was some escape of energy. This can be accounted for in xNLCME through the inclusion of additional modes.

Starting with the same initial conditions, we simulate the NLCME soliton of \( E_{11}^\pm \) with soliton parameters \( v = 0 \) and \( \delta = \frac{\pi}{2} \) and material parameters

\[
\Gamma = 1, \quad N_{\pm 2} = \frac{2}{\pi}, \quad N_{j \neq \pm 2} = 0
\]

in (4.25) resolving only a finite number of harmonics. The primitive electric field is reconstructed from these simulations as

\[
E = \sum_{p = -P_{\text{max}}}^{P_{\text{max}}} E_p^+(Z, T) e^{ip(Z - T)/\epsilon} + E_p^-(Z, T) e^{-ip(Z + T)/\epsilon} + \text{c.c.}
\]

Fig. 10. Evolution of an NLCME soliton in the \( x_{\text{NLCME}} \), resolving odd modes \( |p| \leq 4 \), computed with 4096 grid points in the \( Z \) coordinate. Compare with Figure 6.
E is plotted in Figures 10, and 11, which resolve odd modes up to 3 and 15, respectively. Comparing with Figure 6, we infer that the two smaller pulses symmetrically expelled from the main wave were transferred into $E^+_{1,3}$ since these clearly appear in Figure 10. This addresses the macroscopic discrepancy between NLCME and Maxwell.

Including the additional modes also suggests shock formation by reexamining Figure 9. The sharper, shock-like features can be resolved only by the inclusion of the higher harmonics. The contrast among different truncations is shown in Figure 12. Indeed, we see the Gibbs phenomenon that would be expected from taking a truncated Fourier representation of a discontinuous function.

Despite this, NLCME still gets certain leading order effects correct, such as the main structure in the Maxwell simulations. The robustness of NLCME can also be seen by exploring how energy is partitioned amongst the harmonics. Let

$$e_p = \int (|E^+_p|^2 + |E^-_p|^2 + |E^+|_p|^2 + |E^-|_p|^2) dZ, \quad p = 1, 3, \ldots, p_{\text{max}}.$$  

This is the energy associated with mode $p$. Their sum is conserved. Plotting this for the above simulations in Figure 13, we see that most of the energy remains in mode one, some migrates into mode three, and less is found in the subsequent modes.

6. Summary and discussion. We first numerically simulated the one-dimensional nonlinear Maxwell equations in the regime of weak nonlinearity, low-
contrast periodic structure (weak dispersion) with wave packet data satisfying a Bragg resonance condition, i.e., carrier wavelength equal to twice the medium periodicity. We observe strong evidence of the emergence of a coherent structure evolving as a slowly varying envelope with a carrier-shock train. This violates the nearly monochromatic assumption underlying the classical nonlinear coupled mode equations. We propose our nonlocal integrodifferential equations, governing coupled forward and backward waves and derived via a nonlinear geometrical optics expansion, as the physically correct, mathematically consistent description of waves governed by nonlinear Maxwell in a periodic structure with negligible chromatic (nonlocal in time) dispersion. For solutions which are periodic in the fast (carrier scale) phase, these equations are equivalent to an infinite dimensional system of couple first order PDEs, the xNLCME. The electric field, $E$, obtained from numerical solutions of successively higher truncations of xNLCME, converges toward the envelope carrier-shock trains observed in direct simulations of the nonlinear Maxwell equations.

We also note that our methods could be applied to study the long time-evolution of wave-packet-type initial conditions for the problem of quadratically nonlinear elastic media considered in [18], [24], and [50]. We obtain nonlocal equations by resonant non-linear geometrical optics (or equivalently an infinite family of nonlinear coupled mode equations), governing interacting forward and backward propagating waves [41].

**Fig. 12.** Comparison of the features that develop on the scale of the medium in different truncations of the equations. Including additional harmonics better captures the shocks seen in Figure 9.
difference between the quadratic and cubic cases is that the smallest truncated system that retains nonlinear interactions contains four modes, \( p = \pm 1, \pm 2 \). Nonlinear effects occur through second harmonic generation, a process well known in nonlinear optics.

Open problems and conjectures. As our simulations show, there is agreement between finite mode truncations of the integrodifferential equations and the primitive Maxwell system. Assessing and proving the time of validity of the nonlinear geometrical optics approximation is one open problem. A related question is the local well-posedness theory for the nonlinear geometrical optics approximation/\( xNLCME \) with a good estimate on the time of existence of solutions in terms of the initial data. We expect that solutions of \( xNLCME \) for initial data having a finite number of nonzero mode amplitudes, e.g., \( NLCME \) gap soliton data, will give rise to solutions that develop singularities in finite time. The nature of this blowup is expected to occur via a cascade to high mode amplitudes (higher index, \( p \)), corresponding to modes necessary to resolve the carrier shock structure in the small scale. As we mentioned in the discussion, there is clearly singularity formation when the heterogeneity is turned off (\( N = 0 \)), and either \( E^+ \) or \( E^- \) is initially zero. It is an open problem as to whether this particular mechanism for singularity formation will persist when coupling is restored.
As pointed out in section 1, the success in modeling experiments with NLCME suggests that, although there is such a (weakly turbulent) cascade, it is only a small part of the optical power that is transferred to high wavenumbers and that this energy contributes mainly to resolving the small-scale shocks. To explore this, one needs to simulate the xNLCME equations with many more harmonics. Plotting the Fourier transform (in the Z coordinate) of the simulations in section 5 in Figure 14, we see that the spectral support grows as we increase the number of resolved envelopes (the $E_p^z$’s). A related question is whether or not the primitive Maxwell system, the xNLCME system, or one of its truncations possesses genuine coherent structures. In [45], the authors found such solutions for a first and third harmonic system. This shall be further explored in the forthcoming publication [35].

Finally our computations in section 3 invoked a gas-dynamics entropy condition. Such a condition is necessary to use finite volume methods. Although thermodynamically consistent, we do not know whether this is the correct regularization mechanism of electrodynamics.

![Fig. 14. Fourier transforms of the solutions to truncations of the xNLCME equations. Increasing the number of envelopes expands the support in Fourier space.](image-url)
Appendix A. The NLCME soliton. Using the notation of [12], the NLCME soliton solution of (2.9) is given by

\[ E^+(Z, T) = s\alpha e^{i\eta} \sqrt{\frac{N_2}{2\Gamma}} \frac{1}{\Delta} \sin \delta e^{i\sigma} \text{sech}(\theta - i\delta/2), \]

(A.1a) \quad E^-(Z, T) = -\alpha e^{i\eta} \sqrt{\frac{N_2}{2\Gamma}} \Delta \sin \delta e^{i\sigma} \text{sech}(\theta + i\delta/2),

(A.1b) \quad \theta = \gamma N_2 \sin(\delta(Z - vT)), \quad \sigma = \gamma N_2 \cos(\delta(vZ - T)),

(A.1c) \quad e^{i\eta} = \left( -\frac{e^{i\theta} + e^{-i\delta}}{e^{i\theta} + e^{i\delta}} \right)^{2v/(3-v^2)},

(A.1d) \quad \gamma = 1/\sqrt{1 - v^2}, \quad \Delta = \left( \frac{1 - v}{1 + v} \right)^{1/4},

(A.1e) \quad s = \text{sign}(N_2\Gamma), \quad \alpha = \sqrt{\frac{2(1 - v^2)}{3 - v^2}}.

(A.1f)

We assume that \(N_2 \in \mathbb{R}\). There are two free parameters, \(|v| < 1\) and \(\delta \in \mathbb{R}\).

Appendix B. Simulating the nonlinear Maxwell equations. In vector notation, the rescaled Maxwell system (3.2) and constitutive law (3.3) are expressed as

\[ \partial_t \begin{pmatrix} D \\ B \end{pmatrix} + \partial_z \begin{pmatrix} -B \\ -E(D, z) \end{pmatrix} = 0, \]

(B.1) \quad \partial_t \mathbf{v} + \partial_z f(v, z) = 0.

To simulate this system of conservation laws, we employ a shock capturing finite volume scheme with the CLAWPACK software (see [23] and [24]). Furthermore, we employ the \(f\)-wave method to accommodate the spatially varying flux function (see [3], [24], and [50]).

To use finite volume methods we must provide the algorithm with a solution of the Riemann problem. This introduces a subtlety as our system has a nonconvex flux function. Nonconvex fluxes lead to interesting waves, including rightward (or leftward) traveling rarefaction and shockwaves that are “glued” together. Such waves, sometimes called compound or composite waves, were discussed in [27], [28], [46], and [47] and more recently in [32], [48], [49]. Examples are also given in the texts [24] and [43].

B.1. Finite volume methods for Maxwell. In finite volume numerical methods, at each time step, we must solve a Riemann problem between adjacent grid cells:
\[ v_t + f(v; z_j)_z = 0 \quad \text{for} \quad z_{j-1/2} < z < z_{j+1/2}. \]
\[ v_t + f(v; z_{j+1})_z = 0 \quad \text{for} \quad z_{j+1/2} < z < z_{j+3/2}. \]
\[ v(z, t = t^\circ) = \begin{cases} v^n_j & \text{for} \quad z_{j-1/2} < z < z_{j+1/2}, \\ v^n_{j+1} & \text{for} \quad z_{j+1/2} < z < z_{j+3/2}. \end{cases} \]

(B.2)

\(z_{j+1/2}\) is the interface between the cell centered at \(z_j\) and the cell centered at \(z_{j+1/2}\). The fluxes are assumed to be constant in \(z\) within each computational cell. We aim to provide an exact solution to the Riemann problem, in contrast to an approximate solution such as the Roe average.

In the next few sections, we adopt the notation
\[ v_t + f_l(v) = 0 \quad \text{for} \quad z < 0, \]
\[ v_t + f_r(v) = 0 \quad \text{for} \quad z > 0, \]
\[ v(z, 0) = \begin{cases} v_l & \text{for} \quad z < 0, \\ v_r & \text{for} \quad z > 0, \end{cases} \]

(B.3)

where \(f_l(v) = f(v; z_j)\) and \(f_r(v) = f(v; z_{j+1})\) and we take \(z_{j+1/2} = 0\).

Given any point \(v\) in \((D, B)\) phase space, we construct two entropy conditions (specified below) satisfying manifolds \(W_1(v)\) and \(W_2(v)\). These define the locus of points that can be joined to \(v\) by a left-going wave in the former case and a right-going wave in the latter case. We parameterize them in the \(D\) component. Given a state \(v_0\), \(W_j(D; v_0)\) is the parametric curve such that

\[ \left\{ \left( \begin{array}{c} D \\ W_j(D; v_0) \end{array} \right) \right\} = W_j(v_0) \quad \text{for} \quad j = 1, 2. \]

Were the medium homogeneous, solving the Riemann would correspond to finding a state \(v_* \in W_1(v_l) \cap W_2(v_r)\). In terms of the parametric curves, this point solves

(B.4) \[ W_2 \left( D_r; \left( \begin{array}{c} D_* \\ W_1(D_*; v_l) \end{array} \right) \right) = B_r. \]

As the medium is not homogeneous, we match the flux at the interface. We seek \(v_l^*\) and \(v_r^*\) such that

(B.5a) \[ W_1(D_l^*; v_l) = B_l^*. \]
(B.5b) \[ f_l(v_l^*) = f_r(v_r^*). \]
(B.5c) \[ W_2(D_r; v_r^*) = B_r. \]

\(v_l^*\) is the entropy satisfying state immediately to the left of the interface, and \(v_r^*\) is the entropy satisfying state immediately to the right of the interface.

For this problem, the flux matching condition is

(B.6a) \[ E(D_l^*; z_l) = E(D_r^*; z_r). \]
(B.6b) \[ B_l^* = B_r^*. \]
Defining transfer function, \( T \), that, given \( z_l, z_r \) and a left state \( D^*_l \), the flux matched displacement is

\[
T(D^*_l; z_l, z_r) = D^*_r.
\]  

(B.7)

With this function, (B.5) becomes

\[
W_2(D_r; \left( \frac{T(D^*_l; z_l, z_r)}{W_1(D^*_l, v_l)} \right)) = B_r.
\]  

(B.8)

\( D^*_l \) is the unknown. Once we have this value, we recover \( E^* \) and \( B^* \) allowing us to compute the fluxes. This is a one-dimensional root finding problem, subject to specifying the phase space functions \( W_j \).

**B.2. Nonconvex fluxes and the entropy condition.** It remains to specify the manifolds \( W_j \). This requires an additional, nontrivial assumption on an entropy condition. While such a condition is readily apparent in gas dynamics and elasticity, the appropriate condition for Maxwell is nonobvious.

In this work, we employ a diffusive entropy condition, akin to that found in gas dynamics. This was suggested by Sjöberg [42] as part of an entropy-flux pair involving the Poynting vector. This is also physically consistent as many dielectrics absorb the higher harmonics that would appear as the wave began to shock. In constructing the entropy satisfying \( W_j \) functions, we closely follow [27], [28], [32], [47] and particularly the \( p \)-system example in [46]. Graphically the \( W_j \) functions can be constructed by tracing an appropriate convex hull of \( E(D; z) \). Shock waves occur when points are joined by chords, rarefaction waves when points are joined along \( E(D; z) \), and composite waves when the convex curve is a combination.

Throughout this section we suppress the \( z \) argument, and \( E'(D) = \partial_D E(D; z) \).

Since the flux function is no longer uniformly convex, the Lax entropy condition may not be appropriate. Instead, the Liu entropy condition (see [27] and [32]) may apply. Recall that if

\[
\sigma(v_0, v) \equiv \frac{-E(D) + E(D_0)}{B - B_0},
\]  

(B.9)

then

- a shock joining \( v_0 \) to \( v_1 \) satisfies the Lax entropy condition if the system is convex and either

\[
\lambda_1(v_1) < \sigma < \lambda_1(v_0), \quad \sigma < 0,
\]  

(B.10a)

\[
\lambda_2(v_1) < \sigma < \lambda_2(v_0), \quad \sigma > 0,
\]  

(B.10b)

where \( \lambda_1 < 0 < \lambda_2 \) are the eigenvalues of

\[
\begin{pmatrix}
0 & -1 \\
-E'(D) & 0
\end{pmatrix};
\]

- a shock joining \( v_0 \) to \( v_1 \) satisfies the Liu entropy condition if

\[
\sigma(v_0, v_1) \leq \sigma(v_0, \tilde{v})
\]  

(B.11)

for all points \( \tilde{v} \) between the two points along the shock curve in phase space.

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B.2.1. Left traveling waves. Given the state $u_0 = (D_0, B_0)^T$, we construct $W_1(D; u_0)$. Since we have an inflection point in $E(D)$ at $D = 0$, we dissect all the possible configurations of $D_0$, $D$ and the inflection point. Let $D_1$ be the value of $D$ at which the line tangent to $(D_1, E(D_1))$ intercepts $(D_0, E(D_0))$.

First suppose that $D < D_0 < 0$, as in Figure 15(a). In this region, there is no difficulty applying the Lax entropy condition (B.10); there is no shock as

$$\lambda_1(D) = -\sqrt{E'(D)} < \lambda_3(D_0) = -\sqrt{E'(D_0)} < 0.$$ Consequently

$$B = B_0 + \int_{D_0}^{D} \sqrt{E'(s)} ds.$$ Still assuming that $D_0 < 0$, if $D_0 < D < D_1$, the Lax condition continues to apply. $D_0$ and $D$ will satisfy (B.10), and we can join the two with a shock, as in Figure 15(b),

$$B = B_0 + \sqrt{|E(D) - E_0| |D - D_0|}.$$
Once $D > D_1$, the solution changes. It is no longer appropriate to apply the Lax condition as we lose convexity here. Applying the Liu condition, (B.11), we see that there is no longer a shock. Indeed, we can compute that were there shock solutions

$$\sigma(v_0, v) = \frac{-E + E_0}{B - B_0} = -\sqrt{\frac{E - E_0}{D - D_0}},$$

$$\sigma(v_0, v_1) = \frac{-E_1 + E_0}{B_1 - B_0} = -\sqrt{\frac{E_1 - E_0}{D_1 - D_0}}.$$

Examining Figure 15(c),

$$\frac{E_1 - E_0}{D_1 - D_0} < \frac{E - E_0}{D - D_0} < 0,$$

implying

$$\sigma(v_0, v_1) < \sigma(v_0, v),$$

which violates (B.11).

As a shock fails to connect the two states, we resort to joining the states by a compound wave. The solution is a shock from $D_0$ to $D_1$ which continues into a rarefaction wave from $D_1$ to $D$. Thus

$$B = B_0 + \sqrt{|E(D_1) - E_0||D_1 - D_0|} + \int_{D_1}^{D} \sqrt{E'(s)} \, ds.$$

At $D_0 = 0$ the system is convex, yielding leftward traveling rarefaction waves for all values of $D$:

$$B = B_0 + \int_{D_0}^{D} \sqrt{E'(s)} \, ds.$$

For $D_0 > 0$, there are again several cases. For $D < D_1$, we have the compound wave again, as in Figure 16(a):

$$B = B_0 - \sqrt{|E(D_1) - E_0||D_1 - D_0|} + \int_{D_1}^{D} \sqrt{E'(s)} \, ds.$$

As $D$ increases in value and $D_1 < D < D_0$, we have a shock solution

$$B = B_0 - \sqrt{|E(D) - E_0||D - D_0|}.$$

See Figure 16(b). Last, for $D > D_0$, we get a leftward traveling rarefaction:

$$B = B_0 + \int_{D_0}^{D} \sqrt{E'(s)} \, ds.$$

**B.2.2. Right traveling waves** For right traveling waves, the structure is similar. Given our point $D_0$, let $(D_2, E_2)$ be the point intercepted by the line tangent to $(D_0, E(D_0))$. 

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Again, we first treat $D_0 < 0$. The different cases are diagramed in Figure 17. For $D < D_0 < 0$, there is a shock,

$$B = B_0 + \sqrt{|E(D) - E_0||D - D_0|}.$$ 

For $D_0 < D < 0$, this changes to a rarefaction wave,

$$B = B_0 - \int_{D_0}^{D} \sqrt{E'(s)} ds.$$ 

Crossing the inflection point, $0 < D < D_2$, it becomes a compound wave which rarefacts to the point $D_\star$ followed by a shock,

$$B = B_0 - \int_{D_0}^{D_\star} \sqrt{E'(s)} ds - \sqrt{|E(D) - E_\star||D - D_\star|}.$$ 

$D_\star$ is the point $(D_\star, E_\star)$ on the curve whose tangent intercepts $(D, E)$. Past $D_2$, the compound wave reduces to a shock as the system now satisfies (B.11),

$$B = B_0 - \sqrt{|E(D) - E_0||D - D_0|}.$$
For $D_0 = 0$, we have a shock in both directions, 

$$B = B_0 - \text{sign}(D) \sqrt{|E(D) - E_0| D - D_0|}.$$ 

For $D_0 > 0$, again, we must consider the different positions of $D$ relative to the other points. These cases appear in Figure 18. If $D < D_2 < 0$, there is the shock solution satisfying (B.11), 

$$B = B_0 + \sqrt{|E(D) - E_0||D - D_2|}.$$ 

For $D_2 < D < 0$, this becomes a compound wave, 

$$B = B_0 - \int_{D_0}^{D} \sqrt{E'(s)} ds + \sqrt{|E(D) - E_0||D - D_2|}.$$ 

$D_0$ is again the point on the curve whose tangent intercepts $(D, E(D))$. For $0 < D < D_0$, this becomes a purely rarefactory wave 

$$B = B_0 - \int_{D_0}^{D} \sqrt{E'(s)} ds.$$
Finally, for $D > D_0$, we again have a shock,

$$B = B_0 - \sqrt{|E(D) - E_0||D - D_0|}.$$ 

**Acknowledgments.** The authors would like to thank R. R. Rosales for discussions during the early stages of this work on the use nonlinear geometrical optics. We also thank M. Pugh, D. Ketcheson, R. J. LeVeque, J. E. Sipe, and C. Sulem for helpful discussions. MIW would also like to acknowledge the hospitality of the Courant Institute of Mathematical Sciences, where he was on sabbatical during the preparation of this article.

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