Nonlinear Optical Solitary Waves in a Photonic Band Gap

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It is suggested that solitary wave solutions exist in the gap region of photonic band gap materials with a Kerr nonlinearity. Using a variational trial function we estimate the amplitude, size scale, and the nature of phase modulation of these nonlinear waves. In two dimensions, we predict the occurrence of a variety of finite energy solitary waves associated with the different symmetry points of the crystalline Brillouin zone. Solutions which preserve the symmetry of the crystal exist for both positive and negative Kerr coefficient whereas solutions which break the symmetry occur only for positive nonlinearity. These states are relevant to the bistable switching properties of photonic band gap materials.

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Photonic band gap materials represent a new class of dielectrics in which there is a complete gap to electromagnetic wave propagation in three dimensions, in analogy to the electronic band gap of a semiconductor [1-9]. It has been shown [3-5] that such structures exist with gaps as large as 20% of the gap center frequency. Materials of this nature have recently been fabricated [5] for applications in the microwave and optical frequency regimes. A number of new physical phenomena have been predicted to occur in these materials including strong localization of light [2], inhibited spontaneous emission from atoms [1,7], and photon-atom bound states [8]. In this paper, we suggest that, in the presence of a Kerr nonlinearity, wave propagation can occur in these dielectrics for frequencies within the forbidden gap. In the low intensity linear regime, illumination of the periodic dielectric at a band gap frequency leads to exponential decay of the electric field amplitude from the surface and strong reflection of all incident light. Winful, Marburger, and Garmire showed that optical bistability can occur in nonlinear distributed feedback structures [10]. Chen and Mills carried out a numerical study of a finite nonlinear one-dimensional periodic dielectric and showed that for frequencies within the forbidden gap solitary waves exist allowing the system to switch from low to high transmissivity [11]. An analytical description of the nonlinear wave equation was subsequently obtained by Mills and Trullinger [12]. Specific calculations for near band-edge solitons in finite 1D superlattices have been performed by de Sterke and Sipe [13]. Dynamical studies of these solitons show that they exhibit relativistic behavior with velocities between zero and the average speed of light in the medium [14-16].

In higher-dimensional photonic band gap materials, the underlying nonlinear wave equation has not been solved exactly. We present in this paper an approximate solution to the nonlinear equation using a new variational method. Our variational method reproduces to a high degree of accuracy the exact soliton solutions in one dimension. It furthermore makes a number of new predictions concerning the existence and properties of solitary waves in higher dimensions. This includes the occurrence of a variety of finite energy solitary waves associated with different symmetry points of the crystalline Brillouin zone. The one-dimensional gap soliton solution with phase and amplitude modulation in the direction of a single reciprocal lattice vector of the crystal is extended in the transverse directions and has an infinite energy in a higher-dimensional system. However, if the Kerr coefficient is positive, we show that localized finite energy solitary waves are in fact possible with phase modulation in the direction of a single Bragg scattering vector. Unlike the one-dimensional case, finite energy solutions, which pick out a specific reciprocal lattice vector and thus break the symmetry of the crystal, do not occur for negative Kerr coefficient. On the other hand, we find a new class of solitary waves of higher symmetry which occur for both positive and negative Kerr coefficients. These new self-localized states involve Bragg scattering by a complete basis set of reciprocal lattice vectors and exhibit phase modulation in each of these directions.

Another distinguishing property of solitary waves in a photonic band gap is the scaling of the total electromagnetic energy contained in the state with the frequency of the underlying radiation. For one-dimensional solitons the total energy vanishes as the frequency approaches a band edge where the effective mass approximation is valid. For a three-dimensional solitary wave, a simple scaling argument suggests that the total energy is minimum near the center of the photonic band gap but in fact diverges as the frequency approaches this band edge. These threshold, gap center, solitary waves may prove valuable for coupling energy from external sources into an otherwise inpenetrable photonic band gap material on scales much longer than the tunneling length.

For the purpose of illustration, we describe in detail solitary wave solutions in a two-dimensional periodic nonlinear dielectric with the point group symmetry of a square lattice. The essential new physics that distinguishes the square lattice from 1D periodic structures is the existence of multiple symmetry points in the crystalline Brillouin zone which determine the photonic band edges [17-21]. Each of these symmetry points plays an important role in determining the nature of nonlinear waves within the gap and accordingly a slowly varying envelope function expansion of the true electric field am-

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plitude must be performed about each point. The linear part of the dielectric constant is taken to have the form $\epsilon(x,y)=\epsilon_0+\Delta\epsilon(\cos Gx+\cos Gy)$ where the reciprocal lattice vector has a magnitude $G=2\pi/a$. It is assumed that the electric field **E** and polarization **P** are perpendicular to the direction in which they vary. Denoting the z component of the complex electric field amplitude of frequency ω by E, the nonlinear wave equation is

$$[\nabla^2+k^2\epsilon(x,y)+12\pi\chi^{(3)}k^2|E|^2]E=0\,, \tag{1}$$

where $k=\omega/c$, ω is the optical frequency, c is vacuum speed of light, and $\chi^{(3)}$ is the nonlinear susceptibility.

The slowly varying envelope approximation to this equation consists of retaining only those Fourier components of $E(x,y)$ which lie near the crystalline band edges. These occur at the symmetry points X and M of the square lattice Brillouin zone (see Fig. 1, inset). We consider first the X symmetry point at $\mathbf{k}_0=(\pi/a)\hat{\mathbf{x}}$ and expand $E(x,y)=E_1(x,y)e^{ik_0x}+E_2(x,y)e^{-ik_0x}$, where E_1 and E_2 are slowly varying envelope functions of spectral width $\Delta k\ll k_0$. Substituting this expansion into (1), collecting terms of order e^{ik_0x} and e^{-ik_0x}, respectively, and keeping only leading terms in the derivative expansion, we obtain a coupled set of nonlinear differential equations for E_1 and E_2. It is straightforward to show [12] that static solutions in which there is no net transport of electromagnetic energy satisfy the condition $|E_1|=|E_2|$ in which case the coupled equations can be conveniently expressed in terms of a two component spinor field:

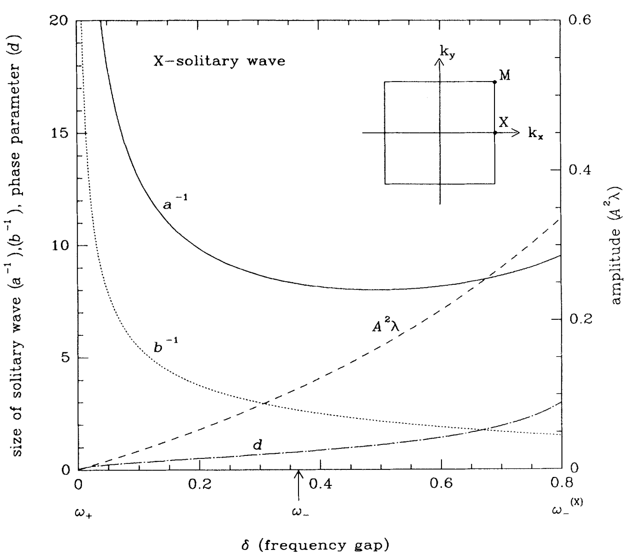

FIG. 1. The size parameters a^{-1} (solid line), b^{-1} (dotted line), phase parameter d (dot-dashed line) (left scale), and amplitude $(A^2\lambda)$ (dashed line) (right scale) of the broken symmetry X-solitary wave are shown as a function of the band gap frequency $\delta=\omega_+^2-\omega^2$. The absolute band gap is marked on the graph as ω_+ and ω_-. These calculations are done for $\Delta\epsilon_0/\epsilon_0=0.7$ and $\lambda>0$.

$$[i\sigma_z\partial_x+\partial_y^2+(\omega^2-1)/4+\omega^2\beta\sigma_x+\omega^2\lambda(\Psi^\dagger\Psi)]\Psi=0\,, \tag{2}$$

where $\Psi^\dagger=(E_1^*,E_2^*)$, x and y are dimensionless coordinate variables measured in units of G^{-1}, $\partial_x=\partial/\partial x$, $\partial_y=\partial/\partial y$, ω is a dimensionless frequency measured in units of the characteristic frequency $\omega_0=c\pi/a\sqrt{\epsilon_0}$, $\beta=\Delta\epsilon/8\epsilon_0$, and $\lambda=9\pi\chi^{(3)}/2\epsilon_0$. σ_x and σ_z are the 2×2 Pauli spin matrices which satisfy an anticommuting algebra. In the absence of the term $\partial_y^2\Psi$, this is precisely the 1D soliton equation [12]. The second derivative term here is essential, however, to render the solitary wave solution finite in the y direction.

The underlying band structure in the envelope approximation (2) is obtained by setting $\lambda=0$ and considering solutions of the form $\Psi=\Phi e^{i\mathbf{q}\cdot\mathbf{r}}$ where $\mathbf{q}$ and $\mathbf{r}$ are 2D vectors in the x-y plane and Φ is independent of $\mathbf{r}$. At $\mathbf{k}=\pi/a$ ($\mathbf{q}=0$) there is a frequency gap bounded by the band edge frequencies $\omega_\pm^{(X)}=(1\mp\Delta\epsilon/2\epsilon_0)^{-1/2}$. In the overall band structure of the crystal the frequency $\omega_+=\omega_+^{(X)}$ plays the role of the upper band edge of the photonic band gap. As a consequence of the anisotropic dispersion, this model has an indirect gap with the lower band edge ω_- occurring at the corner of the Brillouin zone (M point).

Before discussing the precise nature of solitary wave solutions of (2) we describe the possibility of qualitatively different solitary wave states associated with the other symmetry points in the Brillouin zone. Equation (2) clearly breaks the symmetry of the square lattice. By interchanging x and y in Eq. (2) we may obtain solitary waves that are rotated by 90°. To find nonlinear solutions that preserve the symmetry of the crystal it is necessary to perform an envelope expansion about each of the four equivalent X points, $E(x,y)=E_1e^{ik_0x}+E_2e^{-ik_0x}+E_3e^{ik_0y}+E_4e^{-ik_0y}$. Again assuming a static self-localized state with the magnitude of the slowly varying envelope to be the same, the effective equation for the four component spinor field $\Psi^\dagger=(E_1^*,E_2^*,E_3^*,E_4^*)$ is

$$[i(\gamma_1\partial_x+\gamma_2\partial_y)+(\omega^2-1)/4+\omega^2\beta\gamma_3+\omega^2\lambda'(\Psi^\dagger\Psi)]\Psi=0\,, \tag{3}$$

where $\lambda'=(3/2)\lambda$ and γ_1, γ_2, and γ_3 are 4×4 matrices defined as

$$\gamma_1=\begin{bmatrix}\sigma_z & 0\\ 0 & 0\end{bmatrix},\quad \gamma_2=\begin{bmatrix}0 & 0\\ 0 & \sigma_z\end{bmatrix},\quad \gamma_3=\begin{bmatrix}\sigma_x & 0\\ 0 & \sigma_x\end{bmatrix}.$$

Unlike Eq. (2), which requires a second derivative to yield a localized solution, we will show that symmetric localized solutions of Eq. (3) are possible even though we have retained only first order derivatives in both the x and y directions.

A distinct class of solitary wave solutions is associated with the fourfold degenerate M point. Since there are two reciprocal lattice vectors which connect a given M point to symmetry related partners, it is necessary to include all four of the corresponding envelope functions in any expansion of the electric field amplitude. This yields

$$[i(\gamma_1' \partial_x + \gamma_2' \partial_y) + (\omega^2 - 2)/4 + \omega^2 \beta \gamma_3' + \omega^2 \lambda' (\Psi^\dagger \Psi)] \Psi = 0 \quad (4)$$

for the four component envelope field Ψ, where the new 4×4 matrices γ_1' and γ_2' are defined as

$$\gamma_1' = \begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}, \quad \gamma_2' = \begin{pmatrix} \sigma_z & 0 \\ 0 & -\sigma_z \end{pmatrix}, \quad \gamma_3' = \begin{pmatrix} 0 & \sigma_x + I \\ \sigma_x + I & 0 \end{pmatrix}.$$

The underlying photonic band structure near the M point is determined by setting the nonlinear coefficient $\lambda' = 0$. A spectral gap occurs between the two frequencies $\omega_\mp^{(M)} = \sqrt{2}(1 \pm \Delta\epsilon/\epsilon_0)^{-1/2}$.

In order to have a complete photonic band gap, the gaps at the X and M points should overlap. This leads to the requirement that $\Delta\epsilon/\epsilon_0 \gtrsim 0.5$. In this case, the true photonic band gap is indirect and is bounded by the lower band edge $\omega_- = \omega_-^{(M)}$ and the upper band edge $\omega_+ = \omega_+^{(X)}$.

Equations (2), (3), and (4) describe the properties of three distinct types of elementary solitary waves within the two-dimensional photonic band gap. Unlike their counterpart for the one-dimensional stop gap in which a simple analytic soliton solution exist [12] we seek approximate analytic solutions within the gap. Nevertheless, certain features of the one-dimensional solution remain evident in higher dimensions. The first is the exponential decay of the wave amplitude. Physically we may regard the high light intensity at the center of the solitary wave as creating an effective dielectric defect in the otherwise periodic structure leading to a localized state in the gap [22]. Another essential feature of the solitary wave is the existence of a kink in the phase of electric field near the center of the solution. Both of these features play a vital role in the variational trial function we introduce to approximately solve the nonlinear envelope equations. Equation (2) may be regarded as a stationary point of the functional

$$F_1 = \int d^2\mathbf{r} \{ |\partial_y \Psi|^2 - \Psi^\dagger [i\sigma_z \partial_x + (\omega^2 - 1)/4 + \omega^2 \beta \sigma_x + (\omega^2/2)\lambda(\Psi^\dagger \Psi)] \Psi \} \quad (5)$$

with respect to arbitrary functions Ψ. The condition $\delta F_1/\delta \Psi^\dagger = 0$ may be implemented approximately by introducing a trial solution $\Psi^\dagger(x,y) = \varepsilon(\mathbf{r})(e^{-i\Phi(\mathbf{r})}, e^{i\Phi(\mathbf{r})})$ with $\varepsilon(\mathbf{r}) = A\,\mathrm{sech}(ax)\mathrm{sech}(by)$ and $\Phi(\mathbf{r}) = c + \arctan[d \times \tanh(ax)]$ describing a localized state with a kink in the x direction. The functional F_1 can be evaluated analytically and minimized with respect to the variational parameters A, a, b, c, and d. The results are shown in Fig. 1 as a function of the dimensionless detuning frequency $\delta = \omega_+^2 - \omega^2$. The phase shift $c = (n + 1/2)\pi$. For this symmetry breaking solitary wave, a nontrivial solution exists for $\lambda > 0$. Within the two envelope function approximation (2) this solution persists for all frequencies within the X gap: $\omega_-^{(X)} < \omega < \omega_+^{(X)}$. However, for frequencies $\omega_-^{(X)} < \omega < \omega_-^{(M)}$ which lie outside of the true photonic band gap, the solution is unstable to decay by interaction with the continuum modes. As shown in Fig. 1, within the photonic band gap region, the length scales a^{-1}, b^{-1} of the solitary wave diverge as $\delta^{-1/2}$ and the amplitude $A \sim \delta^{1/2}$ near the upper band edge. A similar behavior for a^{-1} and A occurs $\omega_-^{(X)}$ but this is preceded by the occurrence of the indirect lower band edge $\omega_- = \omega_-^{(M)}$. A more elaborate trial wave function is in fact needed to exhibit the divergence of the localization length at the lower direct band edge for $\lambda > 0$ [12]. We refer to the above solution as the "X solitary wave." The total energy of the solitary wave is defined as $U = \int d^d\mathbf{r}(\Psi^\dagger\Psi)$ for each frequency in the gap. In general, the total electromagnetic energy of the solitary wave scales as the square of the amplitude A and the volume a^{-d}. Near the band edge (small δ) it follows that the energy obeys the scaling behavior

$$U \sim [\lambda k_0^d \delta^{1-d/2}]^{-1}. \quad (6)$$

$d = 2$ is a marginal dimension in which U is some finite number throughout the gap. For $d = 1$, $U \to 0$ as the band edge is approached and there is no threshold for creating a soliton. In $d = 3$, however, $U \to \infty$ near a band edge and in fact the threshold energy for creating a solitary wave is realized near the gap center, as far from the band edges as possible.

The variational method we have outlined may be used to obtain an "M solitary wave" as well as a "symmetric X solitary wave." From Eq. (4) it is apparent that the M solitary wave can be regarded as an extremum of the functional

$$F_2 = \int d^2\mathbf{r}\, \Psi^\dagger [i(\gamma_1' \partial_x + \gamma_2' \partial_y) + (\omega^2 - 2)/4 + \omega^2 \beta \gamma_3' + (\omega^2/2)\lambda' (\Psi^\dagger \Psi)] \Psi. \quad (7)$$

A solution can be found for all frequencies in the gap for both positive and negative λ' by inserting the variational function $\Psi^\dagger = \varepsilon(r)(e^{-i\Phi_1}, e^{i\Phi_1}, e^{-i\Phi_2}, e^{i\Phi_2})$ where

$$\varepsilon(\mathbf{r}) = A\,\mathrm{sech}(ax)\,\mathrm{sech}(ay),$$

$$\Phi_1 = c_1 + \arctan[b \tanh(ax)] + \arctan[b \tanh(ay)],$$

and

$$\Phi_2 = c_2 + \arctan[b \tanh(ax)] - \arctan[b \tanh(ay)].$$

Minimizing F_2 with respect to the variational parameters A a, b, and c yields a finite energy solitary wave. The results are given in Fig. 2 for $\lambda' > 0$. Here $c_1 = 2\pi n$ and $c_2 = (2n+1)\pi$. The case for $\lambda' < 0$ is easily found by mirror reflecting the curves about $\delta = 2.75$ in Fig. 2.

We mention finally that a symmetric X solitary wave solution occurs by following essentially the same procedure as above by casting Eq. (3) into a variational form. The trial solution takes a similar form to the symmetric M solitary wave. The results are qualitatively similar to those depicted in Fig. 2 so we do not repeat them here. It is interesting to note, nevertheless, that unlike the broken symmetry X solitary wave, a symmetric solution of finite energy exists for either sign of the non-

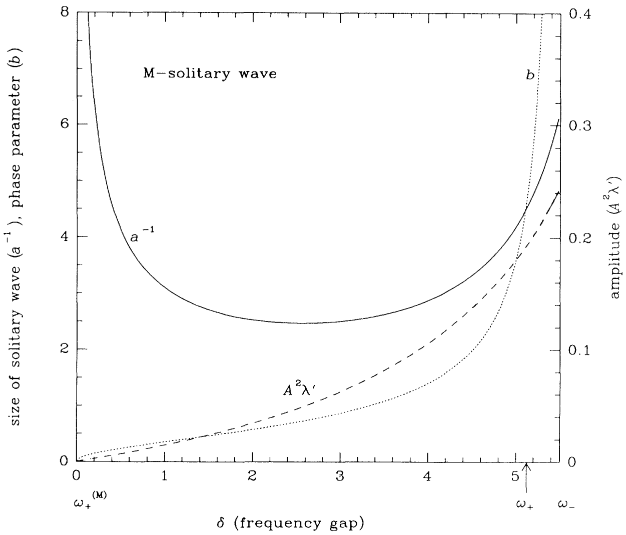

FIG. 2. The size parameter a^{-1} (solid line), phase parameter b (dotted line) (left scale), and amplitude ($A^2\lambda'$) (dashed line) (right scale) of the M solitary wave are shown as a function of the band gap frequency $\delta = \omega_+^{2(M)} - \omega^2$ for $\lambda' > 0$ and $\Delta\epsilon/\epsilon_0 = 0.7$. The absolute band gap is marked on the graph with ω_+ and ω_-.

linear Kerr coefficient.

In summary, we have derived a generalization of the one-dimensional optical gap soliton states to higher-dimensional photonic band gap materials. The variational ansatz reproduces very accurately the exact 1D gap soliton state for most of the band gap. The only significant deviations from the exact solution occur near the lower direct band edge for $\lambda > 0$ and the upper direct band edge for $\lambda < 0$. In our 2D square lattice model with an indirect gap these regions are not relevant to the true photonic band gap. The 1D soliton state exhibits relativistic dynamics when time dependence is included in its governing equation [15]. This follows directly from the anticommutation algebra of the Pauli matrices for the 1D problem. In higher dimensions this relativistic dynamics, we expect, will be lost, since, unlike a true Dirac equation, the γ matrices appearing in Eqs. (3) and (4) fail to anticommute.

The experimental realization of these self-localized solitary waves requires lossless materials with large nonlinear Kerr coefficient. Typical nonresonant nonlinearities in semiconductors are $\chi^{(3)} \sim 10^{-15}$–10^{-17} (cm/V)^2. For certain GaAs-AlAs structures it has been shown that the optical absorption edge falls off very sharply below the electronic band gap whereas the nonlinear constant remains relatively high. In these systems $\chi^{(3)} \sim 10^{-10}$ (cm/V)^2 [23]. If we assume $\delta \sim 10^{-1}$ the solitary wave has a peak intensity of the order of 3 kW/cm^2 corresponding to a field strength of 10^3–10^4 V/cm. Another possible system is a two-dimensional array of InGaAsP disks. Individual disks of this nature have already been utilized as low threshold microcavity lasers [24].

These studies will further elucidate the novel propagative effects of photonic band gap materials. Photonic band gap materials, although "emptier than the vacuum" to linear electromagnetic effects [1] are quite rich in nonlinear phenomena. Materials which exhibit these nonlinear phenomena at modest field strengths may have important technological applications.

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