Photonic crystals, coupled-mode equations, and gap solitons

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References:

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Introduction

Motivations

- Modeling of photonic crystals in one and two dimensions
- Control of linear transmission properties in stop bands
- Persistence and time-evolution of gap solitons in band gaps
Introduction

Motivations

- Modeling of photonic crystals in one and two dimensions
- Control of linear transmission properties in stop bands
- Persistence and time-evolution of gap solitons in band gaps

Plan of the talk

1. Reduction of Maxwell equations to coupled-mode equations
2. Well-posedness of linear boundary value PDE problems (2-D)
3. Linearized stability of gap solitons (1-D)
Linear Maxwell equations

\[ \nabla^2 \mathbf{E} - \frac{n^2}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} = \nabla (\nabla \cdot \mathbf{E}), \quad \nabla \cdot \left( n^2 \mathbf{E} \right) = 0 \]

Three-dimensional vectors \( \mathbf{E} = (E_x, E_y, E_z) \) and \( \mathbf{x} = (x, y, z) \)

\( n = n(\mathbf{x}) \) is the periodic refractive index with \( n(\mathbf{x} + \mathbf{a}) = n(\mathbf{x}) \)

\( c \) is the speed of light
Photonic band gaps in 1-D and 2-D

- Existence of Bloch waves for arbitrary smooth $n(x)$ (Kuchment, 1993)
  \[
  E(x, t) = \Psi(x) e^{i(k \cdot x - \omega t)},
  \]

- $k = (k_x, k_y, k_z)$ is the wave vector
- $\omega = \omega(k)$ is the wave frequency
- $\Psi(x + a) = \Psi(x)$ is the periodic envelope
Low-contrast 3-D photonic crystals

- Small periodicity of the refractive index

\[ n(x) = 1 + \epsilon \sum_{(n,m,l) \in \mathbb{Z}^3} \alpha_{n,m,l} e^{i(nk_1 + mk_2 + lk_3)x} \]

- \( \epsilon \) is small parameter
- \( k_{1,2,3} \) are reciprocal lattice vectors
The incident wave $\mathbf{E} = e_k e^{i(k \cdot x - \omega t)}$ with $\mathbf{k} = \mathbf{k}_{\text{in}}$, where

$$\mathbf{k} \cdot e_k = 0, \quad \omega^2 = c^2 \left( k_x^2 + k_y^2 + k_z^2 \right)$$
Concept of resonances

- The *incident* wave \( \mathbf{E} = e_k e^{i(k \cdot \mathbf{x} - \omega t)} \) with \( k = k_{\text{in}} \), where
  \[
  k \cdot e_k = 0, \quad \omega^2 = c^2 \left( k_x^2 + k_y^2 + k_z^2 \right)
  \]

- *Transmitted* waves \( \mathbf{E} = e_k e^{i(k \cdot \mathbf{x} - \omega t)} \) with \( k = k_{(n,m,l)}^{(\text{out})} \) in
  \[
  k_{\text{out}}^{(n,m,l)} = k_{\text{in}} + nk_1 + mk_2 + lk_3, \quad (n, m, l) \in \mathbb{Z}^3.
  \]
Concept of resonances

○ The *incident* wave \( \mathbf{E} = e_k e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)} \) with \( \mathbf{k} = \mathbf{k}_{\text{in}} \), where

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○ *Transmitted* waves \( \mathbf{E} = e_k e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)} \) with \( \mathbf{k} = \mathbf{k}_{\text{out}}^{(n,m,l)} \) in

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\mathbf{k}_{\text{out}}^{(n,m,l)} = \mathbf{k}_{\text{in}} + nk_1 + mk_2 + lk_3, \quad (n, m, l) \in \mathbb{Z}^3.
\]

○ The transmitted waves are resonant to the incident wave if

\[
\omega(\mathbf{k}_{\text{out}}^{(n,m,l)}) = \omega(\mathbf{k}_{\text{in}}) \quad \text{for some} \ (n, m, l) \in \mathbb{Z}^3
\]
The cubic crystal structure

\[ \mathbf{x}_{1,2,3} = a \mathbf{e}_{1,2,3}, \quad \mathbf{k}_{1,2,3} = \frac{2\pi}{a} \mathbf{e}_{1,2,3}, \]

where \( \mathbf{e}_{1,2,3} \) are unit vectors in \( \mathbb{R}^3 \) and \( a > 0 \).
Resonances in 3-D cubic crystals

- The cubic crystal structure

\[ x_{1,2,3} = a e_{1,2,3}, \quad k_{1,2,3} = \frac{2\pi}{a} e_{1,2,3}, \]

where \( e_{1,2,3} \) are unit vectors in \( \mathbb{R}^3 \) and \( a > 0 \).

- The set of resonances in low-contrast cubic crystal

\[ S = \left \{ (n, m, l) \in \mathbb{Z}^3 : n(n + p) + m(m + q) + l(l + r) = 0 \right \} \]

where \( (p, q, r) \in \mathbb{R}^3 \) in \( k_{\text{in}} = \frac{\pi}{a}(p, q, r) \).
Resonances in 3-D cubic crystals

- The cubic crystal structure

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- The set of resonances in low-contrast cubic crystal

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where \( (p, q, r) \in \mathbb{R}^3 \) in \( k_{\text{in}} = \frac{\pi}{a} (p, q, r) \).

- The set \( S \) is finite-dimensional and non-empty with \( (n, m, l) = (0, 0, 0) \)

\[
\left( n + \frac{p}{2} \right)^2 + \left( m + \frac{q}{2} \right)^2 + \left( l + \frac{r}{2} \right)^2 < \infty
\]
Particular 1-D and 2-D resonances

- Graphical solution

- Analytical solutions
  - 1-D resonance \( p = q = 0, \ r \in \mathbb{Z} \)
  - 2-D resonance \( (p, q) \in \mathbb{Z}^2, \ r = 0 \)
  - 2-D oblique resonance \( (p, q) \in \mathbb{R}^2, \ r = 0 \)
Formal derivation of coupled-mode equations

- Perturbation series expansions in powers of $\epsilon$:
  \[
  E(x, t) = E_0(x, t) + \epsilon E_1(x, t) + O(\epsilon^2).
  \]

- Bloch waves are plane waves for $\epsilon = 0$:
  \[
  E_0(x, t) = \sum_{j=1}^{N} A_j(X, T) e^{i k_j x - \omega t}.
  \]

- $(X, T)$ are slow normalized variables:
  \[
  X = \frac{\epsilon x}{k}, \quad T = \frac{\epsilon t}{\omega}.
  \]
Formal derivation of coupled-mode equations

- Inhomogeneous equation with resonant terms:

\[ \nabla^2 E_1 - \frac{n_0^2}{c^2} \partial^2 E_1 = F(E_0), \]

- Solvability conditions from orthogonality of \( F(E_0) \) to resonant terms:

\[ i \left( \frac{\partial A_j}{\partial T} + \left( \frac{k_j}{k} \cdot \nabla_X \right) A_j \right) + \sum_{k \neq j} a_{j,k} A_k = 0, \quad j = 1, \ldots, N, \]

- A system of semi-linear hyperbolic PDEs in a bounded domain in \( X \) subject to boundary and initial conditions.
Example: Two waves

\[ S = \{(0, 0, 0), (0, 0, -r)\}, \quad r \in \mathbb{N} \]

\[
i \left( \frac{\partial A_+}{\partial T} + \frac{\partial A_+}{\partial Z} \right) + \alpha A_- = \beta (|A_+|^2 + 2|A_-|^2) A_+, \]

\[
i \left( \frac{\partial A_-}{\partial T} - \frac{\partial A_-}{\partial Z} \right) + \alpha A_+ = \beta (2|A_+|^2 + |A_-|^2) A_- \]
Example: Four waves

\[ S = \{(0, 0, 0), (-p, -q, 0), (-p, 0, 0), (0, -q, 0)\}, (p, q) \in \mathbb{N}^2 \]

\[ i \left( \frac{\partial A_+}{\partial T} + \frac{\partial A_+}{\partial X} + \frac{\partial A_+}{\partial Y} \right) + \alpha A_- + \beta (B_+ + B_-) = 0, \]

\[ i \left( \frac{\partial A_-}{\partial T} - \frac{\partial A_-}{\partial X} - \frac{\partial A_-}{\partial Y} \right) + \alpha A_+ + \beta (B_+ + B_-) = 0, \]

\[ i \left( \frac{\partial B_+}{\partial T} + \frac{\partial B_+}{\partial X} - \frac{\partial B_+}{\partial Y} \right) + \beta (A_+ + A_-) + \alpha B_- = 0, \]

\[ i \left( \frac{\partial B_-}{\partial T} - \frac{\partial B_-}{\partial X} + \frac{\partial B_-}{\partial Y} \right) + \beta (A_+ + A_-) + \alpha B_+ = 0, \]
Problems in progress


Stationary transmission of four waves

- Stationary transmission

\[ A_\pm(X, T) = a_\pm(X + Y)e^{-i\Omega T}, \quad B_\pm(X, T) = b_\pm(X - Y)e^{-i\Omega T} \]

- The four-wave PDE problem:

\[
\begin{align*}
    i \frac{\partial a_+}{\partial x} + \Omega a_+ + \alpha a_- + \beta (b_+ + b_-) &= 0, \\
    -i \frac{\partial a_-}{\partial x} + \alpha a_+ + \Omega a_- + \beta (b_+ + b_-) &= 0, \\
    i \frac{\partial b_+}{\partial y} + \beta (a_+ + a_-) + \Omega b_+ + \alpha b_- &= 0, \\
    -i \frac{\partial b_-}{\partial y} + \beta (a_+ + a_-) + \alpha b_+ + \Omega b_- &= 0.
\end{align*}
\]
Stationary transmission of four waves

- Boundary-value problem on rectangle:

\[ \mathcal{D} = \{(x, y) : 0 \leq x \leq L, 0 \leq y \leq H\}, \]

subject to

\[ a_+(0, y) = \alpha_+(y), \quad a_-(L, y) = 0, \quad b_+(x, 0) = 0, \quad b_-(x, H) = 0 \]
Stationary transmission of four waves

○ Boundary-value problem on rectangle:

\[ D = \{(x, y) : 0 \leq x \leq L, \ 0 \leq y \leq H\}, \]

subject to

\[ a_+(0, y) = \alpha_+(y), \quad a_-(L, y) = 0, \quad b_+(x, 0) = 0, \quad b_-(x, H) = 0 \]

○ Gauge symmetry \((a_+, a_-, b_+, b_-) \mapsto e^{i \phi}(a_+, a_-, b_+, b_-)\) and the flux conservation

\[ \frac{\partial}{\partial x} \left( |a_+|^2 - |a_-|^2 \right) + \frac{\partial}{\partial y} \left( |b_+|^2 - |b_-|^2 \right) = 0. \]
Dispersion relation of stationary transmission

- Dispersion relation $\Omega = \Omega(K_x, K_y)$ for the double Fourier transform with $(K_x, K_y) \in \mathbb{R}^2$:

$$\left(\Omega^2 - \alpha^2 - K_x^2\right)\left(\Omega^2 - \alpha^2 - K_y^2\right) - 4\beta^2(\Omega - \alpha)^2 = 0.$$  

- When $\alpha^2 > 4\beta^2$, no real-valued roots $(K_x, K_y)$ exist for $\Omega = 0$ (stop band)

- When $\alpha^2 < 4\beta^2$, there exist two curves on the $(K_x, K_y)$-plane, which correspond to the real-valued roots (spectral band).

- The case $\Omega = 0$ is considered for simplicity.
Separation of variables:

\[ a_+(x, y) = u_+(x)w_a(y), \quad a_-(x, y) = u_-(x)w_a(y) \]
\[ b_+(x, y) = w_b(x)v_+(y), \quad b_-(x, y) = w_b(x)v_-(y), \]

where

\[ v_+(y) + v_-(y) = \mu w_a(y), \quad u_+(x) + u_-(x) = -\lambda w_b(x), \]

and \((\lambda, \mu)\) are arbitrary.

Separated boundary conditions:

\[ u_+(0) = 1, \quad u_-(L) = 0 \]
\[ v_+(0) = 0, \quad v_-(H) = 0. \]
Linear analysis of stationary transmission

- The inhomogeneous ODE system for \((u_+, u_-)\):

\[
\begin{pmatrix}
    i\partial_x & \alpha \\
    \alpha & -i\partial_x 
\end{pmatrix}
\begin{pmatrix}
    u_+ \\
    u_- 
\end{pmatrix}
= \beta \Gamma^{-1}
\begin{pmatrix}
    1 & 1 \\
    1 & 1 
\end{pmatrix}
\begin{pmatrix}
    u_+ \\
    u_- 
\end{pmatrix}
\]

- The homogeneous ODE system for \((v_+, v_-)\):

\[
\begin{pmatrix}
    i\partial_y & \alpha \\
    \alpha & -i\partial_y 
\end{pmatrix}
\begin{pmatrix}
    v_+ \\
    v_- 
\end{pmatrix}
= \beta \Gamma
\begin{pmatrix}
    1 & 1 \\
    1 & 1 
\end{pmatrix}
\begin{pmatrix}
    v_+ \\
    v_- 
\end{pmatrix},
\]

- \(\Gamma = \lambda/\mu\) is eigenvalue to be found from the homogeneous system
The spectrum of \( \Gamma = (\alpha^2 + k^2)/(2\alpha\beta) \) is defined by roots

\[
\left( \frac{k - \alpha}{k + \alpha} \right)^2 e^{-2ikH} = 1
\]

All roots are simple and located in the first and third open quadrants. For each root, there exists a unique solution for \((u_+, u_-)\).
The set of eigenfunctions $v_j(y) = v_+(y) + v_-(y)$ for roots $k_j$ is orthogonal with respect to

$$\int_0^H v_i(y)v_j(y)dy = \delta_{i,j}$$
The set of eigenfunctions $v_j(y) = v_+(y) + v_-(y)$ for roots $k_j$ is orthogonal with respect to

$$\int_0^H v_i(y)v_j(y)\,dy = \delta_{i,j}$$

Any $C^1([0, H])$ function $\alpha_+(y)$ is uniquely represented by the series of eigenfunctions,

$$\alpha_+(y) = \sum_{\text{all } k_j} c_j v_j(y), \quad c_j = \int_0^H \alpha_+(y)v_j(y)\,dy,$$

which converges uniformly on $0 < y < H$.

Explicit Fourier series solutions for $a_\pm(x, y)$ and $b_\pm(x, y)$ follow from the method of separation of variables.
Example: constant incident wave

○ Boundary conditions

\[ a_+(0, y) = 1, \quad a_-(L, y) = 0, \quad b_+(x, 0) = 0, \quad b_-(x, H) = 0 \]

○ Coefficients of decomposition

\[ c_j = \frac{4i\alpha}{k_j[H(k_j^2 - \alpha^2) + 2i\alpha]} \]

○ The decomposition in series of eigenfunctions,

\[ 1 = \sum_{\text{all } k_j} c_j v_j(y), \quad 0 < y < H. \]
Low transmittance and moderate diffractance

Solution surfaces for $\alpha = 1$, $\beta = 0.25$, $L = H = 20$, and $\alpha_+ = 1$. 
High transmittance and diffractance

Solution surfaces for $\alpha = 1$, $\beta = 0.75$, $L = H = 20$, and $\alpha_+ = 1$. 
Transmission characteristics

- Transmittance
  \[ T = \frac{\mathcal{I}_{\text{out}}}{\mathcal{I}_{\text{in}}}, \quad \mathcal{I}_{\text{out}} = \int_0^H |a_+(L, y)|^2 dy \]

- Reflectance
  \[ R = \frac{\mathcal{I}_{\text{ref}}}{\mathcal{I}_{\text{in}}}, \quad \mathcal{I}_{\text{ref}} = \int_0^H |a_-(0, y)|^2 dy \]

- Diffractance
  \[ D = \frac{\mathcal{I}_{\text{dif}}}{\mathcal{I}_{\text{in}}}, \quad \mathcal{I}_{\text{dif}} = \int_0^L \left(|b_+(x, H)|^2 + |b_-(x, 0)|^2\right) dx \]

- Balance identity:
  \[ R + T + D = 1 \]
Low transmittance and moderate diffractance

Transmission coefficients for $\alpha = 1$, $\beta = 0.25$, $L = H = 20$, and $\alpha_+ = 1$. 
Transmission coefficients for $\alpha = 1$, $\beta = 0.75$, $L = H = 20$, and $\alpha_+ = 1$. 
General symmetric 1-D coupled-mode system

\[
\begin{align*}
&i(u_t + u_x) + v = \partial_{\bar{u}} W(u, \bar{u}, v, \bar{v}) \\
&i(v_t - v_x) + u = \partial_{\bar{v}} W(u, \bar{u}, v, \bar{v})
\end{align*}
\]

- $W$ is invariant with respect to the gauge transformation: 
  \((u, v) \mapsto e^{i\alpha}(u, v), \text{ for all } \alpha \in \mathbb{R}\)
- $W$ is symmetric with respect to the interchange: 
  \((u, v) \mapsto (v, u)\)
- $W$ is analytic in its variables near \(u = v = 0\), such that \(W = O(4)\)
- The quartic part of the potential function \(W\) is given by
  \[
  W = \frac{a_1}{2}(|u|^4 + |v|^4) + a_2 |u|^2 |v|^2 + a_3 (|u|^2 + |v|^2)(v\bar{u} + \bar{v}u) + \frac{a_4}{2} (v\bar{u} + \bar{v}u)^2
  \]
  where \((a_1, a_2, a_3, a_4)\) are parameters.
General characterization of 1-D gap solitons

\[
\begin{align*}
    u_{st}(x, t) &= u_0(x + s)e^{i\omega t + i\theta} \\
    v_{st}(x, t) &= v_0(x + s)e^{i\omega t + i\theta}
\end{align*}
\]

- \((s, \theta) \in \mathbb{R}^2\) are arbitrary parameters and \(-1 < \omega < 1\)
- If \(|u_0|, |v_0| \to 0\) as \(|x| \to \infty\), then \(u_0 = \bar{v}_0\)
- Analytical expressions are available for homogeneous functions \(W\)
  \[
  u_0 = \frac{\sqrt{2(1 - \omega)}}{(\cosh \beta x + i \sqrt{\mu} \sinh \beta x)}, \quad \mu = \frac{1 - \omega}{1 + \omega}, \quad \beta = \sqrt{1 - \omega^2}
  \]
- Explicit gap solitons are stationary solutions. Traveling gap solitons are only available implicitly except few particular examples.
Linearized stability problem for 1-D gap solitons

- Standard linearization, e.g.

\[ u(x, t) = e^{i\omega t} \left( u_0(x) + U_1(x)e^{\lambda t} \right) \]

- Eigenvalue problem

\[ H_{\omega} U = i\lambda \sigma U, \]

where

\[ H_{\omega} = \left( D(\partial_x) + D^2W[u_0(x)] \right) \]

and \( D(\partial_x) \) is the four-component Dirac operator in 1-D

\[
D = \begin{pmatrix}
\omega - i\partial_x & 0 & -1 & 0 \\
0 & \omega + i\partial_x & 0 & -1 \\
-1 & 0 & \omega + i\partial_x & 0 \\
0 & -1 & 0 & \omega - i\partial_x
\end{pmatrix}
\]
There exists an orthogonal similarity transformation $S$ in $\mathbb{C}^4$:

$$S^{-1}H_\omega S = \begin{pmatrix} H_+ & 0 \\ 0 & H_- \end{pmatrix}, \quad S^{-1}\sigma H_\omega S = \sigma \begin{pmatrix} 0 & H_- \\ H_+ & 0 \end{pmatrix}$$

where $H_\pm$ are two-by-two Dirac operators in 1-D

$$H_\pm = \begin{pmatrix} \omega - i\partial_x & \mp 1 \\ \mp 1 & \omega + i\partial_x \end{pmatrix} + \begin{pmatrix} 2|u_0|^2 & u_0^2 \\ \bar{u}_0^2 & 2|u_0|^2 \end{pmatrix},$$
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The linearized stability problem takes the 2-by-2 form:

$$\sigma_3H_-\sigma_3H_+V_1 = \gamma V_1, \quad \sigma_3H_+\sigma_3H_-V_2 = \gamma V_2,$$

where $\gamma = -\lambda^2$. 
Numerical results on unstable eigenvalues

- Chebyshev interpolation with $N$ polynomials

- The advantages of block-diagonalization

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<th>$T_{\text{full}}$</th>
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<td>2500</td>
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<td>$12.723 \cdot 10^3$</td>
</tr>
</tbody>
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- Parameter continuation in $\omega$ on parallel processors
Eigenvalues and instability bifurcations
Summary

*Obtained results:*

- Well-posedness of the radiation boundary-value problem
- Analytical solutions for linear stationary transmission
- Numerical approximations of eigenvalues of 1-D stability problems
Summary

**Obtained results:**

- Well-posedness of the radiation boundary-value problem
- Analytical solutions for linear stationary transmission
- Numerical approximations of eigenvalues of 1-D stability problems

**Open problems:**

- Rigorous derivation of coupled-mode equations
- Bifurcations of solutions for nonlinear stationary transmission
- Numerical modeling of gap solitons in 2-D coupled-mode equations