Photonic crystals, coupled-mode equations, and gap solitons

Dmitry Pelinovsky
Institute of Mathematics, University of Stuttgart, Germany
Department of Mathematics, McMaster University, Canada

References:

D.Agueev, D.P., SIAM J. Appl. Math. 65, 1101 (2005)
M.Chugunova, D.P., SIAM J.Appl.Dyn.Syst. 5, 66 (2006)
D.P., G. Schneider, in preparation (2007)

Colloquium in Applied Mathematics, ETH Zurich, November 29, 2006

Introduction

Motivations

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

Plan of the talk

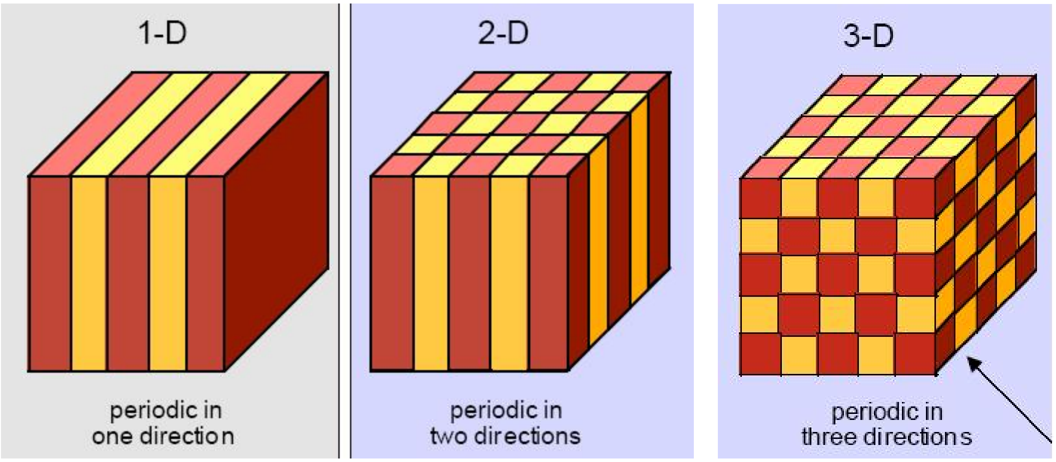
1 Formal reductions of Maxwell equations to coupled-mode equations

2 Well-posedness of linear boundary value PDE problems (2-D)

3 Linearized stability of gap solitons (1-D)

4 Justification of coupled-mode equations (1-D)

Photonic crystals in 1-D, 2-D, and 3-D

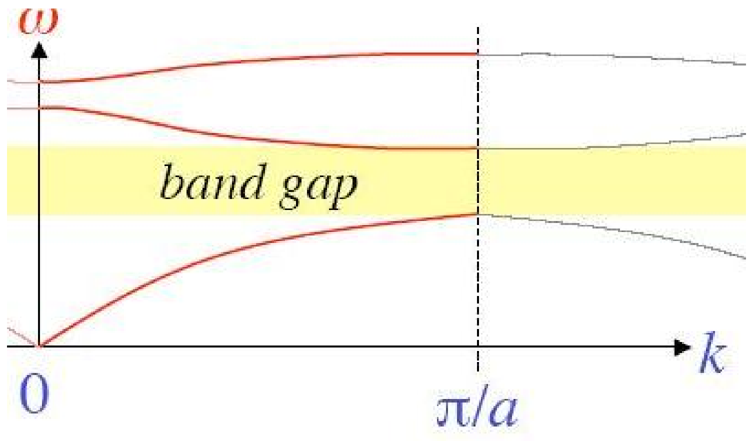


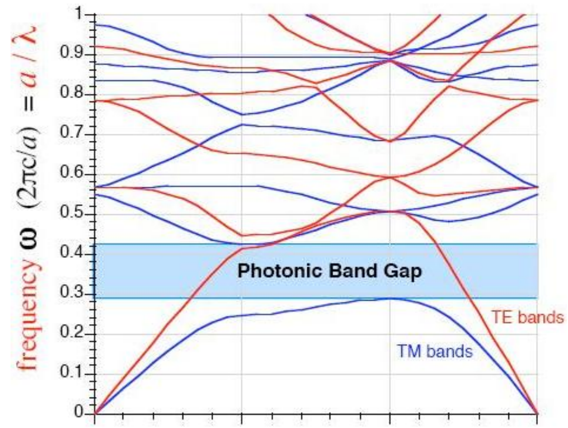
- Linear Maxwell equations

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

- 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



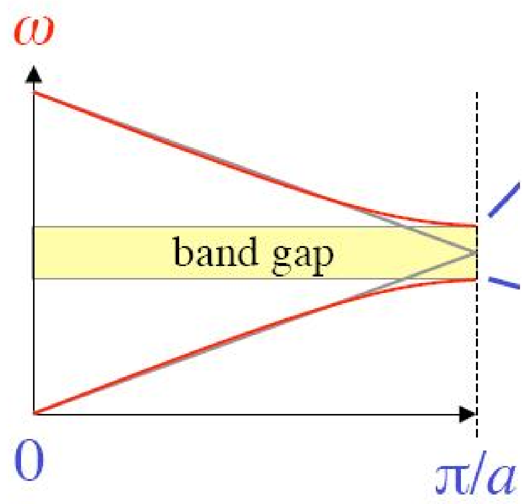


- Existence of Bloch waves for arbitrary smooth $n(\mathbf{x})$ (Kuchment, 1993)

$$\mathbf{E}(\mathbf{x}, t) = \mathbf{\Psi}(\mathbf{x}) e^{i(\mathbf{k}\cdot\mathbf{x} - \omega t)},$$

- $\mathbf{k} = (k_x, k_y, k_z)$ is the wave vector
- $\omega = \omega(\mathbf{k})$ is the wave frequency
- $\mathbf{\Psi}(\mathbf{x} + \mathbf{a}) = \mathbf{\Psi}(\mathbf{x})$ is the periodic envelope

Low-contrast 3-D photonic crystals



- Small periodicity of the refractive index

$$n(\mathbf{x}) = 1 + \epsilon \sum_{(n,m,l)\in\mathbb{Z}^3} \alpha_{n,m,l} e^{i(n\mathbf{k}_1 + m\mathbf{k}_2 + l\mathbf{k}_3)\mathbf{x}}$$

- ϵ is small parameter
- $\mathbf{k}_{1,2,3}$ are reciprocal lattice vectors

Concept of resonances

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

$$\mathbf{k} \cdot \mathbf{e}_{\mathbf{k}} = 0, \qquad \omega^2 = c^2 \left(k_x^2 + k_y^2 + k_z^2 \right)$$

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

$$\mathbf{k}_{\text{out}}^{(n,m,l)} = \mathbf{k}_{\text{in}} + n\mathbf{k}_1 + m\mathbf{k}_2 + l\mathbf{k}_3, \quad (n, m, l) \in \mathbb{Z}^3.$$

- The transmitted waves are resonant to the incident wave if

$$\omega(\mathbf{k}_{\text{out}}^{(n,m,l)}) = \omega(\mathbf{k}_{\text{in}}) \quad \text{for some } (n, m, l) \in \mathbb{Z}^3$$

Resonances in 3-D cubic crystals

- 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 $a > 0$.

- The set of resonances in low-contrast cubic crystal

$$S = \Big\{ (n,m,l) \in \mathbb{Z}^3 : \; n(n+p) + m(m+q) + l(l+r) = 0 \Big\}$$

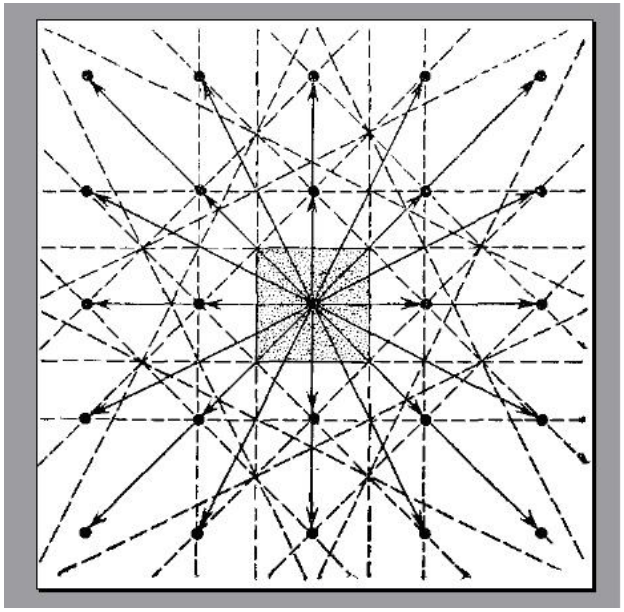
where $(p,q,r) \in \mathbb{R}^3$ in $\mathbf{k}_{\text{in}} = \frac{\pi}{a}(p,q,r)$.

- 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 ϵ:

$$\mathbf{E}(\mathbf{x},t) = \mathbf{E}_0(\mathbf{x},t) + \epsilon \mathbf{E}_1(\mathbf{x},t) + \mathrm{O}(\epsilon^2).$$

- Bloch waves are plane waves for $\epsilon = 0$:

$$\mathbf{E}_0(\mathbf{x},t) = \sum_{j=1}^{N} A_j(\mathbf{X},T)\mathbf{e}_{\mathbf{k}_j} e^{i\left(\mathbf{k}_j \mathbf{x} - \omega t\right)},$$

- $(\mathbf{X},T)$ are slow normalized variables:

$$\mathbf{X} = \frac{\epsilon \mathbf{x}}{k}, \quad T = \frac{\epsilon t}{\omega}$$

Formal derivation of coupled-mode equations

- Inhomogeneous equation with resonant terms:

$$\nabla^2 \mathbf{E}_1 - \frac{n_0^2}{c^2}\frac{\partial^2 \mathbf{E}_1}{\partial t^2} = \mathbf{F}(\mathbf{E}_0),$$

- Solvability conditions from orthogonality of $\mathbf{F}(\mathbf{E}_0)$ to resonant terms

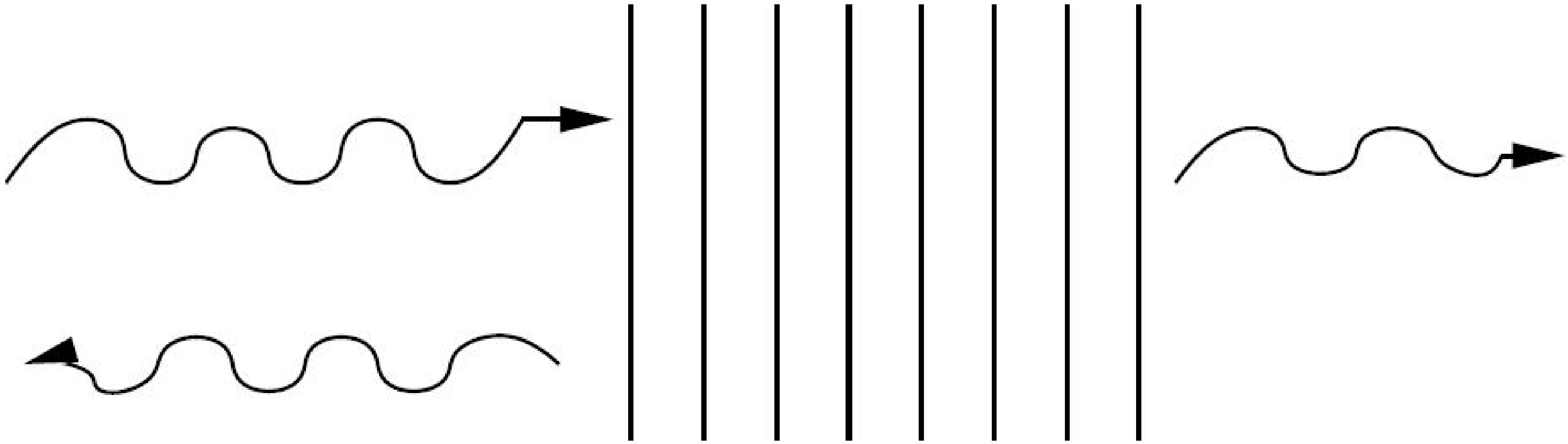
$$i\left(\frac{\partial A_j}{\partial T} + \left(\frac{\mathbf{k}_j}{k}\cdot\nabla_X\right)A_j\right) + \sum_{k\neq j} a_{j,k}A_k = 0, \qquad j = 1, ..., N,$$

- A system of semi-linear hyperbolic PDEs in a bounded domain in $\mathbf{X}$ subject to boundary and initial conditions.

Example: Two waves

$S = \{(0,0,0),(0,0,-r)\}$, $r \in \mathbb{N}$

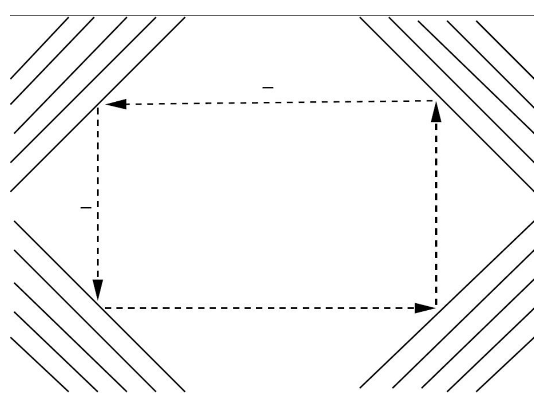
$$\begin{aligned} i\left(\frac{\partial A_+}{\partial T} + \frac{\partial A_+}{\partial Z}\right) + \alpha A_- &= \beta(|A_+|^2 + 2|A_-|^2)A_+, \\ i\left(\frac{\partial A_-}{\partial T} - \frac{\partial A_-}{\partial Z}\right) + \alpha A_+ &= \beta(2|A_+|^2 + |A_-|^2)A_- \end{aligned}$$



Example: Four waves

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

$$\begin{aligned}
i\left(\frac{\partial A_+}{\partial T} + \frac{\partial A_+}{\partial X} + \frac{\partial A_+}{\partial Y}\right) + \alpha A_- + \beta\,(B_+ + B_-) &= 0,\\
i\left(\frac{\partial A_-}{\partial T} - \frac{\partial A_-}{\partial X} - \frac{\partial A_-}{\partial Y}\right) + \alpha A_+ + \beta\,(B_+ + B_-) &= 0,\\
i\left(\frac{\partial B_+}{\partial T} + \frac{\partial B_+}{\partial X} - \frac{\partial B_+}{\partial Y}\right) + \beta\,(A_+ + A_-) + \alpha B_- &= 0,\\
i\left(\frac{\partial B_-}{\partial T} - \frac{\partial B_-}{\partial X} + \frac{\partial B_-}{\partial Y}\right) + \beta\,(A_+ + A_-) + \alpha B_+ &= 0,
\end{aligned}$$



Related Mathematical Problems

- Well-posedness of the Sommerfeld (radiation) boundary-value problem for stationary transmission (D.Agueev, M.Sc. thesis, 2004)

- Existence, stability and propagation of gap solitons, extensions to the relativistic Dirac equations (M. Chugunova, Ph.D. thesis, in progress)

- Rigorous justification of the nonlinear coupled-mode equations for gap solitons (G. Schneider, in progress)

- Derivation of coupled-mode equations for highly-contrast materials with narrow gaps (open project)

Project 1 : well-posedness of transmission proble

- Stationary transmission of four waves

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

- The four-wave PDE problem:

$$\begin{aligned}
i\frac{\partial a_+}{\partial x} + \Omega a_+ + \alpha a_- + \beta\left(b_+ + b_-\right) &= 0,\\
-i\frac{\partial a_-}{\partial x} + \alpha a_+ + \Omega a_- + \beta\left(b_+ + b_-\right) &= 0,\\
i\frac{\partial b_+}{\partial y} + \beta\left(a_+ + a_-\right) + \Omega b_+ + \alpha b_- &= 0,\\
-i\frac{\partial b_-}{\partial y} + \beta\left(a_+ + a_-\right) + \alpha b_+ + \Omega b_- &= 0.
\end{aligned}$$

Stationary transmission of four waves

- Boundary-value problem on rectangle:

$$\mathcal{D} = \{(x, y):\ 0 \le x \le L,\ 0 \le y \le H\},$$

subject to

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

Dispersion relation of stationary transmission

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

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

- 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.

Linear analysis of stationary transmission

- Separation of variables:

$$a_+(x,y) = u_+(x)w_a(y), \qquad a_-(x,y) = u_-(x)w_a(y)$$
$$b_+(x,y) = w_b(x)v_+(y), \qquad b_-(x,y) = w_b(x)v_-(y),$$

where

$$v_+(y) + v_-(y) = \mu w_a(y), \qquad u_+(x) + u_-(x) = -\lambda w_b(x),$$

and (λ, μ) 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_-):

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

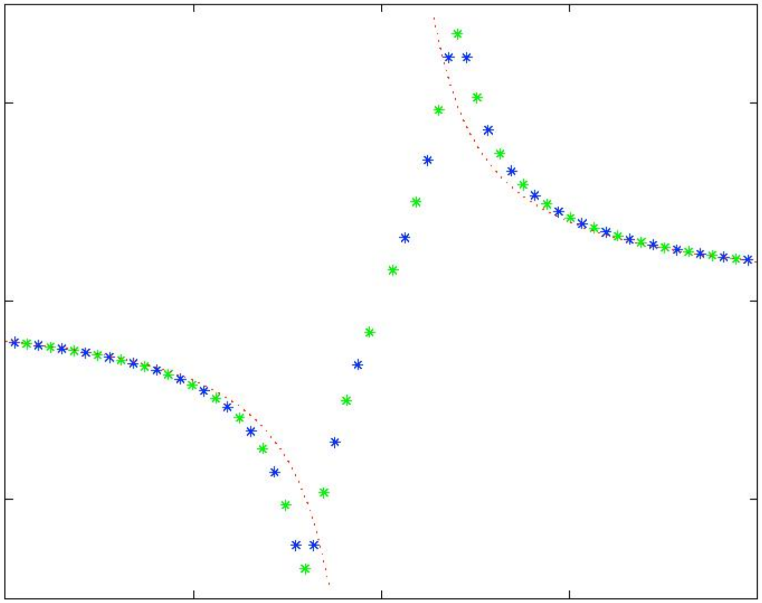
- $\Gamma = \lambda/\mu$ is eigenvalue to be found from the homogeneous system

Linear analysis of stationary transmission

- 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_-).



Linear analysis of stationary transmission

- 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,

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

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

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

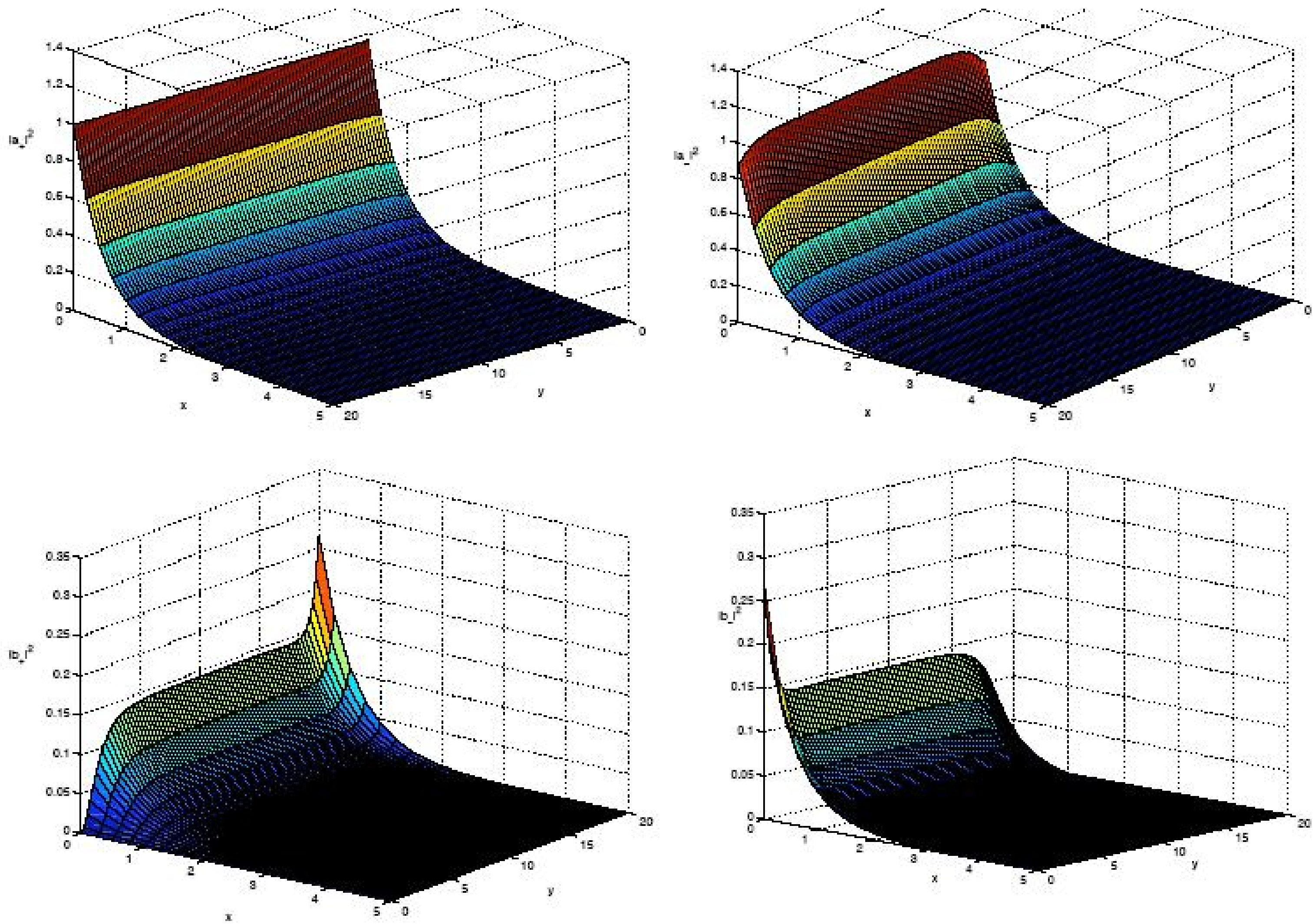
- Coefficients of decomposition

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

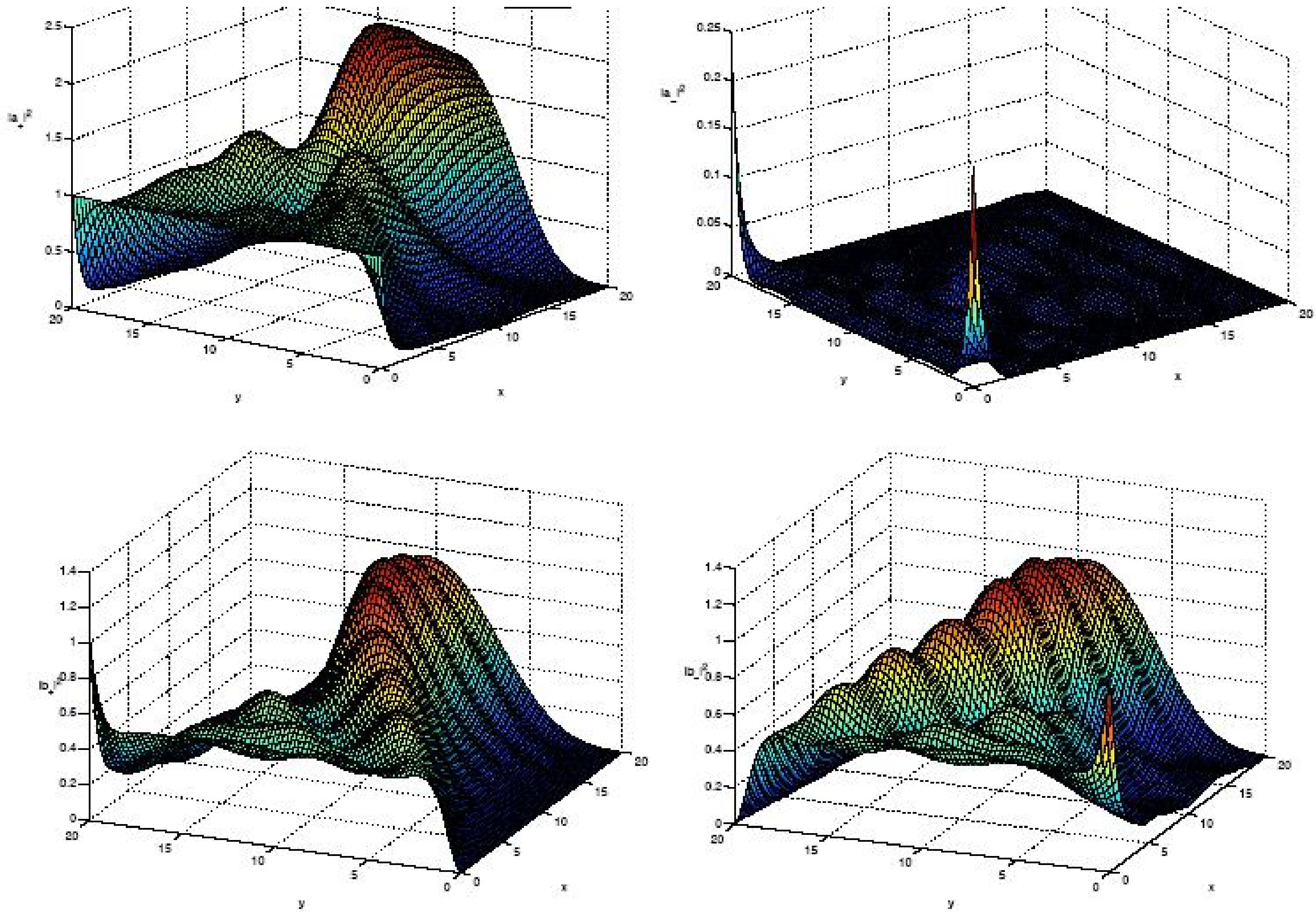
- The decomposition in series of eigenfunctions,

$$1 = \sum_{\text{all } k_j} c_j v_j(y), \qquad 0 < y < H.$$

Low transmittance and moderate diffractance



Solution surfaces for the stop band.



Solution surfaces for the spectral band.

Project 2: existence and stability of gap solitons

General symmetric 1-D coupled-mode system:

$$\begin{cases} i(u_t + u_x) + v = \partial_{\bar{u}} W(u, \bar{u}, v, \bar{v}) \\ i(v_t - v_x) + u = \partial_{\bar{v}} W(u, \bar{u}, v, \bar{v}) \end{cases}$$

- W is invariant with respect to the gauge transformation: $(u, v) \mapsto e^{i\alpha}(u, v)$, 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

Stationary solutions of the coupled-mode system:

$$\begin{cases} u_{\text{st}}(x,t) = u_0(x+s)e^{i\omega t + i\theta} \\ v_{\text{st}}(x,t) = v_0(x+s)e^{i\omega t + i\theta} \end{cases}$$

- $(s,\theta) \in \mathbb{R}^2$ 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

$$u_0 = \frac{\sqrt{2(1-\omega)}}{(\cosh \beta x + i\sqrt{\mu} \sinh \beta x)}, \qquad \mu = \frac{1-\omega}{1+\omega}, \quad \beta = \sqrt{1-\omega^2}$$

- Explicit gap solitons are *stationary* solutions. *Traveling* gap solitons are only available implicitly except few special 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

$$H_\omega \mathbf{U} = i\lambda\sigma\mathbf{U}, \quad \mathbf{U} \in \mathbb{C}^4,$$

where

$$H_\omega = D(\partial_x) + D^2 W[u_0(x)]$$

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

$$D = \begin{pmatrix} \omega - i\partial_x & 0 & -1 & 0 \\ 0 & \omega + i\partial_x & 0 & -1 \\ -1 & 0 & \omega + i\partial_x & 0 \\ 0 & -1 & 0 & \omega - i\partial_x \end{pmatrix}$$

Block-diagonalization of the stability problem

- There exists an orthogonal similarity transformation S in $\mathbb{C}^4$:

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

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

$$H_\pm = \begin{pmatrix} \omega - i\partial_x & \mp 1 \\ \mp 1 & \omega + i\partial_x \end{pmatrix} + \begin{pmatrix} 2|u_0|^2 & u_0^2 \\ \bar{u}_0^2 & 2|u_0|^2 \end{pmatrix},$$

- The linearized stability problem takes the 2-by-2 form:

$$\sigma_3 H_- \sigma_3 H_+ \mathbf{V}_1 = \gamma \mathbf{V}_1, \qquad \sigma_3 H_+ \sigma_3 H_- \mathbf{V}_2 = \gamma \mathbf{V}_2,$$

where $\gamma = -\lambda^2$.

Numerical results on unstable eigenvalues

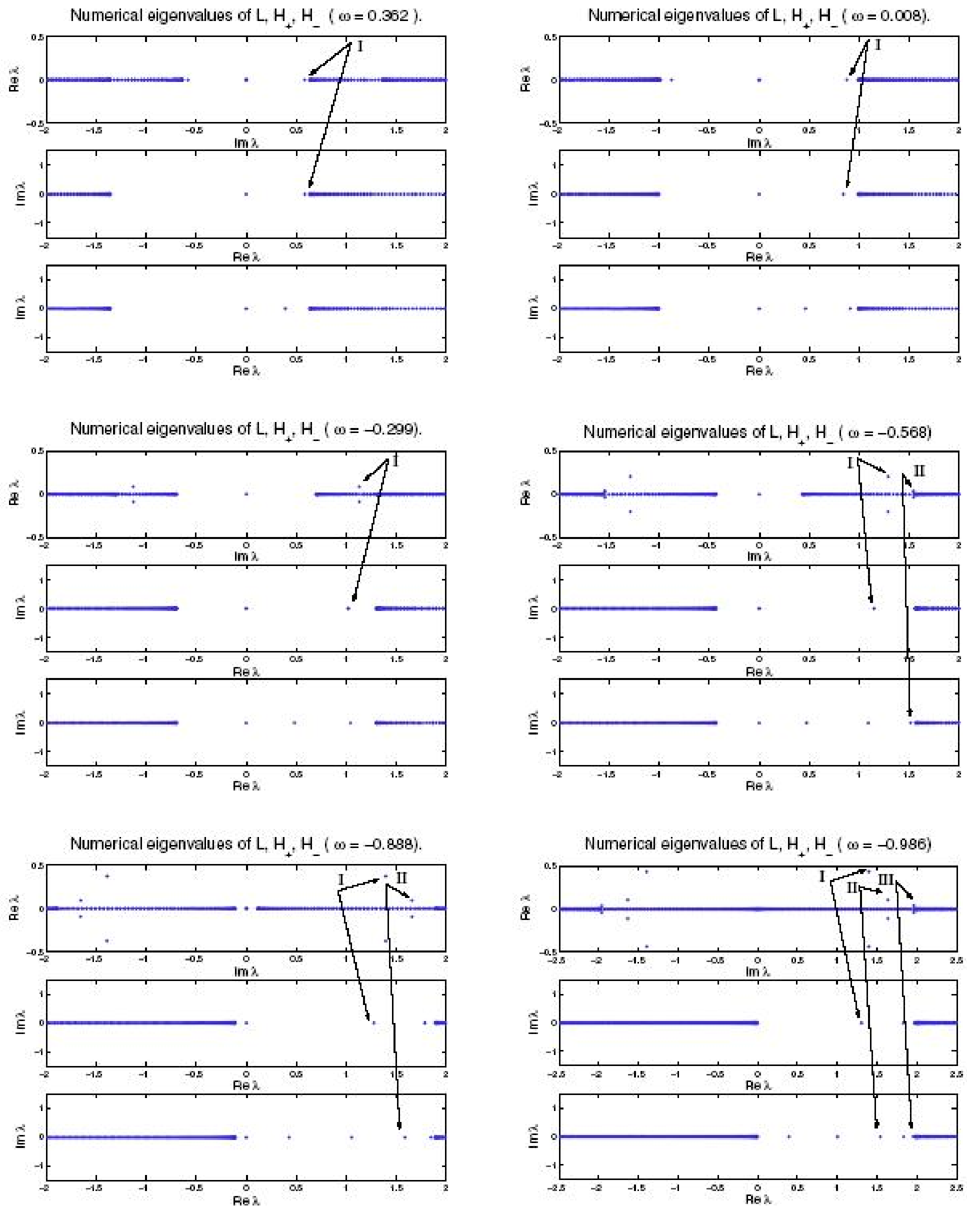
- Chebyshev interpolation with N polynomials

- The advantages of block-diagonalization

N	T_{block}	T_{full}
100	1.656	1.984
200	11.219	12.921
400	130.953	207.134
800	997.843	$1.583 \cdot 10^3$
1200	$3.608 \cdot 10^3$	$6.167 \cdot 10^3$
2500	$7.252 \cdot 10^3$	$12.723 \cdot 10^3$

- Parameter continuation in ω on parallel processors

Eigenvalues and instability bifurcations



Project 3: justification of coupled-mode system

- A simple (toy) problem:

$$\left(\omega^2 + \partial_x^2 + \epsilon W(x)\right) U(x) = \sigma |U|^2 U,$$

where ϵ is small parameter, $\sigma = \pm 1$, $W(x+2\pi) = W(x)$ is real-valued, and $U(x)$ is complex-valued.

- Let $W(x) = \sum_{m\in\mathbb{Z}} e^{imx}$ and $U(x) = \sum_{m\in\mathbb{Z}} u_m e^{imx}$ in the space

$$\|\mathbf{U}\|^2_{l^2_s(\mathbb{Z})} = \sum_{m\in\mathbb{Z}} (1+m^2)^s |u_m|^2 < \infty,$$

for some $s \geq 0$. The Fourier representation corresponds to the periodic solutions $U(x+2\pi) = U(x)$.

- The differential problem is equivalent to the nonlinear lattice system

$$\mathcal{L}\mathbf{U} = -\epsilon \mathbf{W} \star \mathbf{U} + \sigma \mathbf{U} \star \bar{\mathbf{U}} \star \mathbf{U},$$

where $\star$ is the convolution operator and $\mathcal{L}$ is diagonal operator with entries $\mathcal{L}_{m,m} = \omega^2 - m^2$ on $m \in \mathbb{Z}$.

Fixed-point iterations

- The convolution operators map $l^2_s(\mathbb{Z})$ to itself for $s > \frac{1}{2}$.

- When $\omega \in \mathbb{R}\backslash\mathbb{Z}$, the nonlinear lattice system has a unique trivial solution $\mathbf{U} = \mathbf{0}$ in a local neighborhood of $\epsilon = 0$.

- When $\omega^2 = n^2 + \epsilon\Omega$ for some $n \in \mathbb{Z}$, the nonlinear lattice system has a non-trivial solution for $\mathbf{U} \in l^2_s(\mathbb{Z})$ with $s > \frac{1}{2}$ in a local neighborhood of $\mathbf{U} = \mathbf{0}$ and $\epsilon = 0$ if and only if there exists a nontrivial solution for $(a, b) \in \mathbb{C}^2$ of the bifurcation equations

$$\begin{aligned} (\Omega + w_0)a + w_n b - \sigma(|a|^2 + 2|b|^2)a &= \epsilon A_\epsilon(a, b) \\ (\Omega + w_0)b + w_{-n} a - \sigma(2|a|^2 + |b|^2)b &= \epsilon B_\epsilon(a, b), \end{aligned}$$

where

$$\max\{|A_\epsilon|, |B_\epsilon|\} \leq C(|a| + |b|).$$

The system of bifurcation equations is the coupled-mode system for stationary periodic solutions.

Methods of analysis

- Lyapunov–Schmidt reductions

$$\mathrm{Ker}(\mathcal{L}) = \mathrm{Span}\,(\mathbf{e}_n, \mathbf{e}_{-n}) \subset l_s^2(\mathbb{Z}),$$

  such that

$$\mathbf{U} = \sqrt{\epsilon}\,[a\mathbf{e}_n + b\mathbf{e}_{-n} + \mathbf{g}]$$

  and

$$\mathbf{g} \in \mathrm{Ker}(\mathcal{L})^{\perp} = \{\mathbf{g} \in l_s^2(\mathbb{Z}') : \quad g_n = g_{-n} = 0\}.$$

- Operator $(\mathcal{L} + \epsilon\mathbf{W}\star)$ is continuously invertible on $\mathbf{g} \in \mathrm{Ker}(\mathcal{L})^{\perp}$, such that there exists a unique map $\mathbf{g}_\epsilon = \epsilon\mathbf{G}_\epsilon(a,b)$, where

$$\|\mathbf{G}_\epsilon\|_{l_s^2} \leq C(|a| + |b|).$$

- Bifurcation equations follow from projection of the lattice system to $\mathrm{Ker}(\mathcal{L})$.

Extensions

- Bifurcations of antiperiodic solutions $U(x+2\pi) = -U(x)$ occurs at $\omega = \frac{n}{2}$ for any $n \in \mathbb{Z}$.

- The method can be extended for gap soliton solutions in

$$\|U(x)\|^2_{H^s(\mathbb{R})} = \int_{\mathbb{R}} \left(1+k^2\right)^s |\hat{U}(k)|^2 dk < \infty$$

  for $\frac{1}{2} < s < \frac{3}{2}$.

- In two dimensions, bifurcations of periodic and antiperiodic solutions can be proved with this technique in $l^2_s(\mathbb{Z})$ with $s > 1$. Bifurcations of 2D gap soliton solutions can not be proved as the bounds $s > 1$ and $s < 1$ become contradictory.

- Time evolution of gap solitons can be studied on finite time intervals as in H. Uecker & G. Schneider (2001)

Summary

Obtained results:

- **Well-posedness of the radiation boundary-value problem**
- **Analytical solutions for linear stationary transmission**
- **Approximations of eigenvalues of stability problems**
- **Full analysis of stability and bifurcations of gap solitons**
- **Rigorous justification of coupled-mode equations**

Open problems:

- **Bifurcations of nonlinear stationary solutions**
- **Modeling of gap solitons in 2-D coupled-mode equations**
- **Reductions of Maxwell equations beyond the coupled-mode theory**