

Photonic crystals, coupled-mode equations, and gap solitons

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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

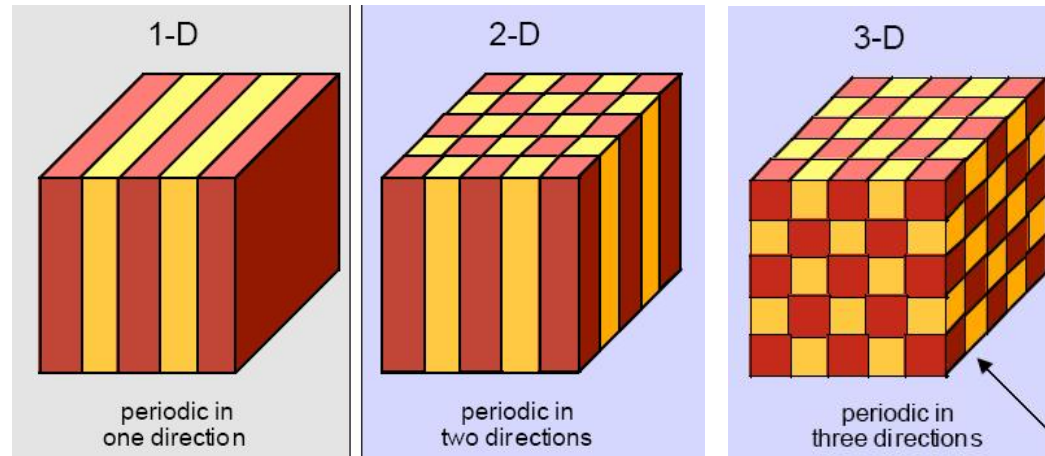
■ *Motivations*

- 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

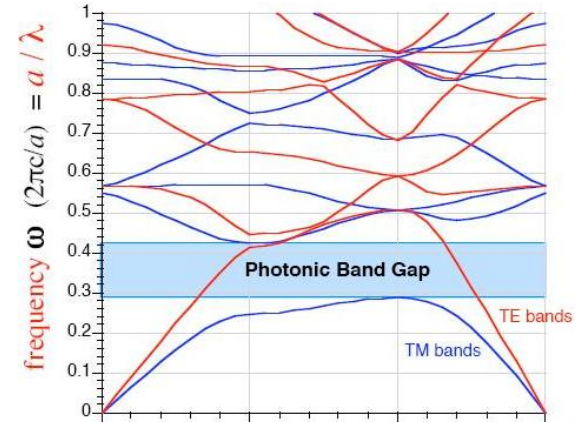
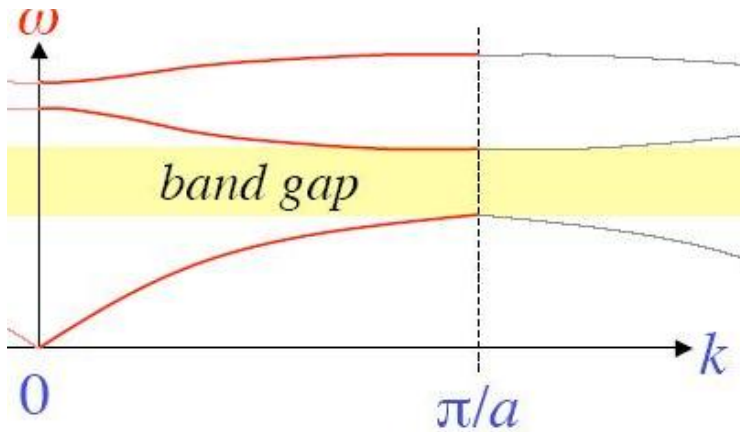


- Linear Maxwell equations

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

- 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

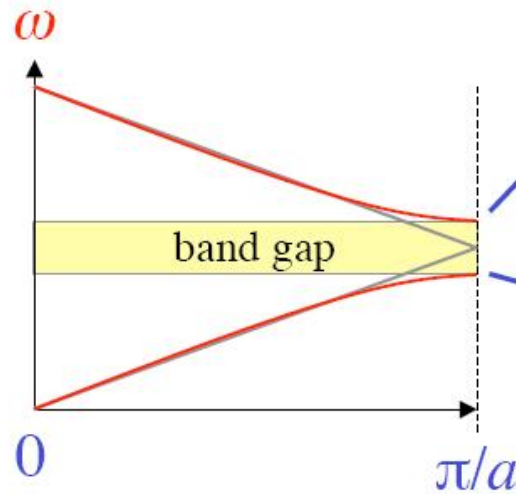


- Existence of Bloch waves for arbitrary smooth $n(\mathbf{x})$ (Kuchment, 1993)

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

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

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

- *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

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

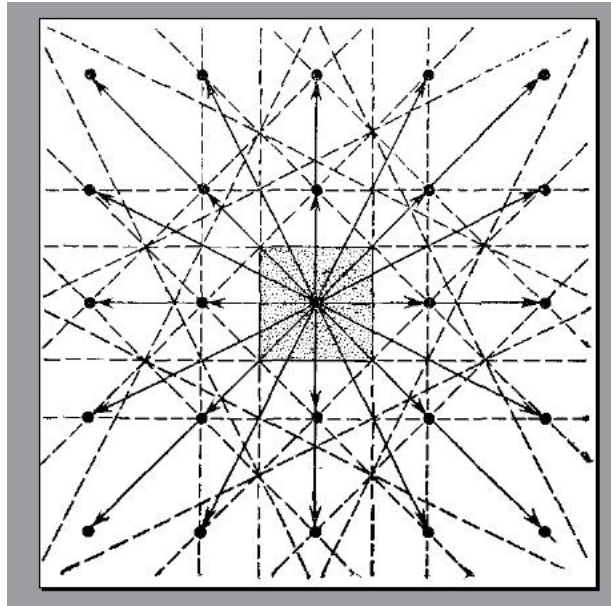
where $(p, q, r) \in \mathbb{R}^3$ in $\mathbf{k}_{\text{in}} = \frac{\pi}{a}(p, q, r)$.

- 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 :

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

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

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

- (\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

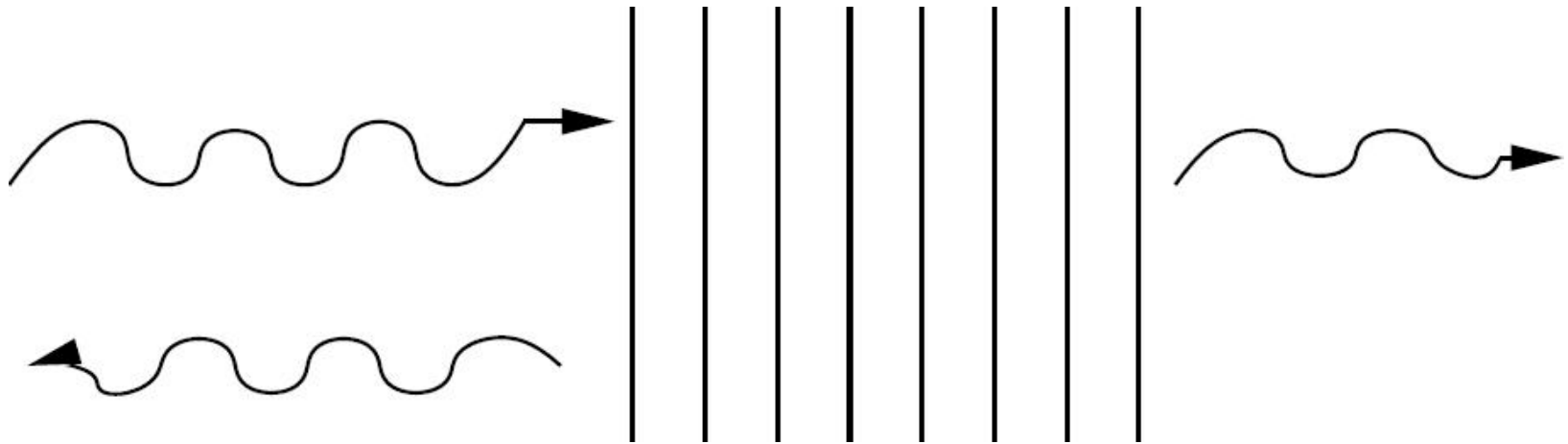
$$i \left(\frac{\partial A_j}{\partial T} + \left(\frac{\mathbf{k}_j}{k} \cdot \nabla_X \right) A_j \right) + \sum_{k \neq j} a_{j,k} A_k = 0, \quad j = 1, \dots, N,$$

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

Example: Two waves

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

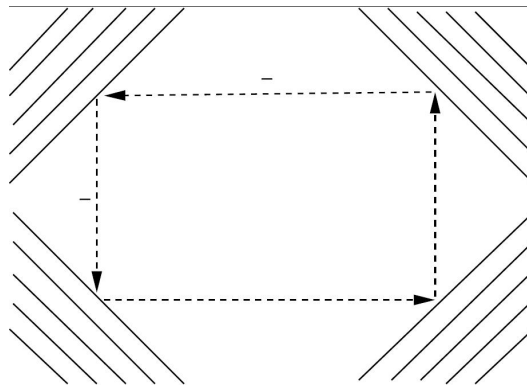
$$i \left(\frac{\partial A_+}{\partial T} + \frac{\partial A_+}{\partial Z} \right) + \alpha A_- = \beta (|A_+|^2 + 2|A_-|^2) A_+,$$
$$i \left(\frac{\partial A_-}{\partial T} - \frac{\partial A_-}{\partial Z} \right) + \alpha A_+ = \beta (2|A_+|^2 + |A_-|^2) A_-$$



Example: Four waves

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

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



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 problem

- 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:

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

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

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

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:

$$\begin{aligned}a_+(x, y) &= u_+(x)w_a(y), & a_-(x, y) &= u_-(x)w_a(y) \\ b_+(x, y) &= w_b(x)v_+(y), & b_-(x, y) &= w_b(x)v_-(y),\end{aligned}$$

where

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

and (λ, μ) are arbitrary.

- Separated boundary conditions:

$$\begin{aligned}u_+(0) &= 1, & u_-(L) &= 0 \\ v_+(0) &= 0, & v_-(H) &= 0.\end{aligned}$$

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_-) :

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

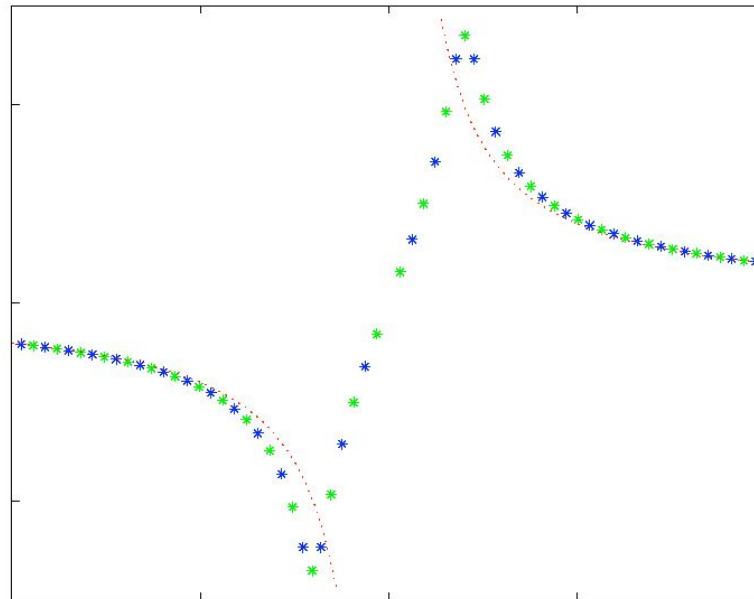
- $\Gamma = \lambda/\mu$ is eigenvalue to be found from the homogeneous system

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,

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

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

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

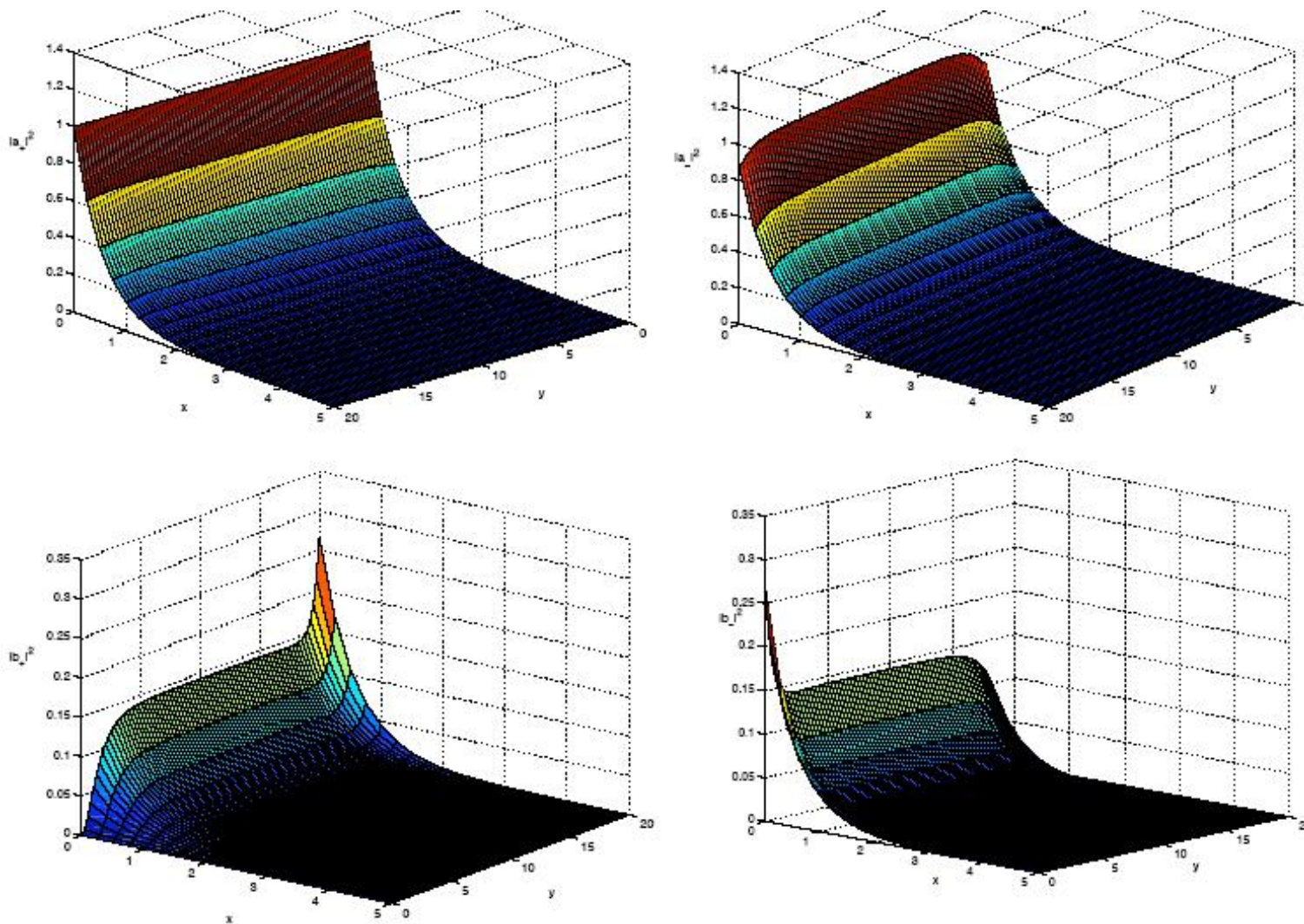
- Coefficients of decomposition

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

- The decomposition in series of eigenfunctions,

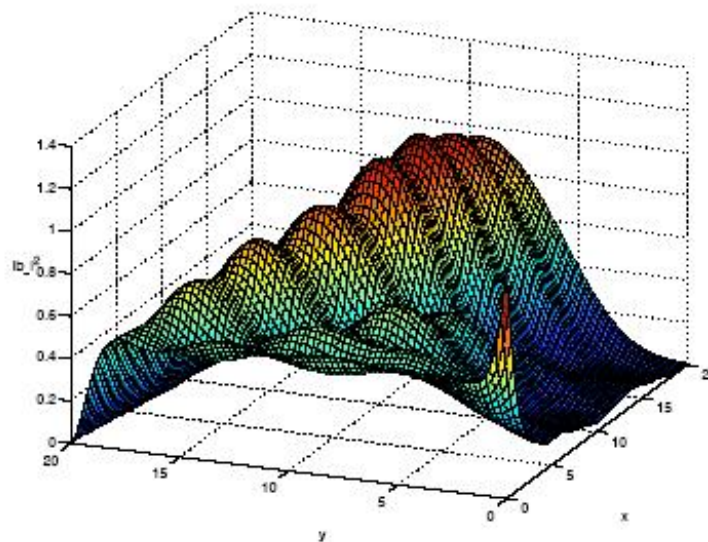
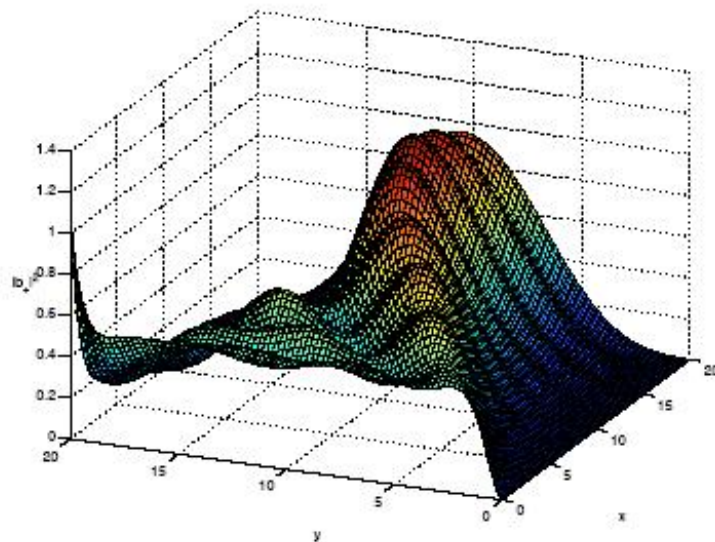
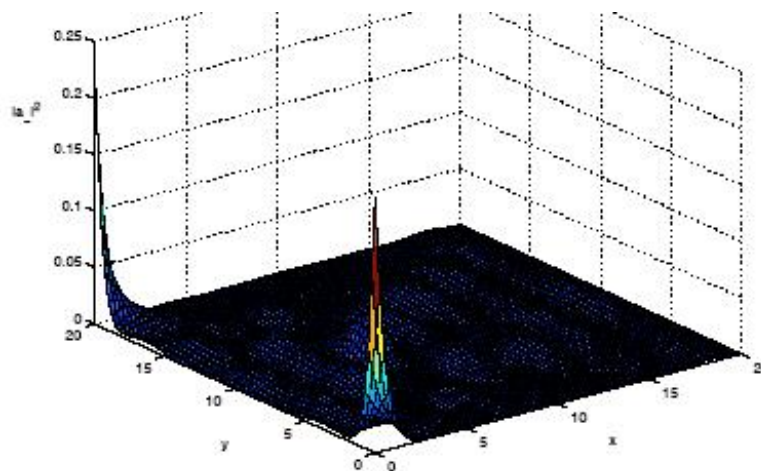
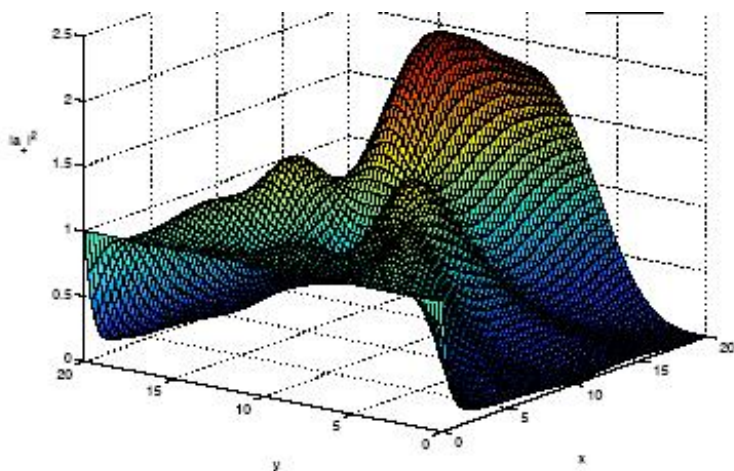
$$1 = \sum_{\text{all } k_j} c_j v_j(y), \quad 0 < y < H.$$

Low transmittance and moderate diffractance



Solution surfaces for the stop band.

High transmittance and diffractance



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 $|u_0|, |v_0| \rightarrow 0$ as $|x| \rightarrow \infty$, 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 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 :

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

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

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

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

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

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

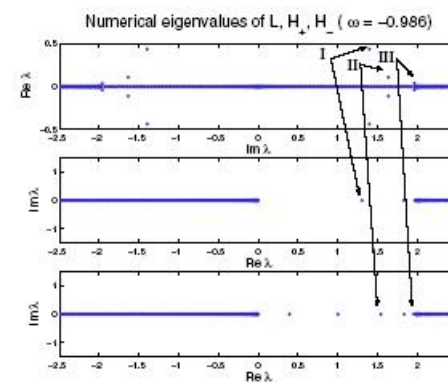
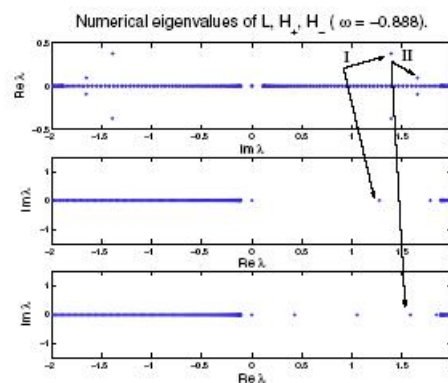
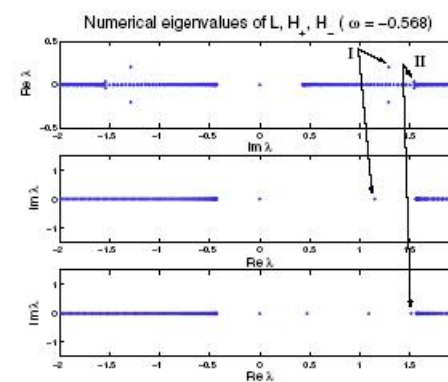
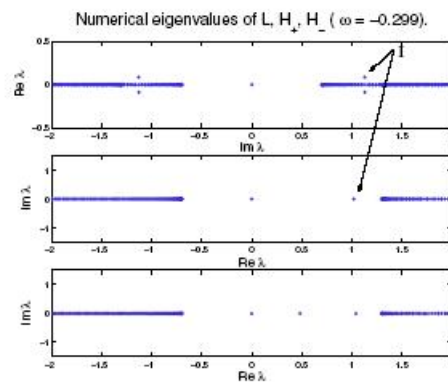
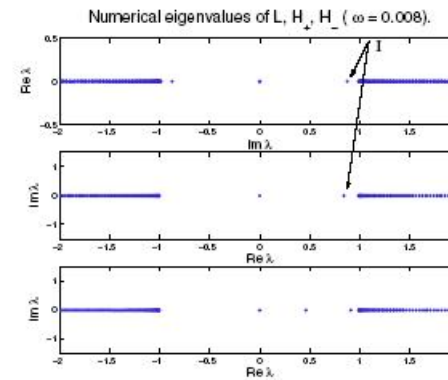
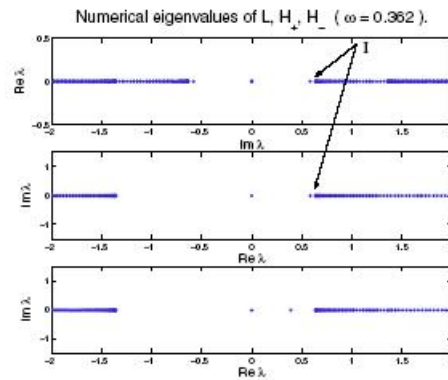
Numerical results on unstable eigenvalues

- 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

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

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 $l_s^2(\mathbb{Z})$ to itself for $s > \frac{1}{2}$.
- When $\omega \in \mathbb{R} \setminus \mathbb{Z}$, 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 $\mathbf{U} \in l_s^2(\mathbb{Z})$ 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

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

such that

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

and

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

- Operator $(\mathcal{L} + \epsilon \mathbf{W}\star)$ is continuously invertible on $\mathbf{g} \in \text{Ker}(\mathcal{L})^\perp$, 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 $\text{Ker}(\mathcal{L})$.

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

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

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

- In two dimensions, bifurcations of periodic and antiperiodic solutions can be proved with this technique in $l_s^2(\mathbb{Z})$ 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