Computing eigenmodes on the torus: photonic crystals using second-kind integral equations

IPAM, Feb 12, 2009

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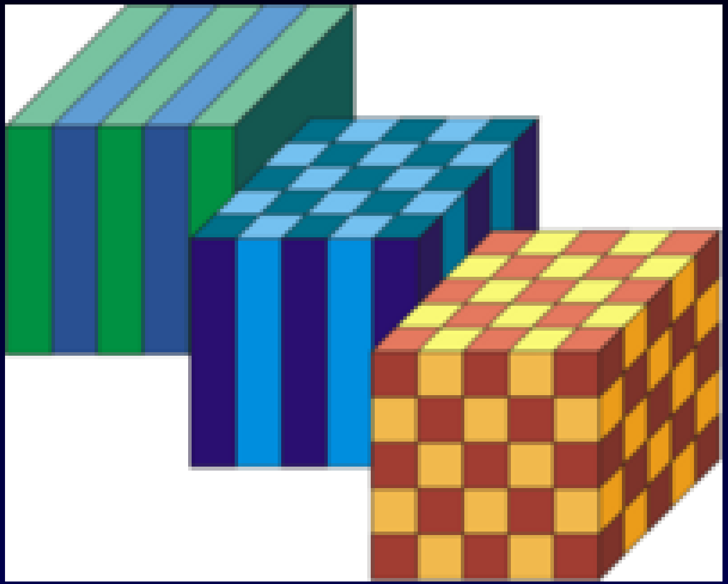
joint work with Leslie Greengard, Courant Institute

Photonic crystals

periodic dielectric structures

period $\approx$ wavelength of light $\approx 1\mu$m

control optical propagation in ways impossible in homogeneous media



(Joannopoulos group)

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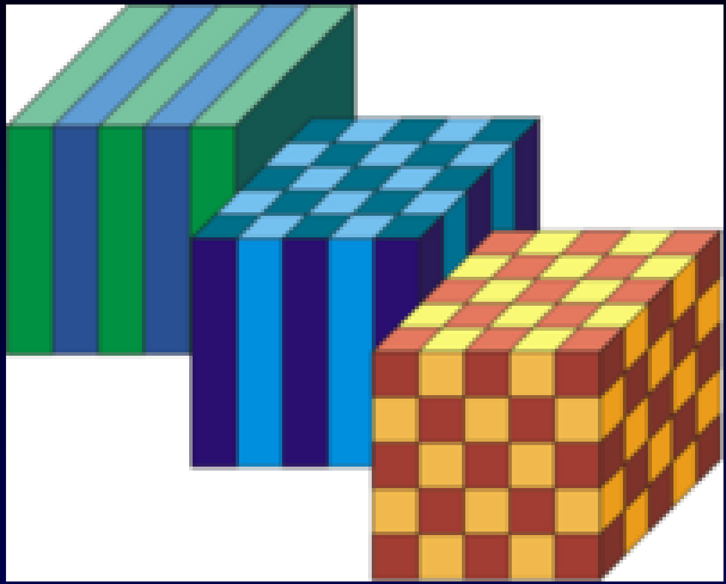

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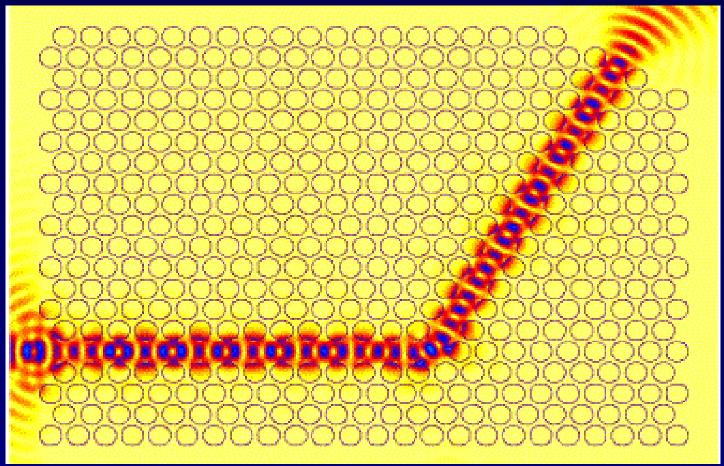
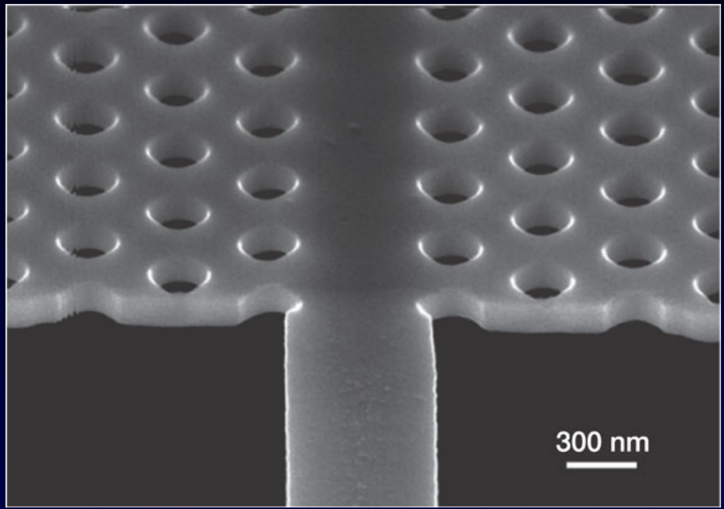


2D lattice of cylinders (INFM, U. Pavia)

e.g. 'bandgap' medium: $\exists$ freqs. s.t. all waves evanescent (non-propagating)

- 'insulators' with embedded waveguides
- unlike dielectric guides, sharp bends ok

Photonic crystal examples



Si, $\lambda = 1.6\mu$m (Vlasov '05)

- Slab w/ 2D-periodic air holes

couples to external dielectric guide

manipulate guide dispersion to give v slow group velocity ($c/300$)

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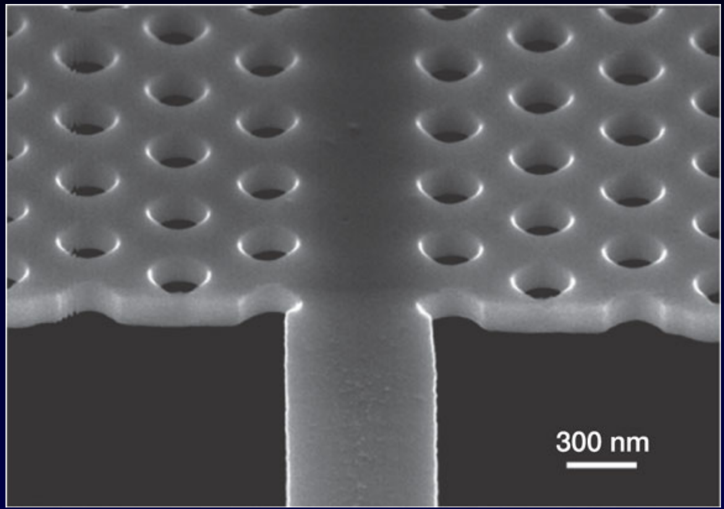

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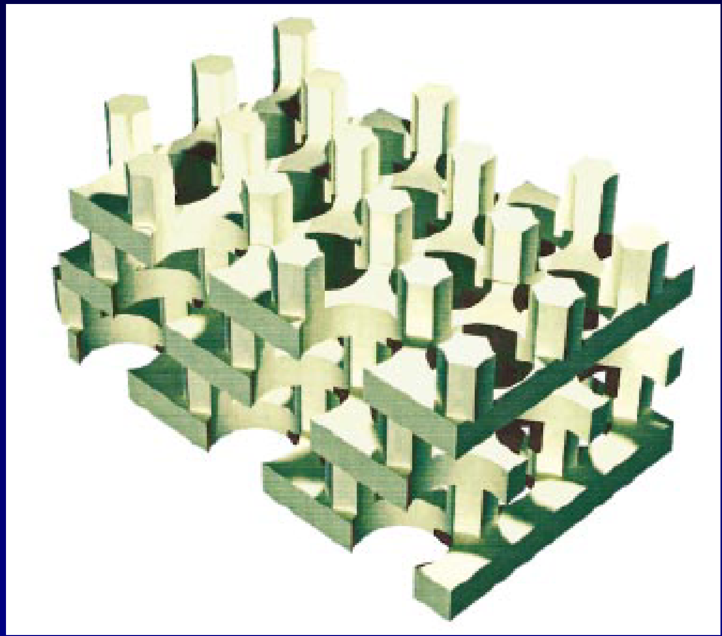
- Full 3D bandgap (all polarizations)

'Yablonovite' (cm scale) (Yablonovich '91)
'woodpile' $\lambda = 12\mu$m (Lin *et al.* '98)
'inverse opals' (spherical air 'bubbles')
stacked slabs (built $\lambda = 1.3\mu$m, Qi *et al.* '04)

- complex geometry (not just cylinders!)

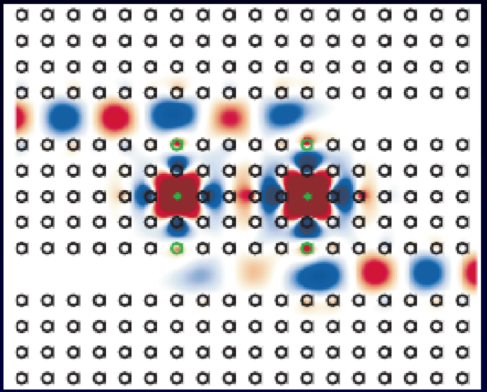


(Johnson *et al.* '00)

Applications

Build low-loss optical signal paths on 1μm scale:
integrated optical devices, signal-processing,
Big goal: optical ($\Rightarrow$ *high* speed!) computing

e.g. high-Q resonators, couplers, junctions



channel-drop filter in 2D crystal

(Johnson *et al.* '00)

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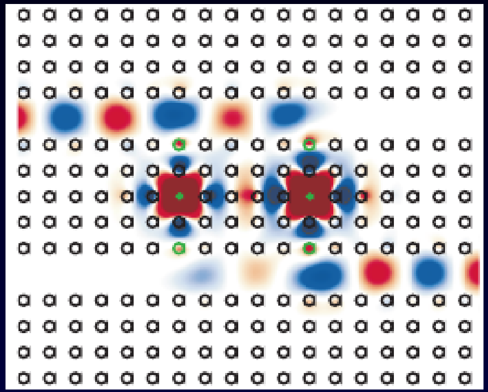

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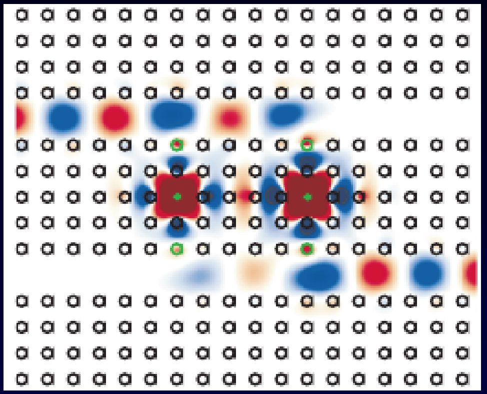

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Common features

- piecewise-homogeneous dielectric media, wavenumber low
- each medium linear, may be dispersive *e.g.* metals (plasmons)
- manufacturing costly $\Rightarrow$ numerical design/modeling/optimization

Outline

1. Band structure of a photonic crystal: eigenmodes on a torus
2. Existing numerical approaches
3. Potential theory, boundary integral equations
4. New (& better!) way to periodize the problem
5. Preliminary results

Scalar waves in $\mathbb{R}^2$: 'free space'

dimensionless wave equation $\hat{u}_{tt} = \Delta u$ (Δ = laplacian)

const frequency ω: time-harmonic solns $\hat{u}(\mathbf{x}, t) = u(\mathbf{x})e^{-i\omega t}$

becomes Helmholtz eqn: $(\Delta + \omega^2)u = 0$

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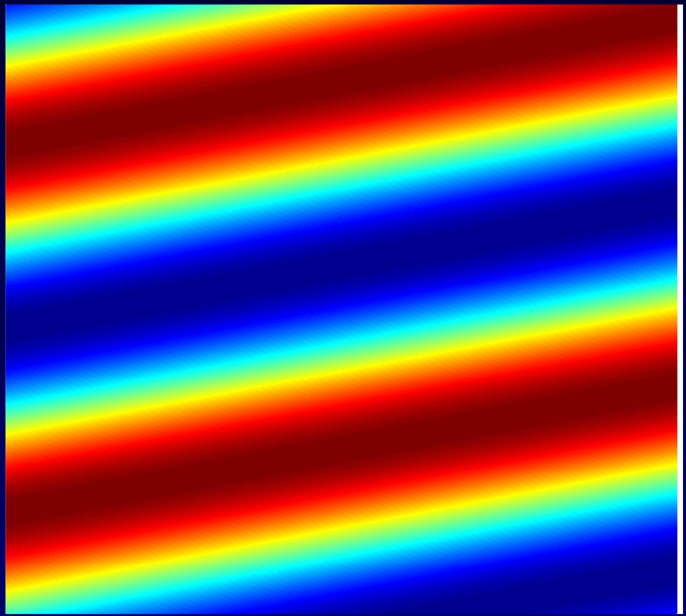
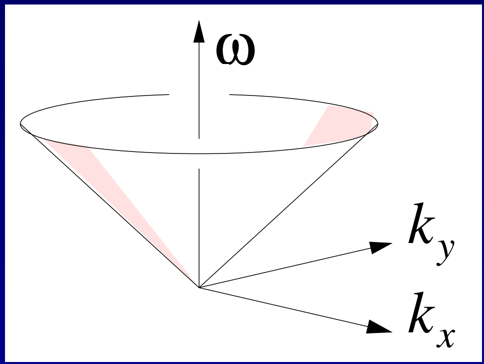


u is generalized eigenfunc. (EF) of $-\Delta$

One choice: $u(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}$
plane waves, $\mathbf{k} \in \mathbb{R}^2$

Shown: $\mathrm{Re}[u]$ for $\mathbf{k} = (-0.39, 2.08)$

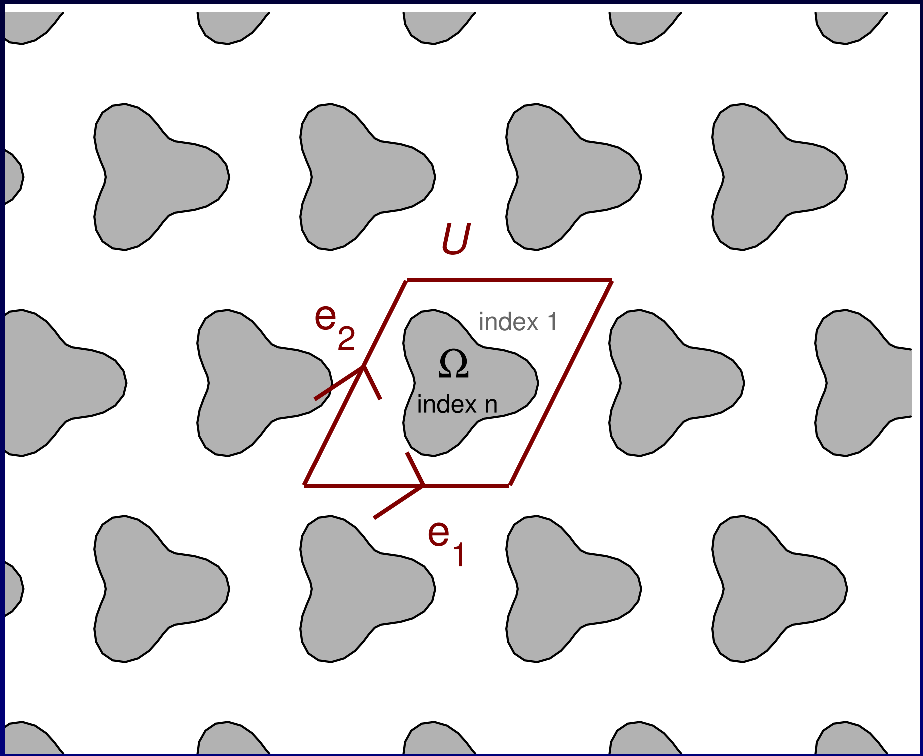


- 'band structure' = dispersion relation

$\omega = |\mathbf{k}|$ is cone in (ω, k_x, k_y)

Waves in a crystal lattice

U = unit cell $\quad\quad \Omega$ = smooth inclusion, refr. index n
Bravais lattice $\Lambda := \{m\mathbf{e}_1 + n\mathbf{e}_2 : n, m \in \mathbb{Z}\}$
dielectric inclusions $\Omega_\Lambda; = \{\mathbf{x} : \mathbf{x} + \mathbf{d} \in \Omega$ for some $\mathbf{d} \in \Lambda\}$



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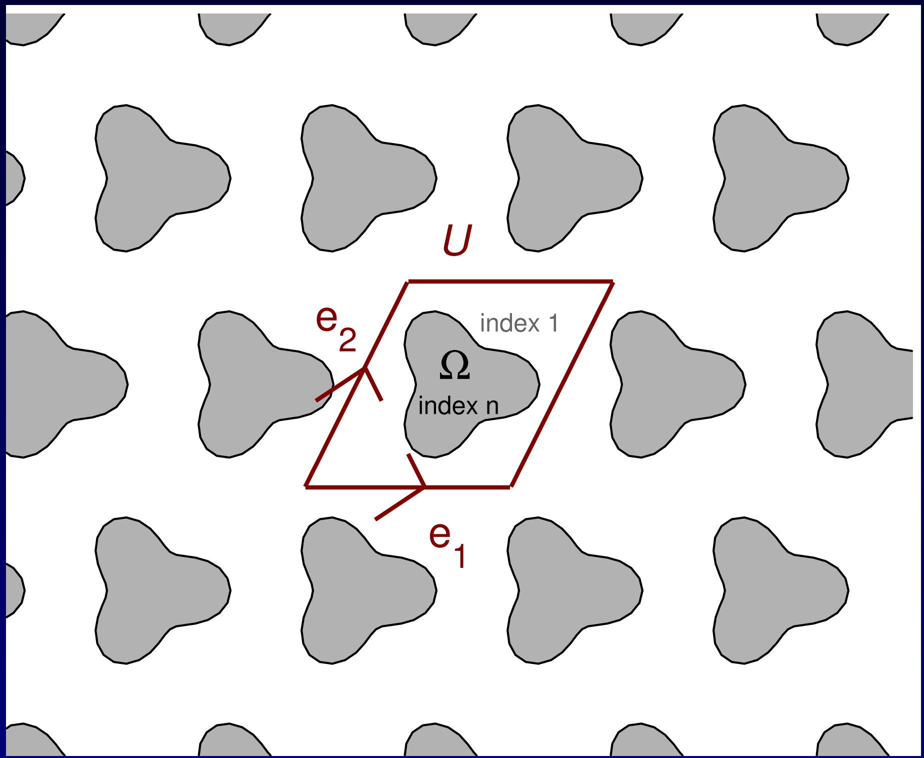


PDE:

$$\begin{aligned}(\Delta + n^2\omega^2)u &= 0 \ \text{ in } \Omega_\Lambda \\ (\Delta + \omega^2)u &= 0 \ \text{ in } \mathbb{R}^2 \setminus \Omega_\Lambda\end{aligned}$$

continuity (matching) BCs:

$$\begin{aligned}u^+ - u^- &= 0 \ \text{ on } \partial\Omega_\Lambda \\ u_n^+ - u_n^- &= 0 \ \text{ on } \partial\Omega_\Lambda\end{aligned}$$

(z-invariant Maxwell, TM polarization)

‘Bloch Theorem’

In infinite periodic medium, can choose gen. EFs as Bloch waves

$$u(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}\tilde{u}(\mathbf{x}) \quad \text{where } \tilde{u} \text{ is periodic}$$

> *‘When I started to think about it, I felt that the main problem was to explain how the electrons could sneak by all the ions in a metal. . . By straight Fourier analysis I found to my delight that the wave differed from the plane wave of free electrons only by a periodic modulation’*

(F. Bloch, 1928)

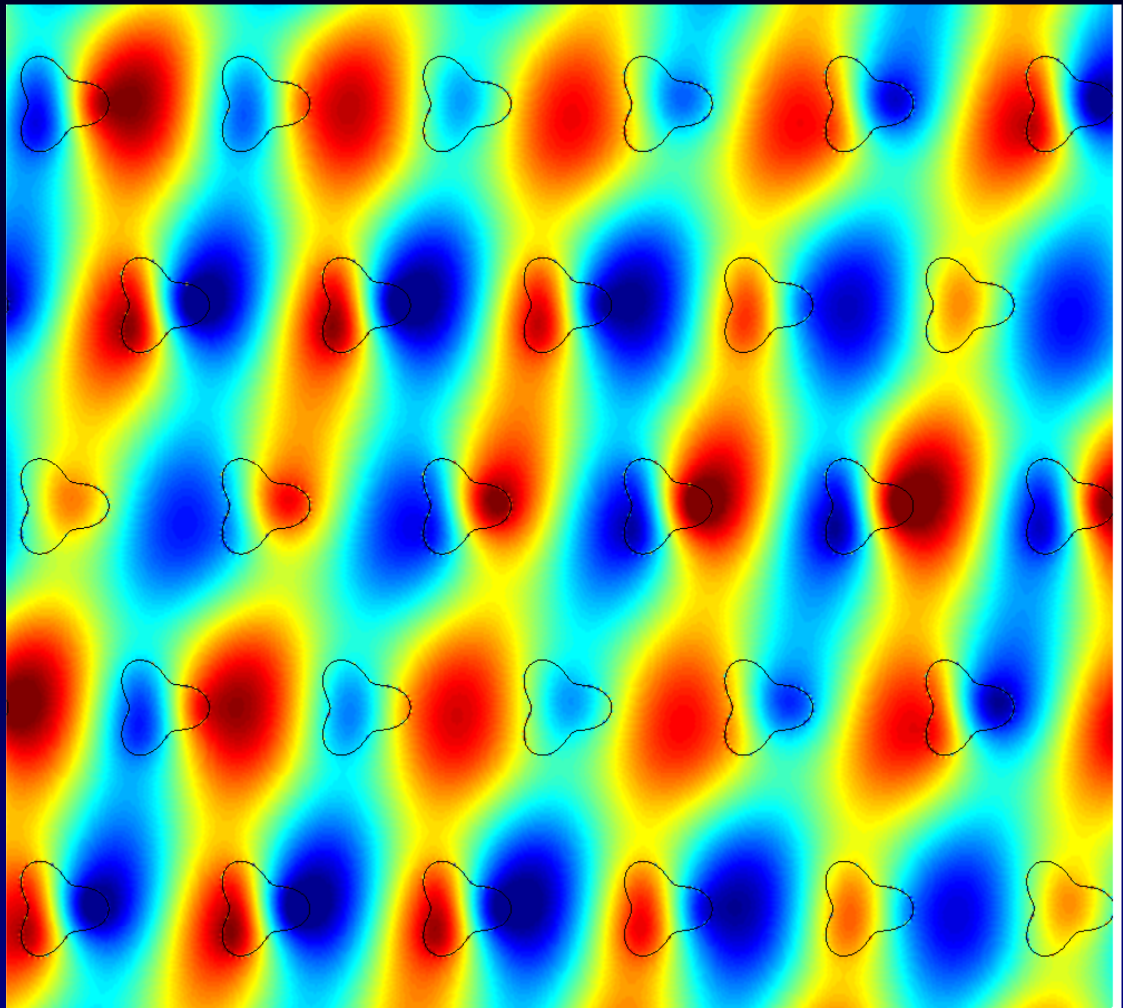
(indep. prediscovered by Hill 1877, Floquet 1883, Lyapunov 1892)

Why?

- differential operator commutes w/ translations $T_{\mathbf{e}_1}$, $T_{\mathbf{e}_2}$
  $\Rightarrow$ can choose simultaneous EFs of PDE, $T_{\mathbf{e}_1}$, and $T_{\mathbf{e}_2}$
- EFs of translations are complex exponentials

Bloch wave

Example soln $u(\mathbf{x})$ to PDE and dielectric BCs on $\partial\Omega$, of form $e^{i\mathbf{k}\cdot\mathbf{x}}\tilde{u}(\mathbf{x})$



Re$[u]$ shown

Bloch wavevector $\mathbf{k}$ (same as earlier plane wave)

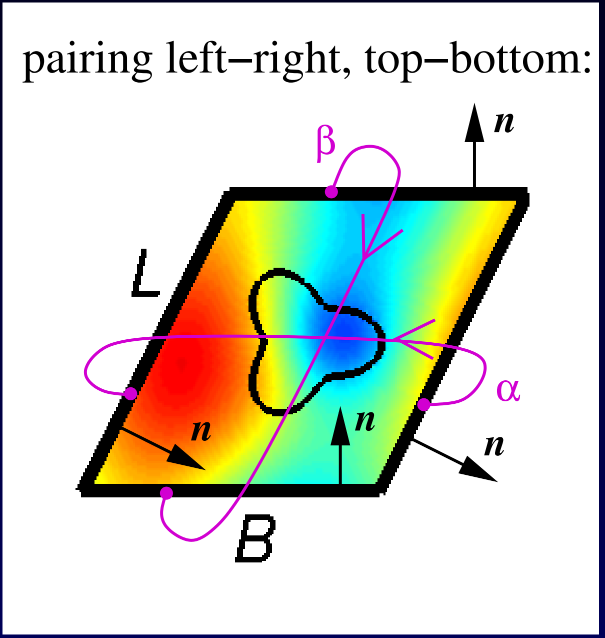
$\mathbf{e}_1 = (1, 0)$
$\mathbf{e}_2 = (\frac{1}{2}, 1)$
$\omega = 5$

- Task: find the set of (ω, k_x, k_y) s.t. non-trivial Bloch EF u exists

Bloch eigenvalue problem on torus

Bloch wave condition equiv. to quasi-periodic BCs on ∂U:

Require vanishing unit cell discrepancy:



$$
\begin{aligned}
f &:= u|_L - \alpha^{-1} u|_{L+\mathbf{e}_1} &= 0 \\
f' &:= u_n|_L - \alpha^{-1} u_n|_{L+\mathbf{e}_1} &= 0 \\
g &:= u|_B - \beta^{-1} u|_{B+\mathbf{e}_2} &= 0 \\
g' &:= u_n|_B - \beta^{-1} u_n|_{B+\mathbf{e}_2} &= 0
\end{aligned}
$$

Bloch phases $\alpha := e^{i\mathbf{k}\cdot\mathbf{e}_1}$, $\beta := e^{i\mathbf{k}\cdot\mathbf{e}_2}$, $|\alpha| = |\beta| = 1$

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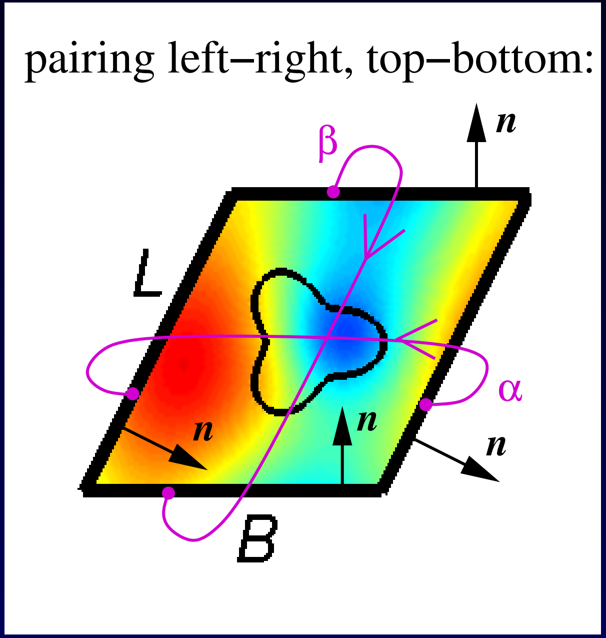

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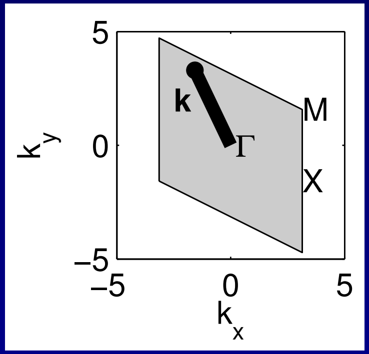
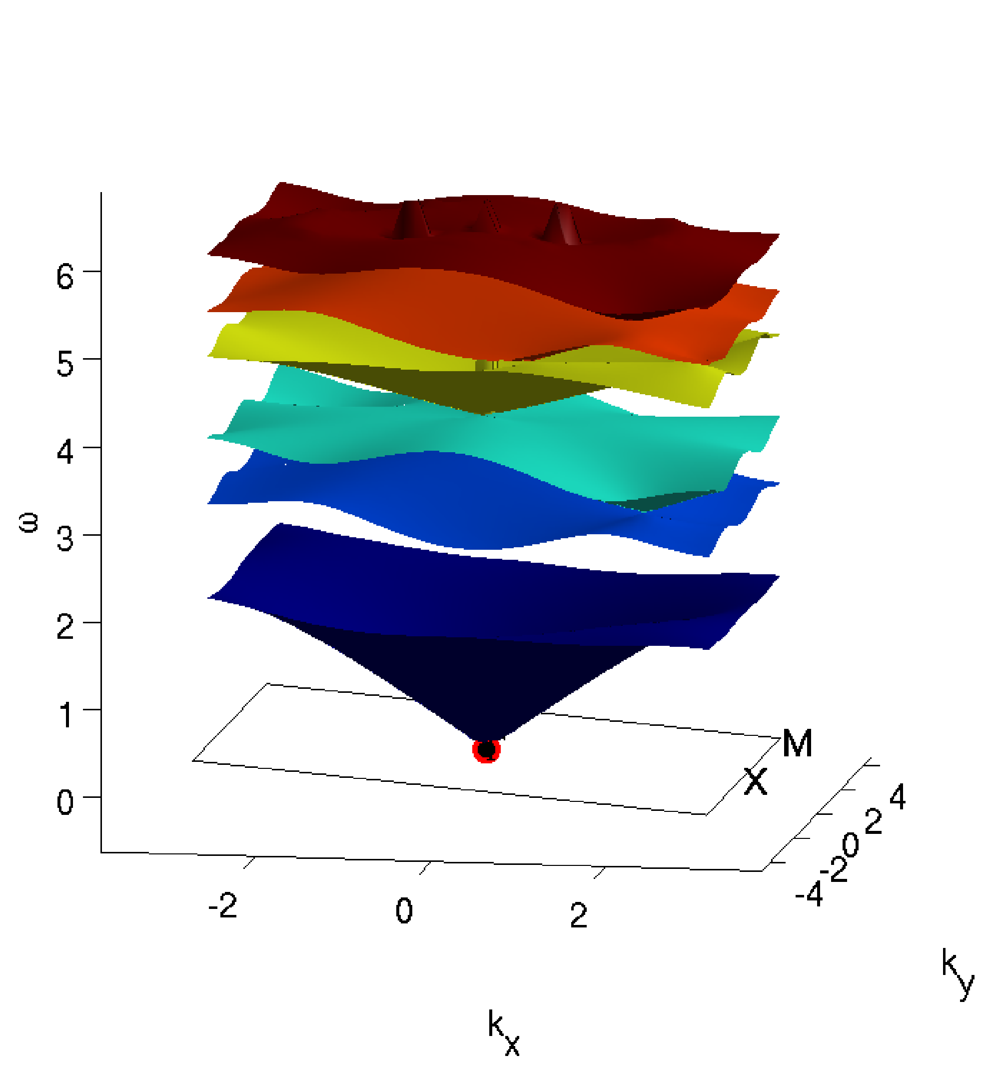
- $\alpha, \beta \in S^1$, thus $\mathbf{k}$ equiv. to $\mathbf{k} + 2\pi\mathbf{q}$ $\quad \forall \mathbf{q} \in \Lambda^*$ dual (reciprocal) lattice

…need consider only $\mathbf{k} \in$ *Brillouin zone* (BZ):



Combine quasi-periodicity w/ PDE, BCs on $\partial\Omega$: eigenvalue problem on (phased) torus

Band structure



For each parameter $\mathbf{k} \in$ BZ (Bloch wavevector) $\exists$ eigenvalues

$$\omega_1(\mathbf{k}) \leq \omega_2(\mathbf{k}) \leq \cdots \nearrow \infty$$

form 'sheets' above the BZ (BZ is also a torus)

note: conical near $\omega = 0$

note: bandgap

- is most important property of photonic crystal for applications
- *e.g.* bandgaps, Snell's law, group vel. $\nabla_{\mathbf{k}}\omega$, group dispersion ...

Main numerical approaches

Time domain

- time-stepping on finite-difference grid (FDTD) (*e.g.* Yee '66)

  low order (inaccurate), close freqs $\Rightarrow$ large t reqd (inefficent)

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- multiple-scattering, cylinder geometry only (McPhedran *et al.*)
- Plane-wave method: all in Fourier space (Joannopoulos, Johnson, Sözüer)

  discont. dielectric $\Rightarrow$ Gibbs phenom, slow $(1/N)$ convergence

- Finite element (FEM) discretization in U (Chew, Dobson, Dossou)

  better for discontinuity, N large, meshing and high-order complicated

Note: above two give $A\mathbf{x} = \omega^2 B\mathbf{x}$, but become non-linear EVP in dispersive media

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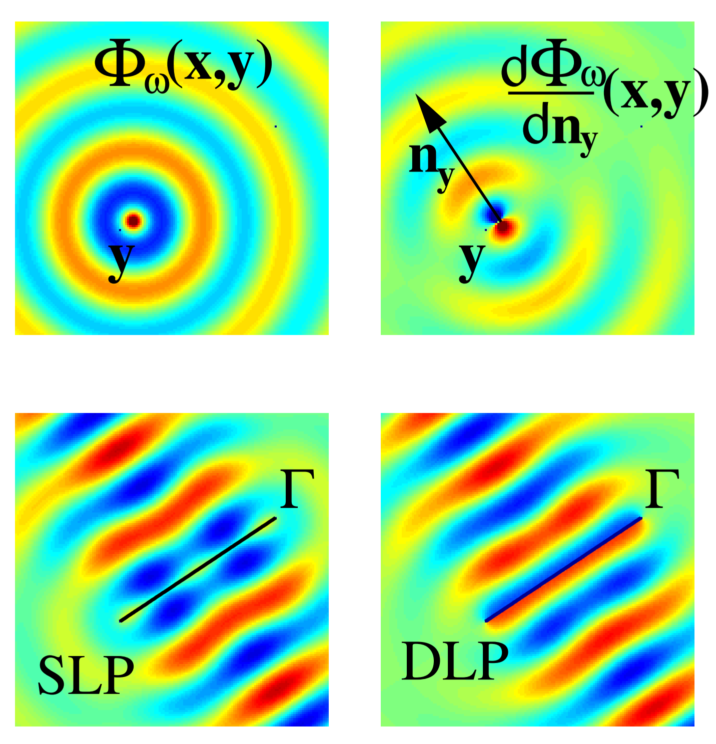
- Integral equations: formulate problem *on* the discontinuity $\partial\Omega$

  reduced dimensionality (small N), good tools for scattering, Fast Multipole (FMM)

  high order (quadratures): high accuracy with small effort

Integral equations

'charge' (sources of waves) distributed along curve Γ w/ density func.



single-, double-layer potentials, $\mathbf{x} \in \mathbb{R}^2$:

$$u(\mathbf{x}) = \int_\Gamma \Phi_\omega(\mathbf{x},\mathbf{y})\sigma(\mathbf{y})ds_\mathbf{y} := (\mathcal{S}\sigma)(\mathbf{x})$$

$$v(\mathbf{x}) = \int_\Gamma \frac{\partial \Phi_\omega}{\partial n_\mathbf{y}}(\mathbf{x},\mathbf{y})\tau(\mathbf{y})ds_\mathbf{y} := (\mathcal{D}\sigma)(\mathbf{x})$$

$$\Phi_\omega(\mathbf{x},\mathbf{y}) := \Phi_\omega(\mathbf{x}-\mathbf{y}) := \frac{i}{4}H_0^{(1)}(k|\mathbf{x}-\mathbf{y}|)$$

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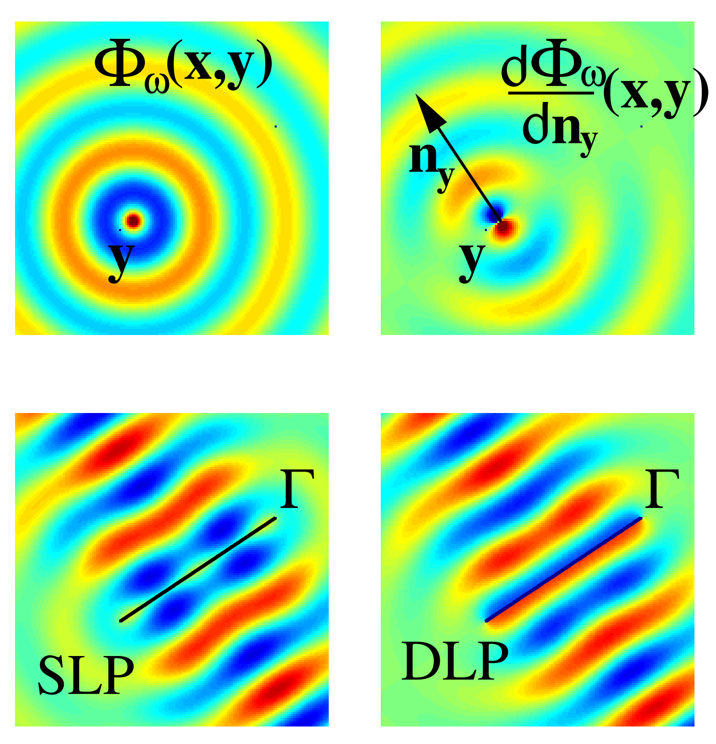

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Jump relations: limit as $\mathbf{x} \to \Gamma$ may depend on which side ($\pm$):

$$u^\pm = S\sigma$$
$$u_n^\pm = D^T\sigma \mp \tfrac{1}{2}\sigma$$
$$v^\pm = D\tau \pm \tfrac{1}{2}\tau$$
$$v_n^\pm = T\tau$$

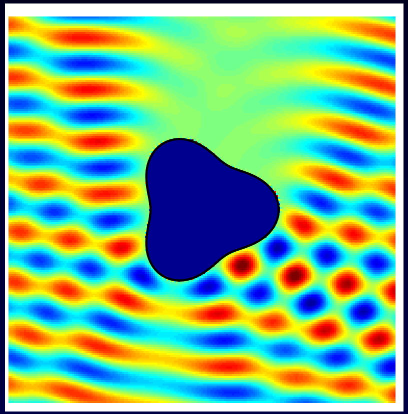
S, D are integral ops with above kernels

but defined on $C(\Gamma) \to C(\Gamma)$

T has kernel $\frac{\partial^2 \Phi_\omega}{\partial n_\mathbf{x} \partial n_\mathbf{y}}(\mathbf{x},\mathbf{y})$

Integral equations for scattering (overview)

e.g. Dirichlet obstacle: represent $u = u^{\text{inc}} + \mathcal{D}\tau$ DLP on $\partial\Omega$



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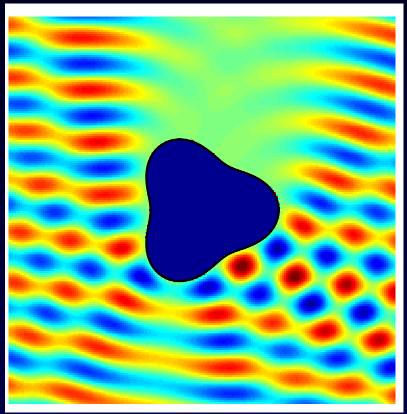

BC $0 = u^+ = u^{\text{inc}}|_{\partial\Omega} + (D + \frac{1}{2})\tau$ by JR3

integral eqn on $\partial\Omega$: $(I + 2D)\tau = -2u^{\text{inc}}$

2nd-kind, D compact op so $(I + 2D)$ sing. vals. $\not\to 0$

Why important?

condition # small, iterative solvers (GMRES) fast

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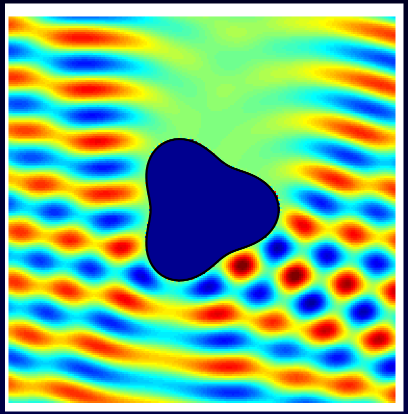

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Quadrature scheme, choose N nodes $\mathbf{y}_j \in \partial\Omega$, weights w_j

Nyström discretization: N-by-N linear system for vector $\{\tau_k^{(N)}\}_{k=1}^N$

$$\tau_k^{(N)} + 2\sum_{j=1}^N w_j D(\mathbf{y}_k, \mathbf{y}_j)\tau_j^{(N)} = -2u^{\text{inc}}(\mathbf{y}_k), \qquad k = 1, \ldots, N$$

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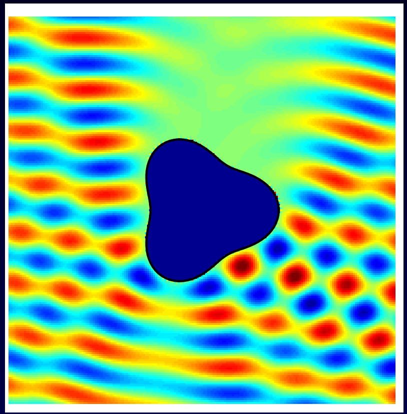

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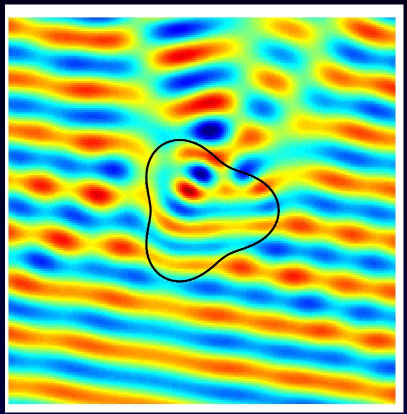
Thm: (Anselone, Kress) $\|\tau^{(N)} - \tau\|_\infty$ converges at *same rate* as quadrature scheme for the true integrand $D(\mathbf{y}, \cdot)\tau$.

- Analytic curve & data, periodic trapezoid rule: spectral convergence
- *e.g.* above: $N = 60$ enough for 10^{-6} error, $N = 100$ for 10^{-12}
- error $\sim e^{-\gamma N}$, rate $\gamma \approx$ distance to nearest singularity of τ in $\mathbb{C}$

Dielectric (transmission) scattering



Represent $u = u^{\text{inc}} + \mathcal{D}\tau + \mathcal{S}\sigma$ outside wavenumber ω

$u = \mathcal{D}_i\tau + \mathcal{S}_i\sigma$ inside wavenumber $n\omega$

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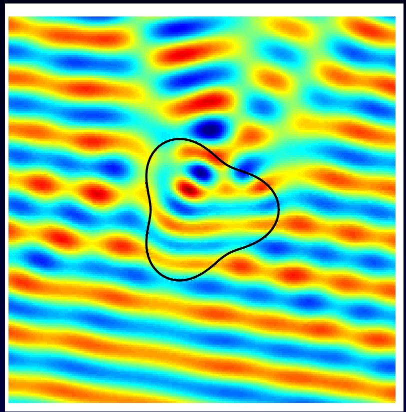

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mismatch on $\partial\Omega$: $h := u^+ - u^-$, $h' := u_n^+ - u_n^-$

BCs: mismatch $m := [h; h']$ vanishes, use JRs...

$$\begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} u^{\text{inc}}|_{\partial\Omega} \\ u_n^{\text{inc}}|_{\partial\Omega} \end{bmatrix} + \left(\underbrace{\begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} + \begin{bmatrix} D - D_i & S_i - S \\ T - T_i & D_i^T - D^T \end{bmatrix}}_{A} \right) \underbrace{\begin{bmatrix} \tau \\ -\sigma \end{bmatrix}}_{\eta}$$

block 2nd-kind A maps densities to their effect on mismatch

- hypersingular part of T cancels, so $A = \text{Id} + \text{compact}$ (Rokhlin '83)
- kernel weakly singular, but exists spectral product quadrature for $f(s) + \log(4\sin^2\frac{s}{2})g(s)$, f, g analytic 2π-periodic (Kress '91)

Standard way to periodize

replace kernel $\Phi_\omega(\mathbf{x})$ by $\Phi_{\omega,\mathrm{QP}}(\mathbf{x}) := \sum_{m,n\in\mathbb{Z}} \alpha^m \beta^n \Phi(\mathbf{x} - m\mathbf{e}_1 - n\mathbf{e}_2)$
Thus the layer potential integral operator A becomes A_{QP}

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- common way to do: lattice sums (Ewald, ..., McPhedran *et al.* , Linton)

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  e.g. band structures (Leung '93, Moroz '99)
  e.g. scattering from 2D gratings (Otani '08)

  ...modifies top-level of FMM, easy in 2D, nightmare in 3D

Standard way to periodize

replace kernel $\Phi_\omega(\mathbf{x})$ by $\Phi_{\omega,\text{QP}}(\mathbf{x}) := \sum_{m,n\in\mathbb{Z}} \alpha^m \beta^n \Phi(\mathbf{x} - m\mathbf{e}_1 - n\mathbf{e}_2)$
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For band structure:

$$\boxed{\text{Null } A_{\text{QP}} \neq \{0\} \quad \Leftrightarrow \quad (\omega, k_x, k_y) \text{ is eigenvalue}}$$

- note no u^{inc}, has become eigenvalue problem

But not robust: $\Phi_{\omega,\text{QP}}(\mathbf{x}) \to \infty \;\; \forall \mathbf{x}$ at certain params (ω, k_x, k_y) !

Spurious resonance problem

$\Phi_{\omega,\mathrm{QP}}(\mathbf{x})$ is Helmholtz Greens function in *empty* (index 1) torus

$$= \frac{1}{\mathrm{Vol}(U)} \sum_{\mathbf{q}\in 2\pi\Lambda^*} \frac{e^{i(\mathbf{k}+\mathbf{q})\cdot\mathbf{x}}}{\omega^2 - |\mathbf{k}+\mathbf{q}|^2}$$

torus spectral representation

has simple pole wherever (ω, k_x, k_y) is eigenvalue of empty torus…

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Simply by forming $\Phi_{\omega,\text{QP}}$ we must cause blow-up of roundoff errors

- problem not widely appreciated
- also true for scattering from gratings and arrays (Linton '07)
- a non-issue for … Laplace, Poisson $(\omega = 0)$ (Ethridge '01)
  modified Helmholtz $(\omega^2 < 0)$ (Cheng '06)
  inhomogeneous Helmholtz (resonance *is* physical) (Beylkin '08)

Our cure: robust way to periodize

represent $u = \mathcal{D}\tau + \mathcal{S}\sigma +$ (densities ξ on walls of U) outside

$\uparrow$ $\uparrow$

can enforce mismatch $m = 0$ can enforce discrepancy $d := [f; f'; g; g'] = 0$

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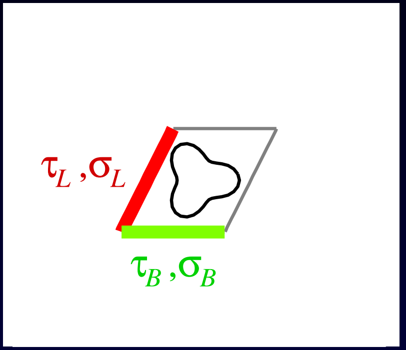
- gain robustness: no matrix element blow-up at spurious resonances

$$\boxed{\text{Null } M \neq \{0\} \quad \Leftrightarrow \quad (\omega, k_x, k_y) \text{ Bloch eigenvalue}}$$

- idea of extra sources of waves not new (*e.g.* Hafner '02)
- what is new is $M = \text{Id} + \text{compact}$ ideal for large-scale, iterative, FMM

How choose new densities on unit cell walls?

- to control 4 discrepancies (f, f', g, g')
  need 4 densities $\xi = [\tau_L; \sigma_L; \tau_B; \sigma_B]$



$Q = \frac{1}{2}\text{Id} + \text{(self-interactions)} + \text{(other interactions)}$

JRs $\quad \sigma_L \to u|_L \quad \sigma_L \to u|_B$

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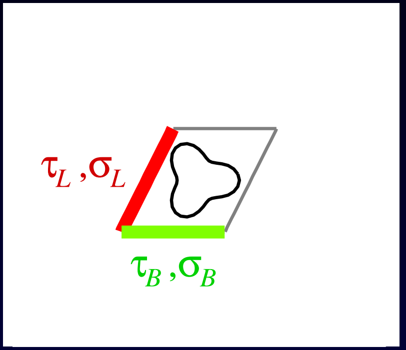

$Q = \frac{1}{2}\mathrm{Id}$ + (self-interactions) + (other interactions)

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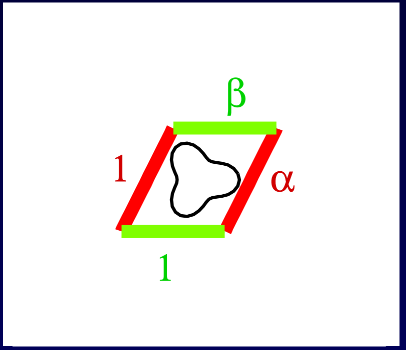
- add phased ghost copies on other 2 walls

  recall $f := u|_L - \alpha^{-1} u|_{L+\mathbf{e}_1}$



$$\left.\begin{array}{l}\text{effect of } \sigma_L \text{ on } u_n|_L \\ \text{effect of } \alpha\sigma_L \text{ on } \alpha^{-1} u_n|_{L+\mathbf{e}_1}\end{array}\right\} \text{cancel apart from Id}$$

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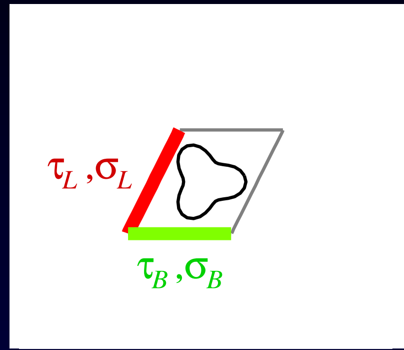

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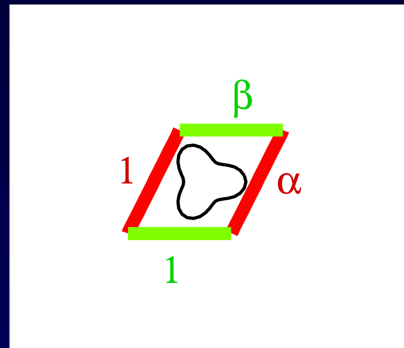
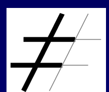
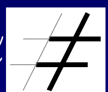


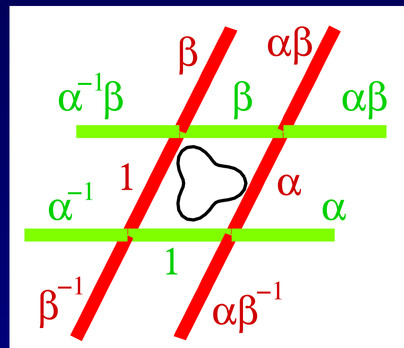
- add more ‘sticking-out’ ghost images

effect of  on $u_n|_L$

effect of α  on $\alpha^{-1}u_n|_{L+\mathbf{e}_1}$

} cancel apart from Id

$\Rightarrow$ all corner interactions vanish!

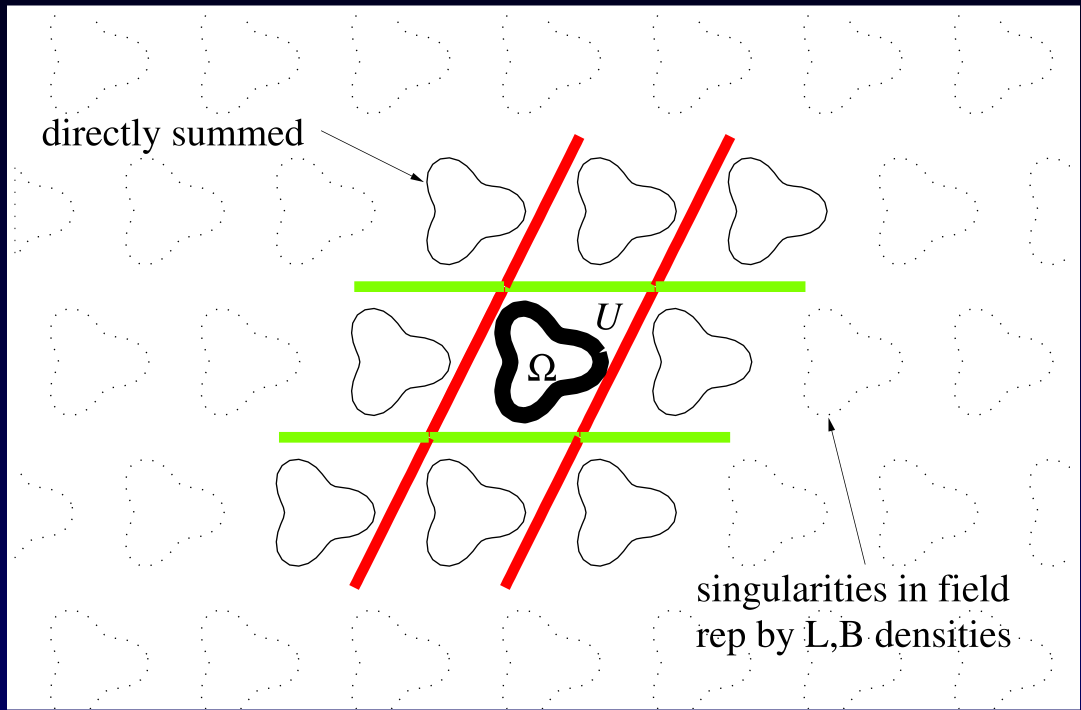


- result: $\quad Q = I +$ (interactions of distance ≥ 1)

  $\Rightarrow$ low rank, rapid convergence: 20-pt Gauss quadr. on L, B $\Rightarrow 10^{-12}$ error

Full scheme

Finally we add 3x3 phased image copies of densities on $\partial\Omega$, giving:



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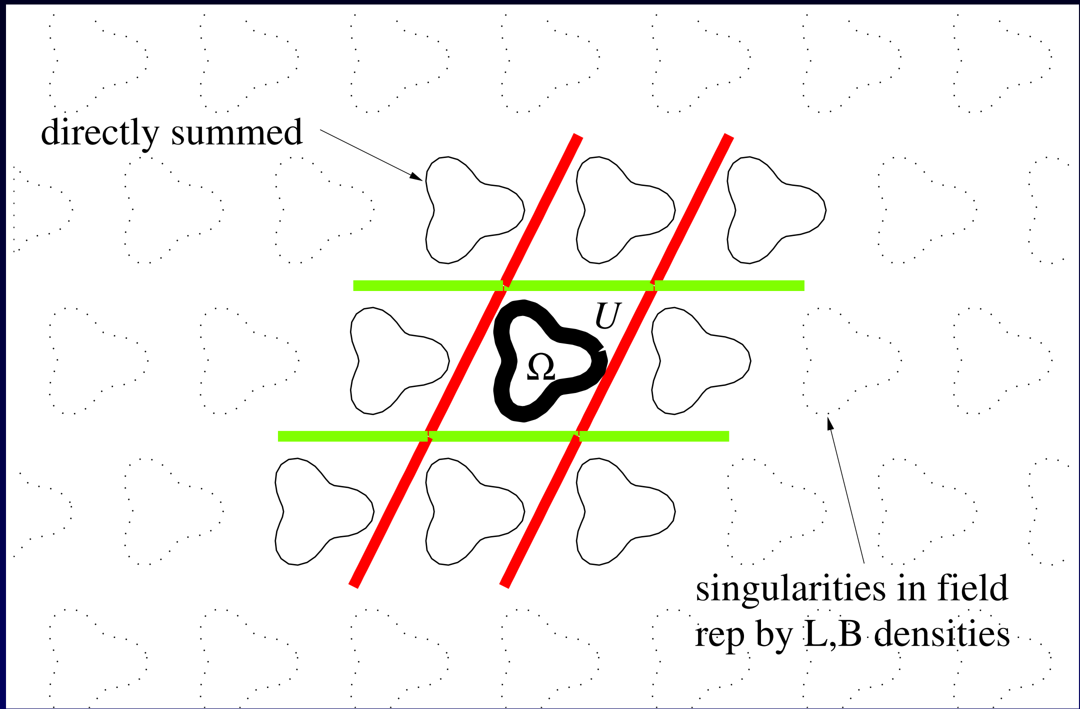

- C cancels similarly to Q, so all its interaction distances ≥ 1
- B does have closer interactions; need tricks if $\mathrm{dist}(\Omega, \partial U) \to 0$

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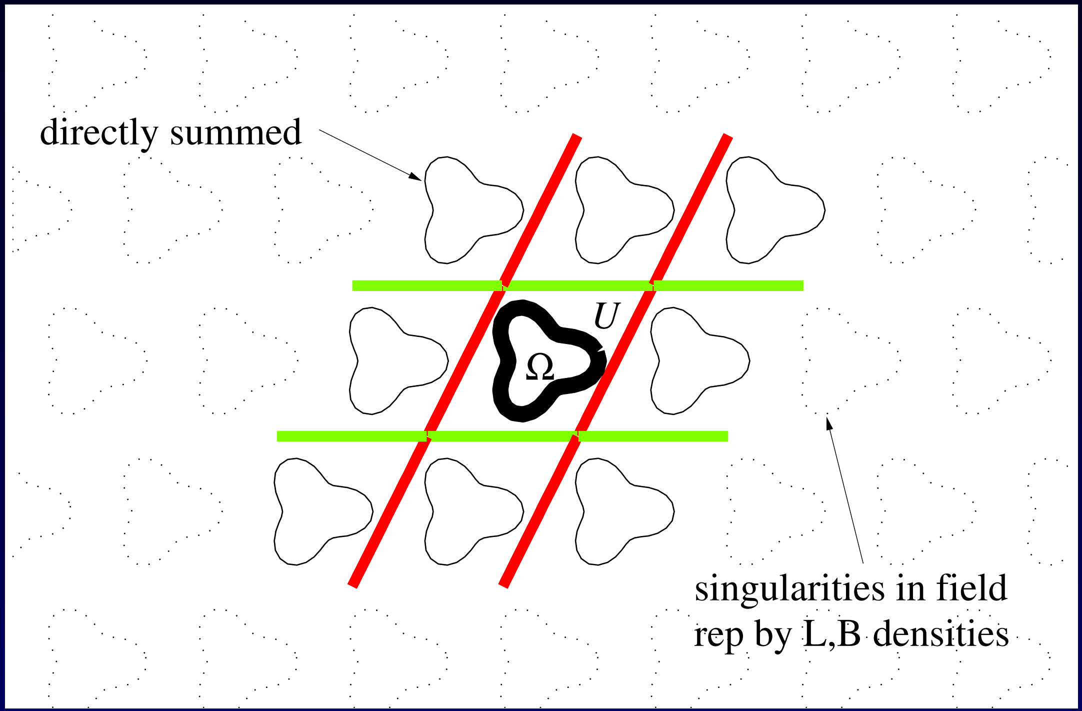

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Philosophy: sum neighboring image sources directly so fields due to remaining lattice have distant singularities

Results: small inclusion

band structure: simply plot log min sing. val. of M vs (ω, k_x, k_y) …

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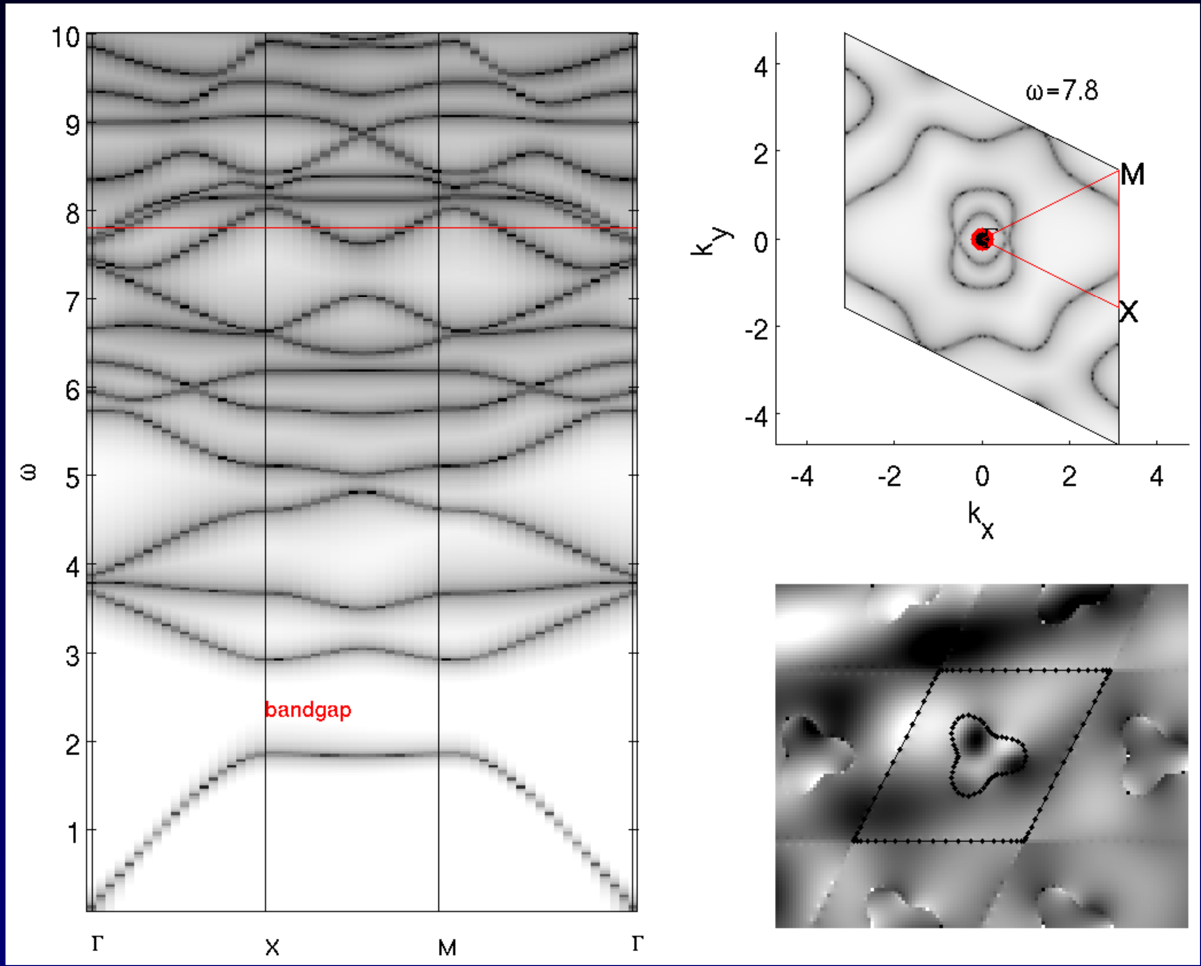


0.1 sec per eval

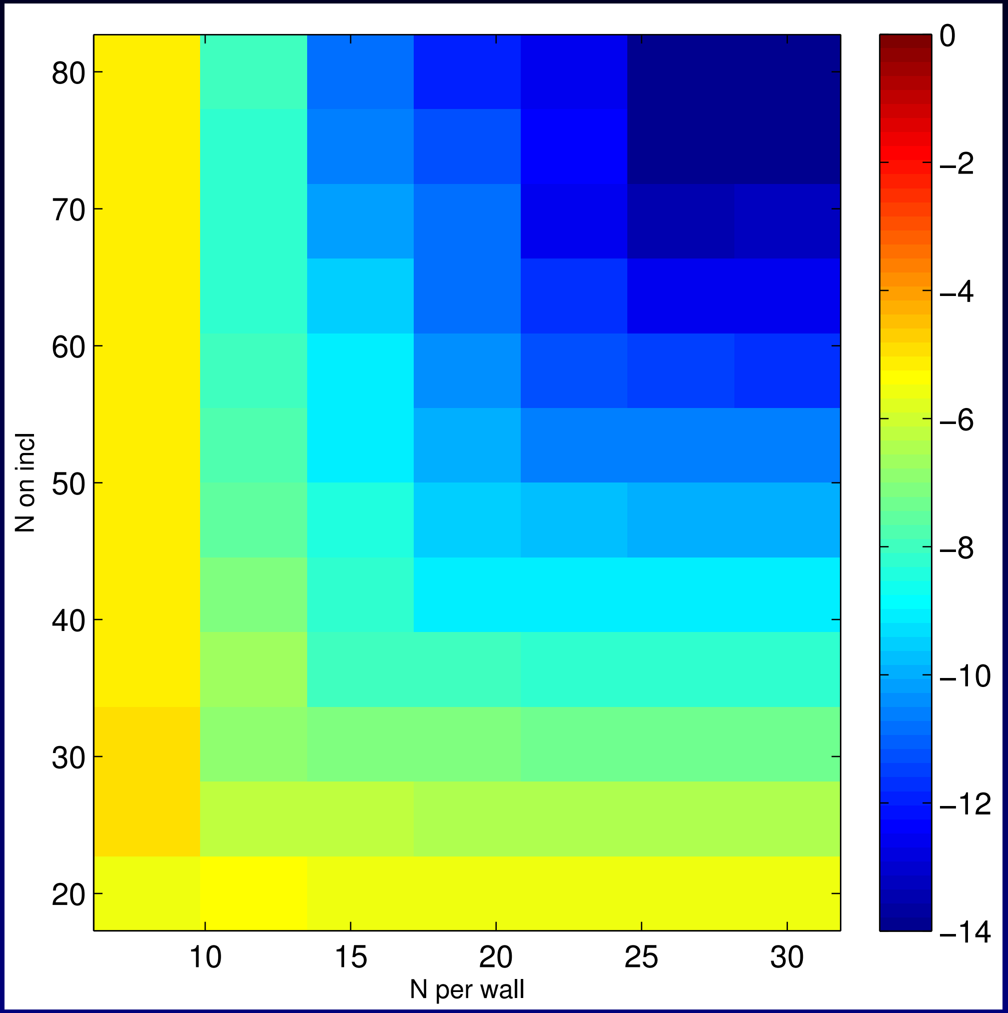
1 min per const-ω slice

movie in ω

- errors 10^{-9} for 40 pts on $\partial\Omega$, 20 per wall (total $N = 160$)
- need search in (ω, k_x, k_y) for where M singular: non-linear EVP

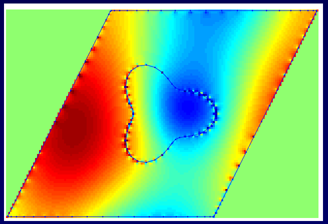
Error convergence

$\log_{10}$ min sing. val M for known Bloch eigenvalue (should be zero):



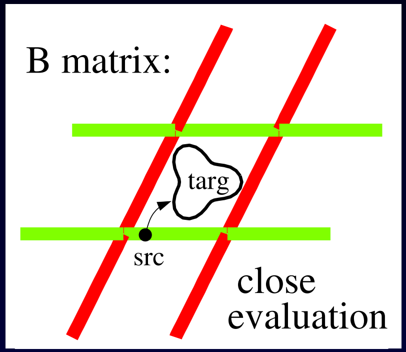
Note: is eigenvalue error up to $O(1)$ const

$\omega = 5, \mathbf{k} = (-0.39\ldots, 2.08\ldots)$

mode: 

- spectral (exponential) convergence: error $\sim e^{-cN}$

Large inclusion passing through unit cell



As $\mathrm{dist}(\Omega, \partial U) \to 0$ standard quadrature v. poor

- fix via adaptive quadrature of Lagrange interpolant
- faster: project wall densities onto J-expansion using addition thm (now $N{=}35$ per wall)

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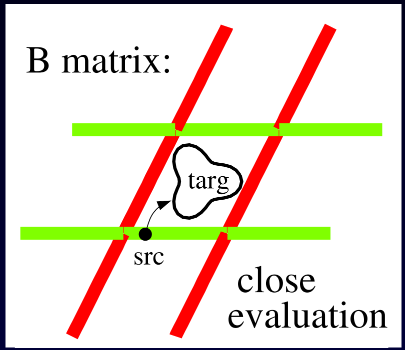

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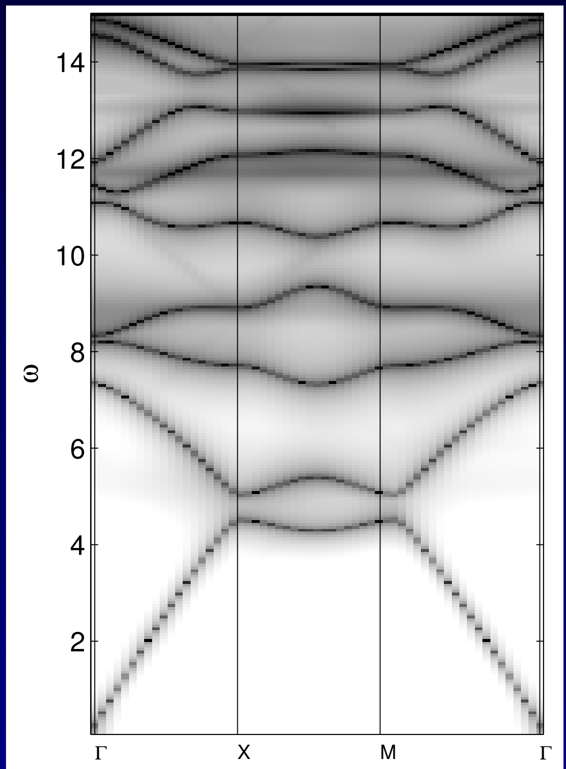
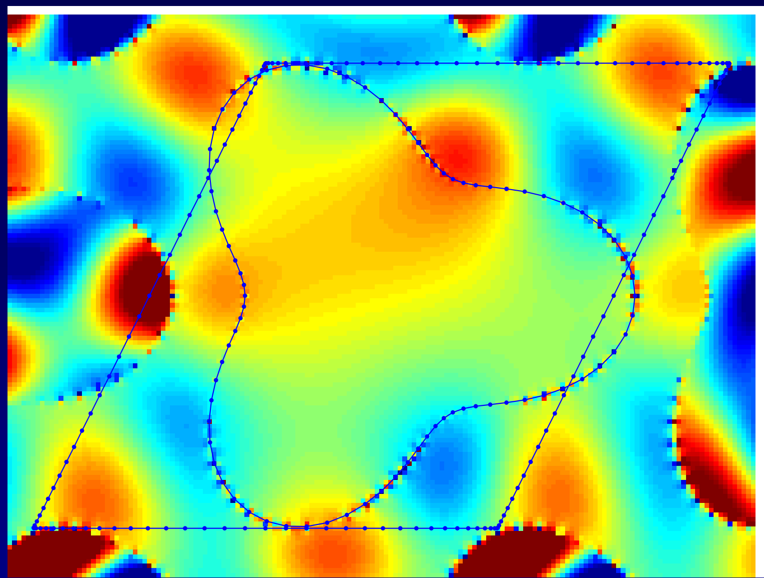


Amazingly (due to far singularities), J-exp analytically continues the field to outside U:



$\omega = 4.47$

$\mathbf{k} \approx (0.17, 2.11)$

n=1 inside

n=3.3 outside

movie

Avoiding the root search

Holding ω constant, can rapidly explore the slice (ω, α, β):

operator (hence matrix) M is of the form $\sum_{m,n=-2}^{1} \alpha^m \beta^n M_{mn}$

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- pre-store coeffs M_{nm} for quick filling of M at any (α, β)

- fix ω, β so get a cubic (polynomial) eigenvalue problem in α
  – only eigenvalues with $|\alpha| = 1$ are traveling Bloch waves
  – can be turned into $3N$-by-$3N$ dense generalized EVP (slow)
  – could use iterative methods since only couple eigvals wanted
  – similar linearizations known (Yuan '08, Dossou '06)

Hope: find an approximate linearization in ω, as in scaling method ?

Scaling method

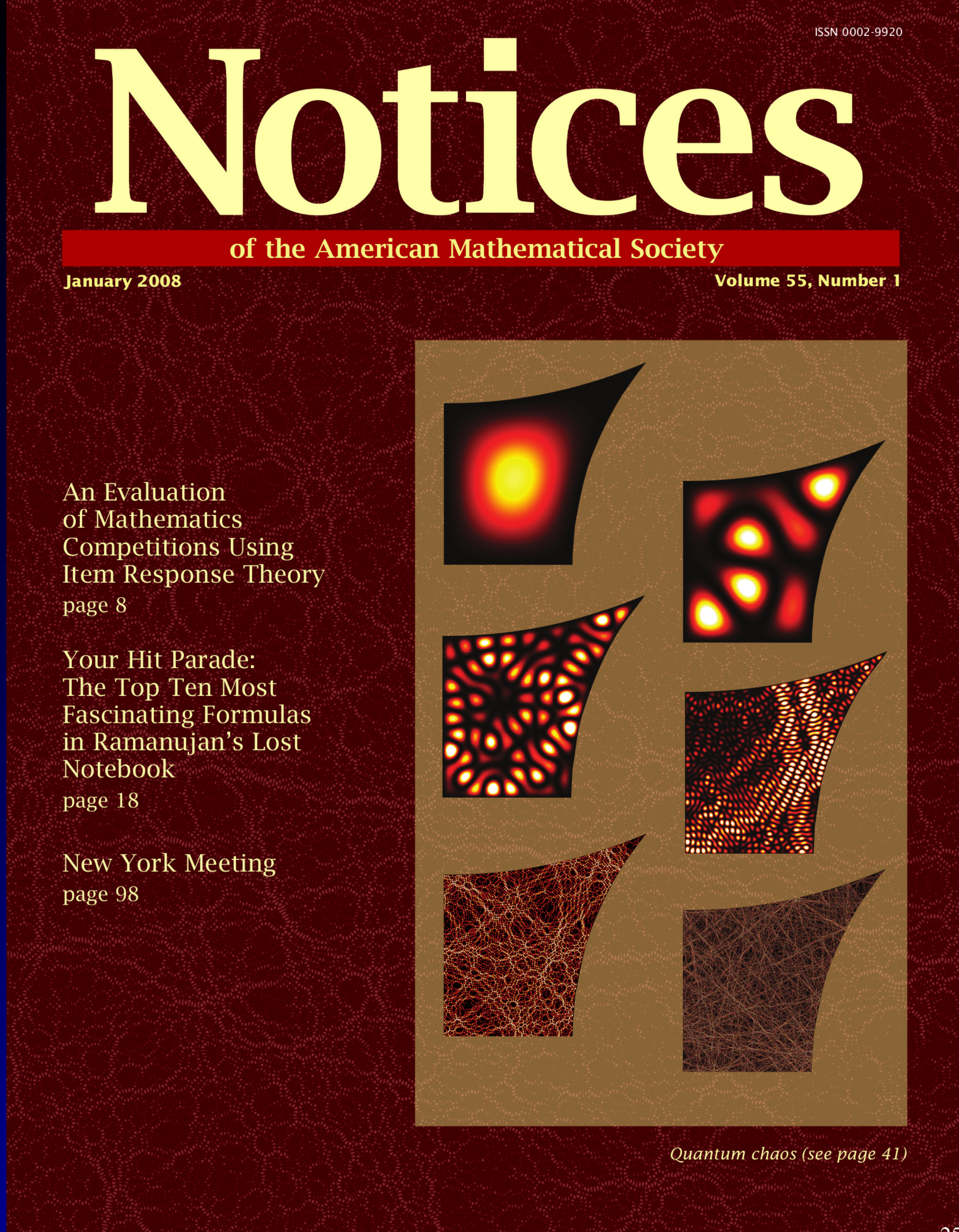
Dirichlet eigenvalue prob:

$(\Delta + E_j) u_j = 0, \quad u_j|_{\partial\Omega} = 0$

- Scaling method:
  star-shaped domains
  no root search
  fastest by factor 10^3
  (Vergini '94, B '00)

- High-freq. asymptotic study of Ω with chaotic ray dynamics (B '06)

shown: mode numbers $j =$
$1, 10, 10^2, 10^3, 10^4, 10^5$



Conclusions

- efficient integral-eqn formulation for photonic crystal EVP
- periodize via small # extra degrees of freedom on cell walls
- more robust and flexible than quasi-periodic Greens function:
  – no spurious breakdown at empty resonances
  – search for Bloch phases via cubic EVP
  – extends simply to 3D (unlike lattice sums)

Future:

- fast iterative root search for min sing val $M(\omega, \alpha, \beta) = 0$
- insert Fast Multipole (FMM) scattering code from inclusion
- theorems bounding distance to nearest eigenvalue? (cf. B SINUM '09)

code:

http://code.google.com/p/mpspack

funding: NSF DMS-0507614
DMS-0811005

Preprints, talks, movies:

http://math.dartmouth.edu/∼ahb

made with: Linux, LaTeX, Prosper