Robust and efficient computation of two-dimensional photonic crystal band structure using second-kind integral equations

LSU, March 1, 2010

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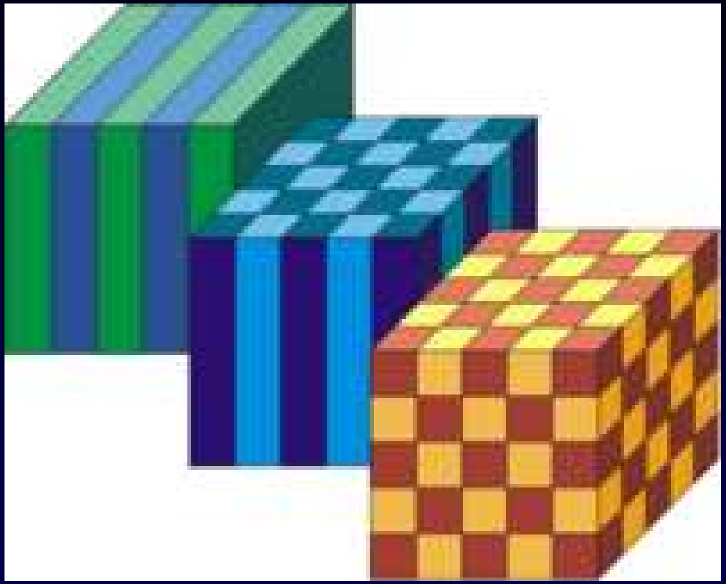
Photonic crystals



(Joannopoulos group)

periodic dielectric structures

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

control optical propagation in ways impossible in homogeneous media

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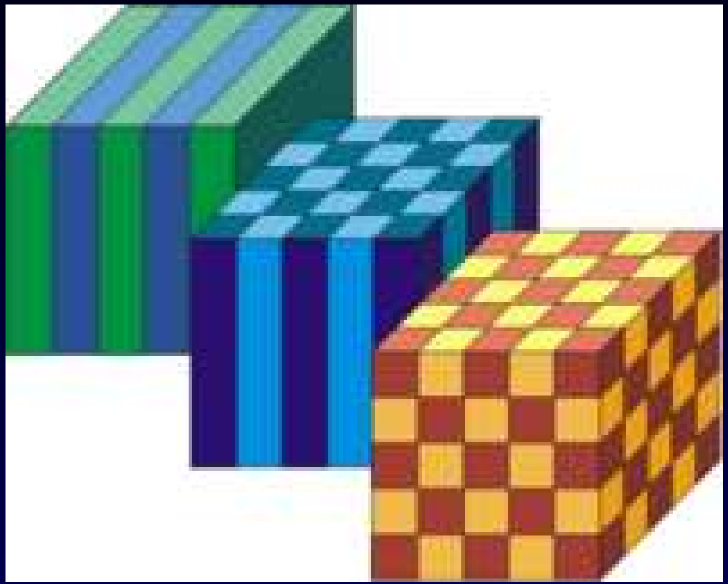

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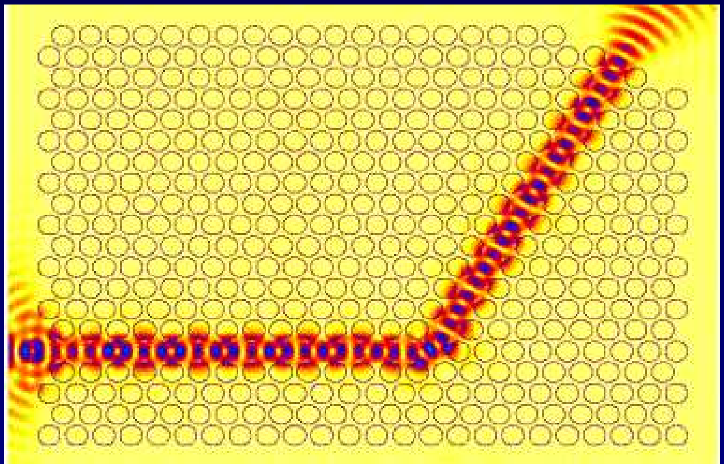
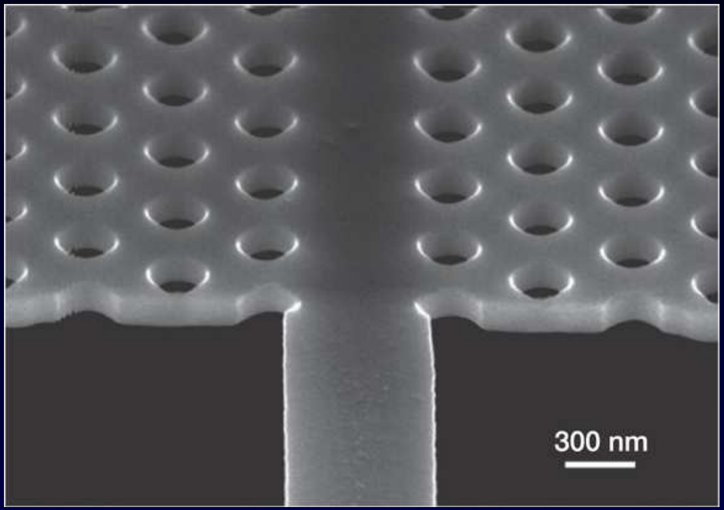


2D lattice of cylinders (INFM, U. Pavia)

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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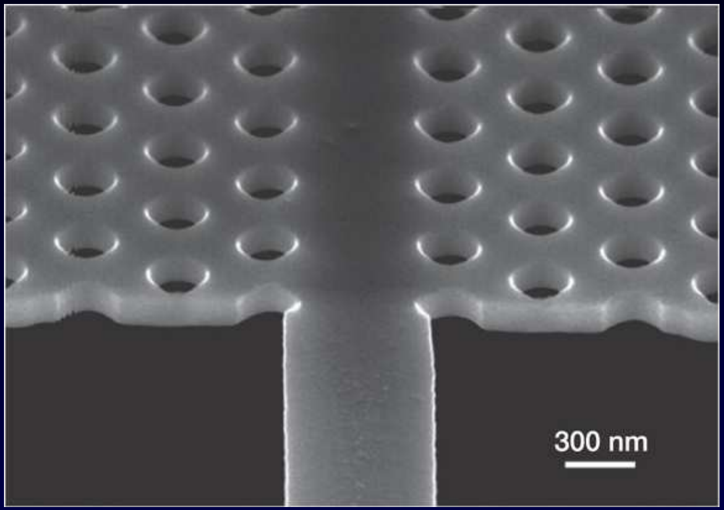

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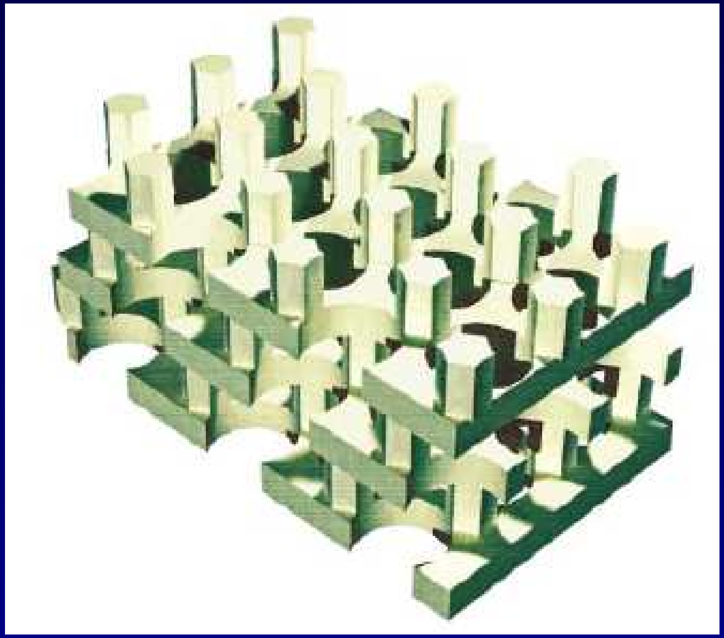
- Full 3D bandgap (all polarizations)

'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!)



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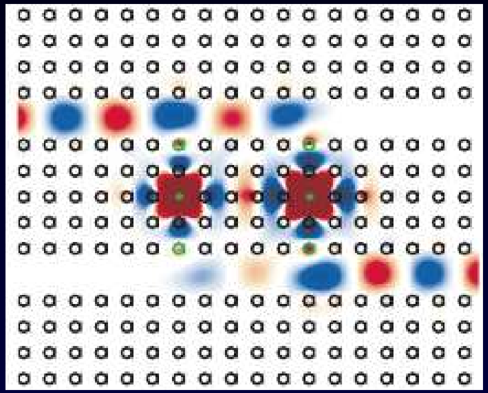
Applications

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

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

channel-drop filter in 2D crystal



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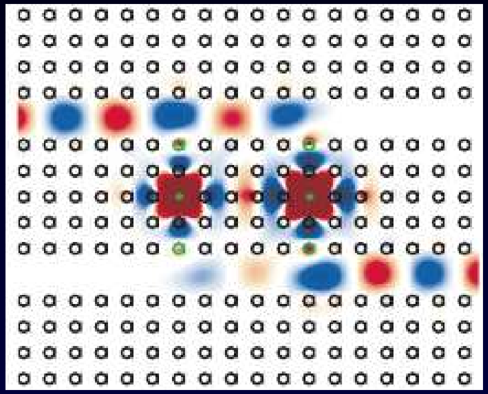

(Johnson *et al.* '00)

- Meta-materials *e.g.* negative refractive index ($-1 =$ 'perfect' lens)
- Solar cells and LEDs: control the density of states
  $\Rightarrow$ spontaneous emission/absorption rates, directions (S. Fan '97)

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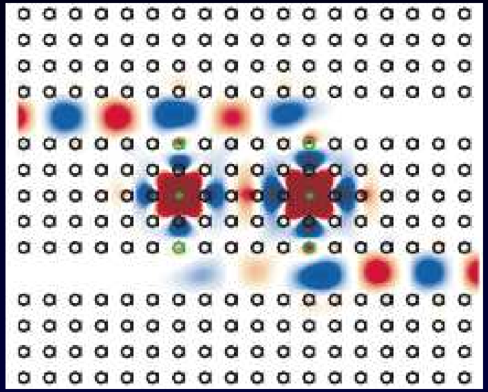

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Common features

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

Outline

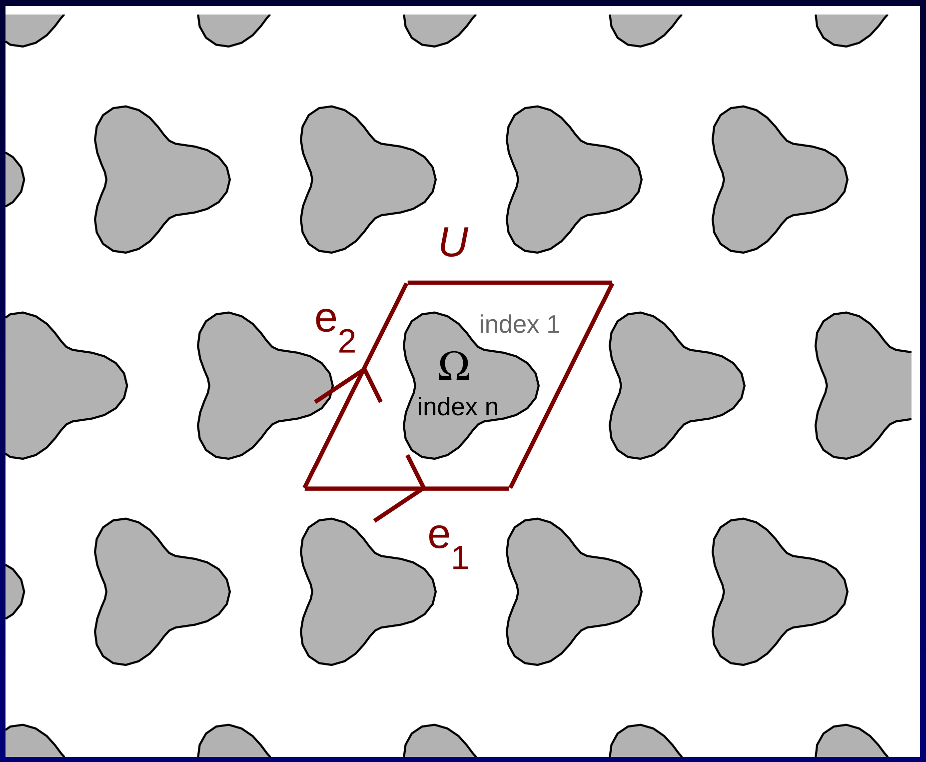
1. Band structure: eigenmodes on a torus
2. Boundary integral equations
3. Periodizing: standard way & new way
4. Interpolation of bands
5. Software environment

2D dielectric crystal (*z*-invariant Maxwell, TM polarization)

unit cell U smooth inclusion $\Omega \Subset U$, refractive index n

lattice $\Lambda := \{m\mathbf{e}_1 + n\mathbf{e}_2 : n, m \in \mathbb{Z}\}$

dielectric inclusions $\Omega_\Lambda := \{\mathbf{x} : \mathbf{x} + \mathbf{d} \in \Omega \text{ for some } \mathbf{d} \in \Lambda\}$



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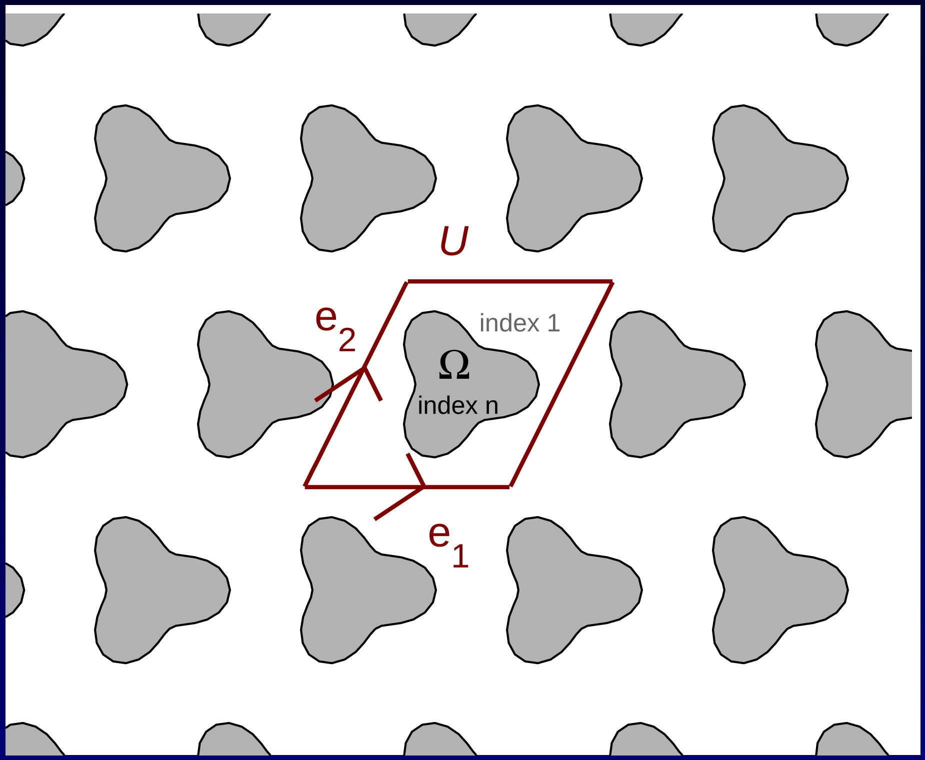

scalar wave $u : \mathbb{R}^2 \to \mathbb{C}$ obeys

PDE (fixed frequency ω):

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

material matching conditions:

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

Bloch 'theorem'

Solutions to PDE w/ periodic coeffs have form (or are sum of forms)

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

- called Bloch waves, $\mathbf{k} \in \mathbb{R}^2$ Bloch wavevector

'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)

Bloch wave and eigenvalue problem

- Bloch eigenvalues: set of $(\omega, \mathbf{k})$ s.t. non-trivial Bloch waves u exist

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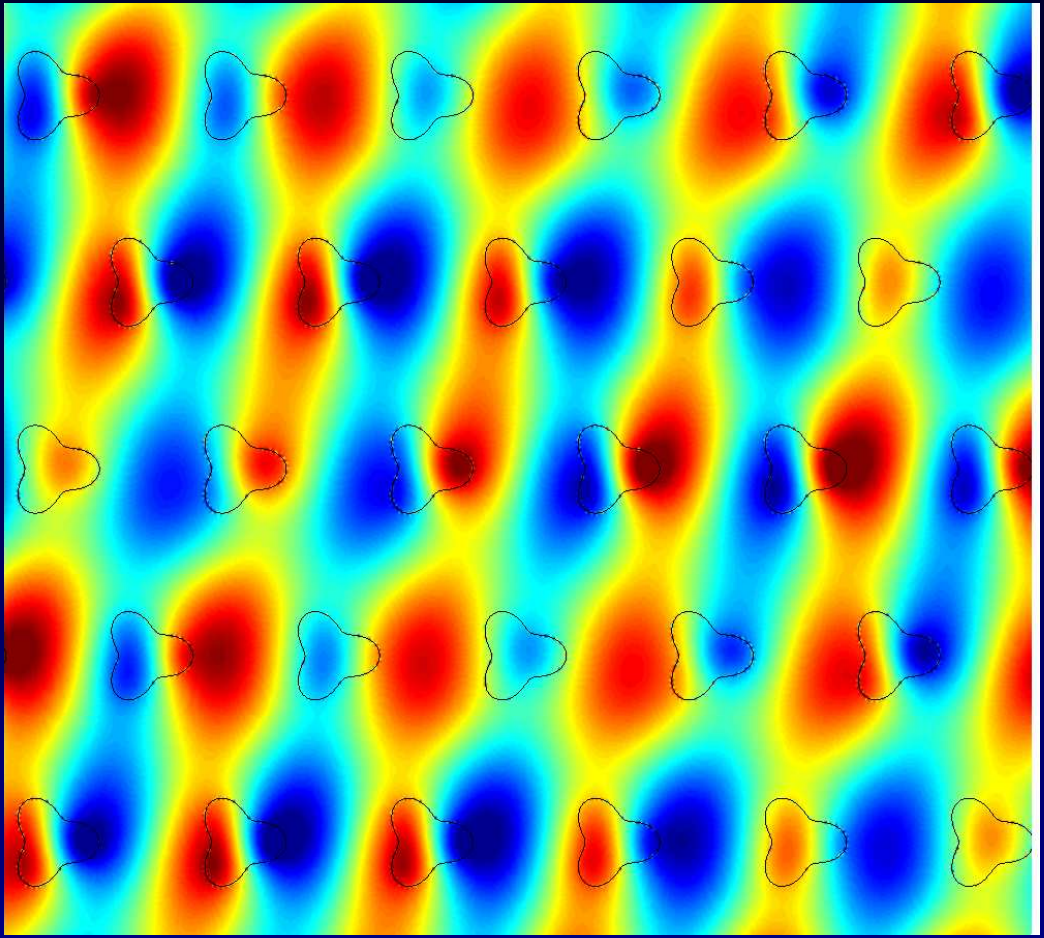

Shown: $\mathrm{Re}[u]$ for

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

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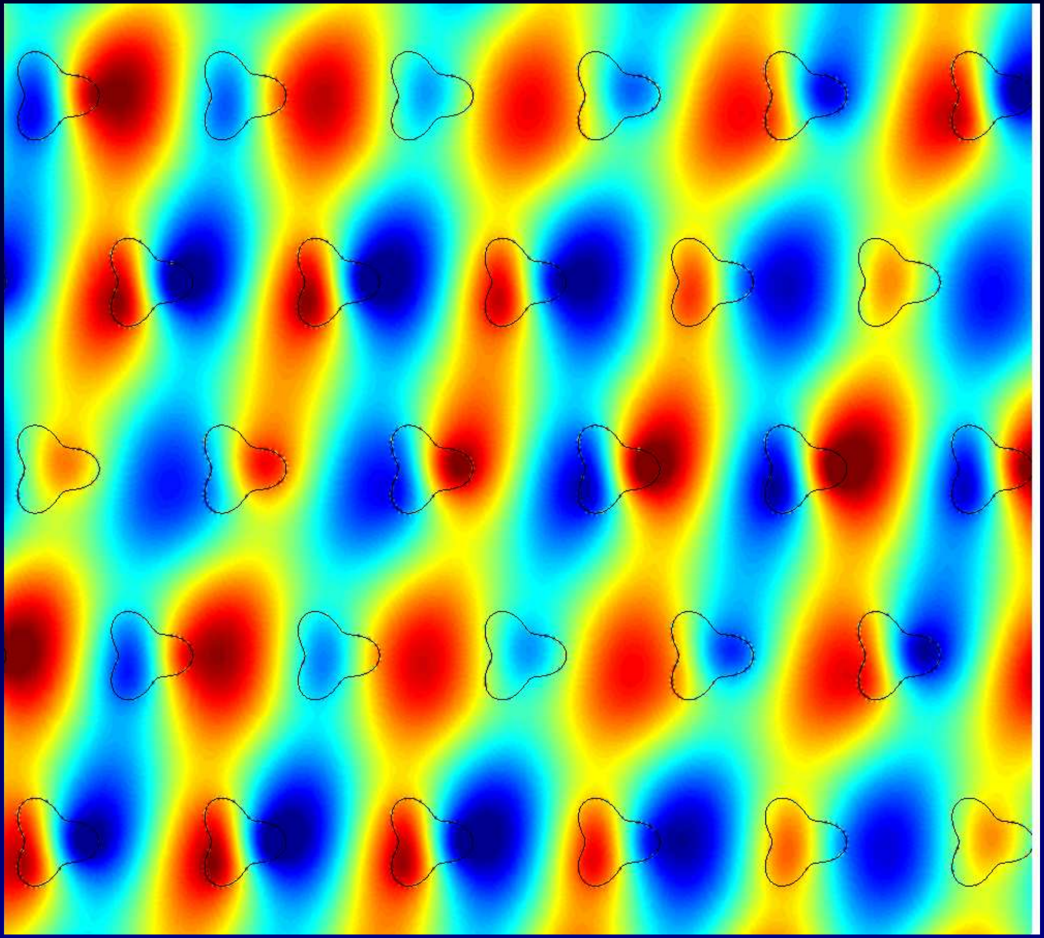

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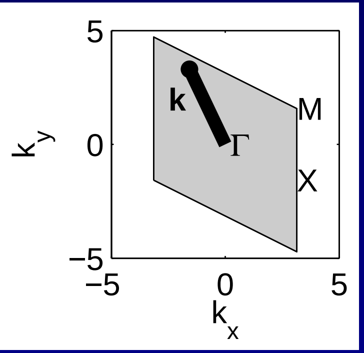
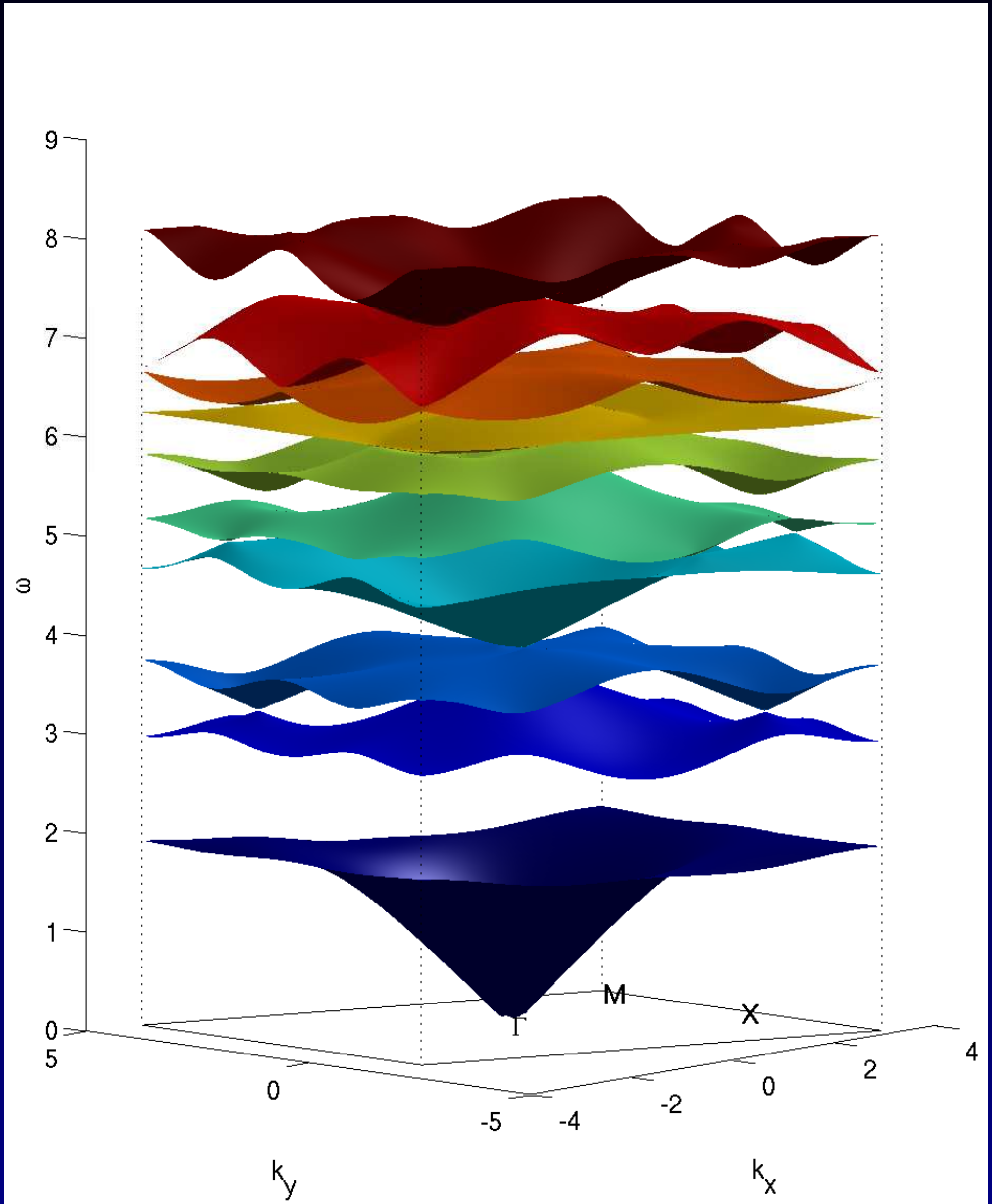
$\mathbf{k}$ equiv. to $\mathbf{k} + \mathbf{q}$, $\forall \mathbf{q} \in 2\pi\Lambda^*$

$\Lambda^* =$ dual (reciprocal) lattice

$\mathbf{k}$ lives on a torus, consider only *fundamental domain* (FD):



Band structure



For each wavevector $\mathbf{k} \in$ FD, $\exists$ discrete Bloch eigenvalues

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

- form ‘sheets’ above the FD

note: conical at low freq ω

note: bandgap

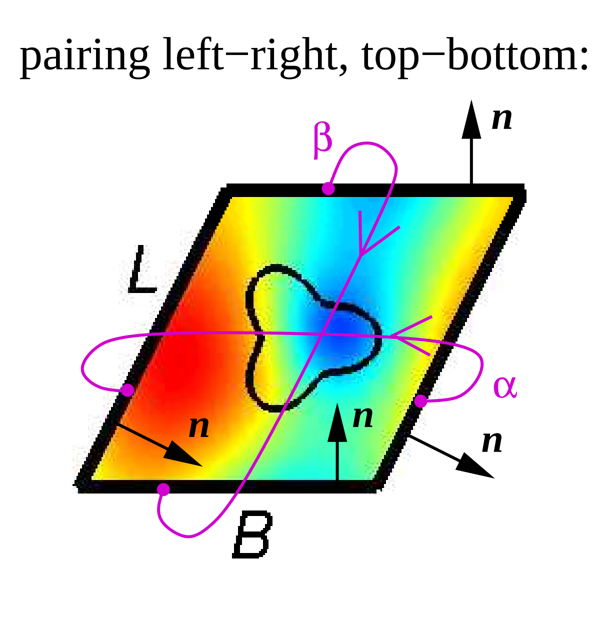
- is most important property of photonic crystal for applications

Recast problem on compact domain (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 phase parameters $\alpha := e^{i\mathbf{k}\cdot\mathbf{e}_1}$, $\beta := e^{i\mathbf{k}\cdot\mathbf{e}_2}$, $|\alpha| = |\beta| = 1$

- Task: find Bloch eigenvalue triples (ω, k_x, k_y), i.e. (ω, α, β)

Main numerical approaches

Time domain

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

low order (inaccurate); close freqs → need large t (inefficent)

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b) multiple-scattering, KKR, cylinders only (McPhedran, Moroz)

c) Plane-wave method: all in Fourier space (Joannopoulos, Johnson, Sözüer)

discont. dielectric $\Rightarrow$ Gibbs phenom, slow ($1/N$ or $1/N^2$) convergence

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

reduced dimensionality (small N)

high order (quadratures): high accuracy w/ small effort ($\Rightarrow$ sensitivity analysis)

scarcely used for band structure (Yuan '08)

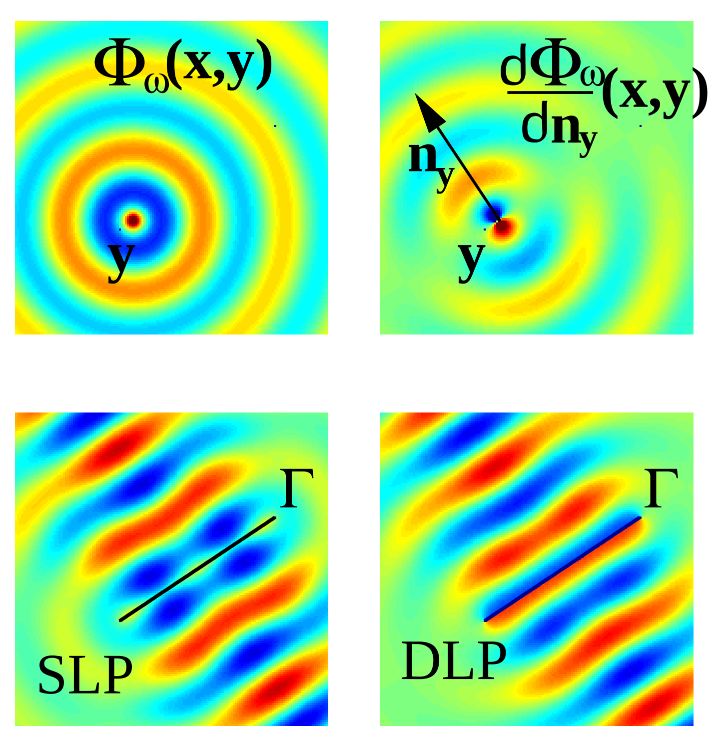
Potential theory

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

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

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

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



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

Helmholtz fundamental soln

aka free space Greens func

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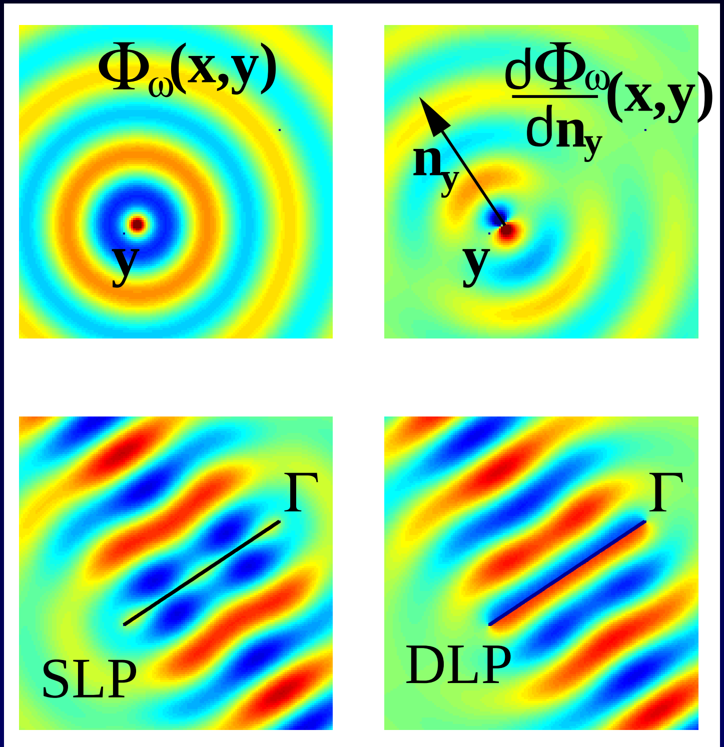


Jump relations: limit as $\mathbf{x} \to \Gamma$ may depend on which side ($\pm$):

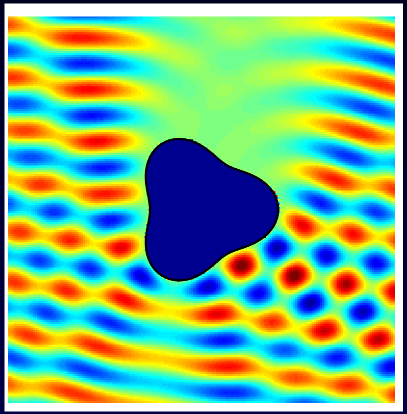
$$u^\pm = S\sigma$$
$$u_n^\pm = D^T\sigma \mp \tfrac{1}{2}\sigma$$
$$v^\pm = D\tau \pm \tfrac{1}{2}\tau$$
$$v_n^\pm = T\tau$$

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 (sketch)

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



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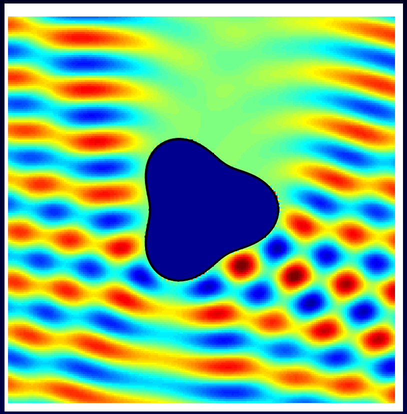

BC $\quad 0 = u^+ = u^{\text{inc}}|_{\partial\Omega} + (D + \frac{1}{2})\tau$ by JR3

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

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

Why important? when scale up...

condition # small, iterative solvers (GMRES) fast

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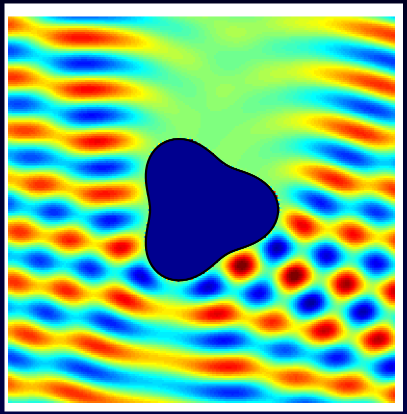

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Nyström discretization: N-by-N linear system for vector $\{\tau_k^{(N)}\}_{k=1}^N$

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

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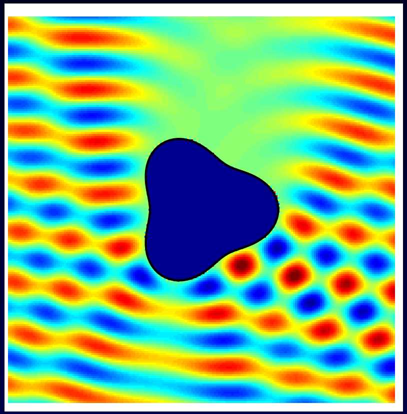

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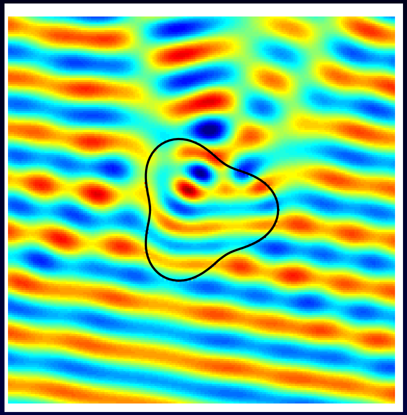
Thm: (Anselone, Kress) $\|\tau^{(N)} - \tau\|_\infty$ converges at *same rate* as quadrature scheme for the true integrand $D(\mathbf{y}, \cdot)\tau$.

- Analytic curve & data, periodic trapezoid rule: spectral convergence
- *e.g.* above: $N = 60$ enough for 10^{-6} error, $N = 100$ for 10^{-12}
- error $= O(e^{-\gamma N})$, 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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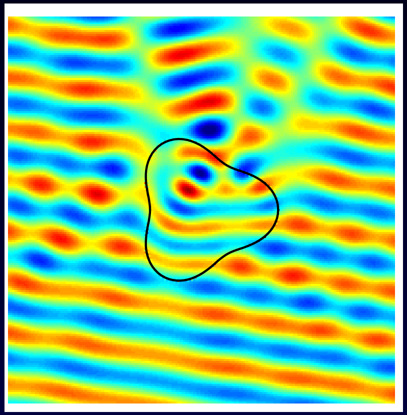

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mismatch on $\partial\Omega$: $h := u^+ - u^-$, $h' := u_n^+ - u_n^-$

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

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

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)

The standard way to periodize

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

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Theorem (*integral formulation of band structure*) :

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

note: no u^{inc} since eigenvalue problem homogeneous

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Not a robust method: A_{QP} does not exist for certain parameters (ω, k_x, k_y)

since there $\Phi_{\omega,\mathrm{QP}}(\mathbf{x}) \to \infty, \ \forall \mathbf{x}$

why. . . ?

Failure at spurious resonances

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

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

spectral representation on torus

has simple pole wherever (ω, k_x, k_y) is eigenvalue of empty torus…
but physical field u well-behaved here: breakdown is non-physical!

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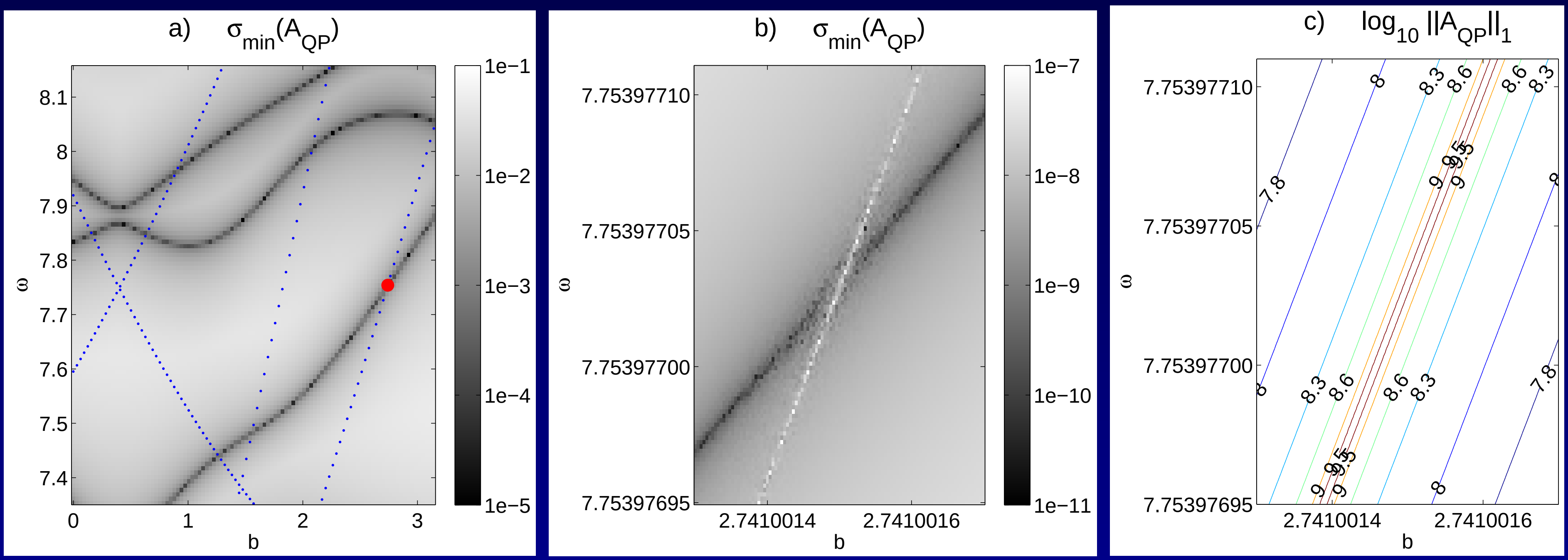
$$= \frac{1}{\mathrm{Vol}(U)} \sum_{\mathbf{q}\in 2\pi\Lambda^*} \frac{e^{i(\mathbf{k}+\mathbf{q})\cdot\mathbf{x}}}{\omega^2 - |\mathbf{k}+\mathbf{q}|^2} \qquad \text{spectral representation on torus}$$

has simple pole wherever (ω, k_x, k_y) is eigenvalue of empty torus. . .
but physical field u well-behaved here: breakdown is non-physical!



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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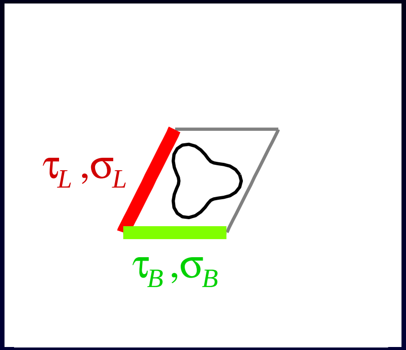
- added extra degrees of freedom (a small #, indep. of complexity of Ω)
- gain robustness: no matrix element blow-up at spurious resonances

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

- idea of extra sources of waves not new (*e.g.* Hafner '02)
- what is new: $M = \text{Id} + \text{compact}$ 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 $\xi = [\tau_L; \sigma_L; \tau_B; \sigma_B]$



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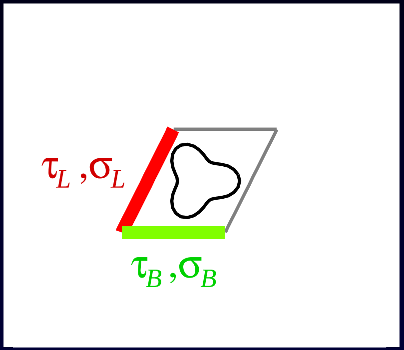

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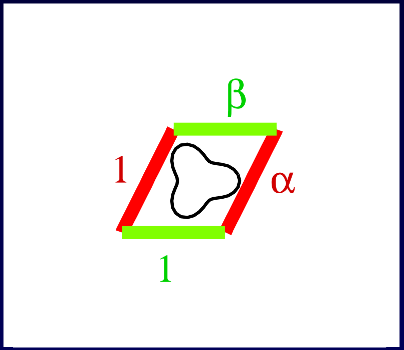
  recall $f := u|_L - \alpha^{-1} u|_{L+\mathbf{e}_1}$



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

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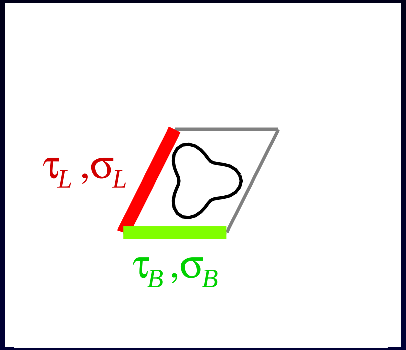

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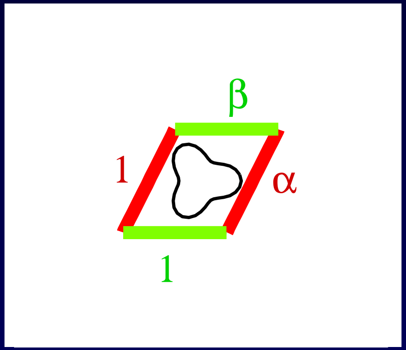
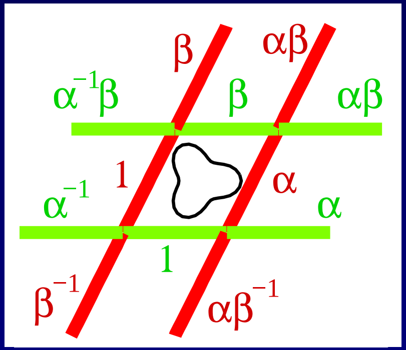


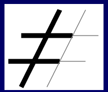
effect of σ_L on $u_n|_L$

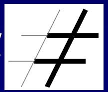
effect of $\alpha\sigma_L$ on $\alpha^{-1} u_n|_{L+\mathbf{e}_1}$

} cancel apart from Id

- 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

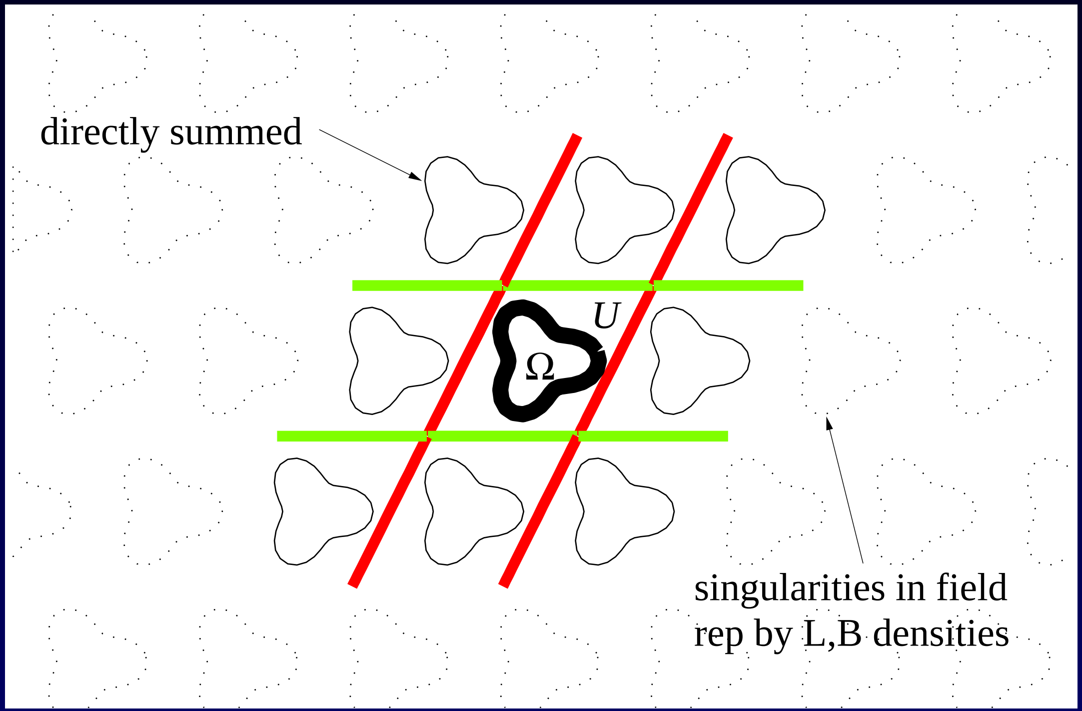
$\Rightarrow$ all corner interactions vanish!

- 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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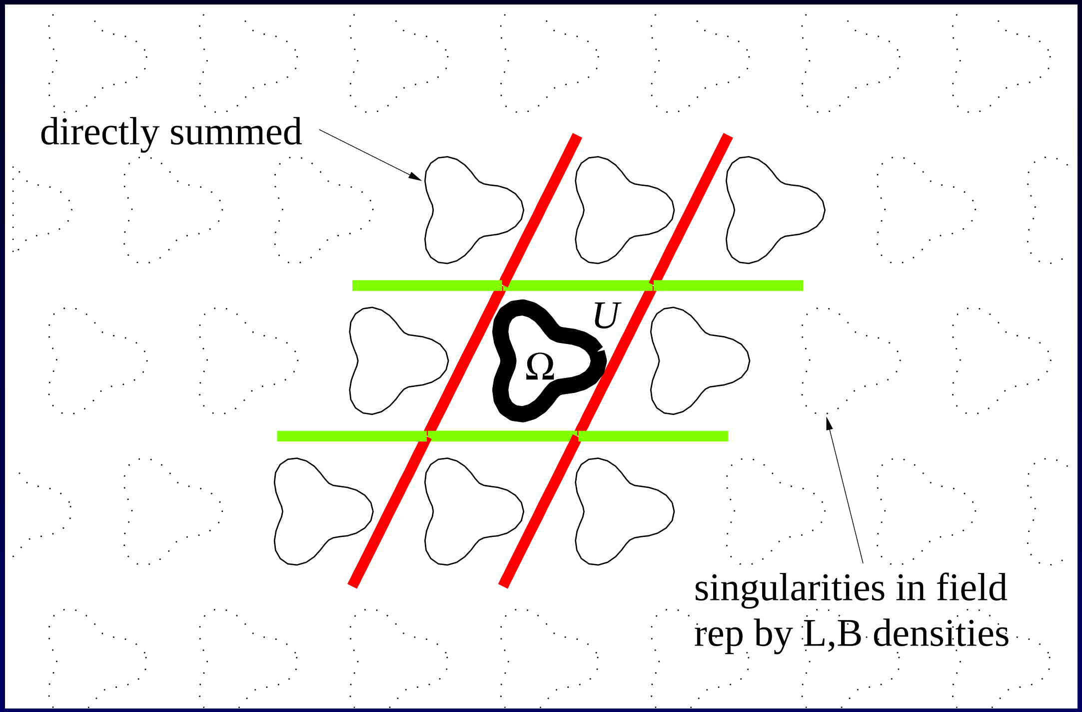
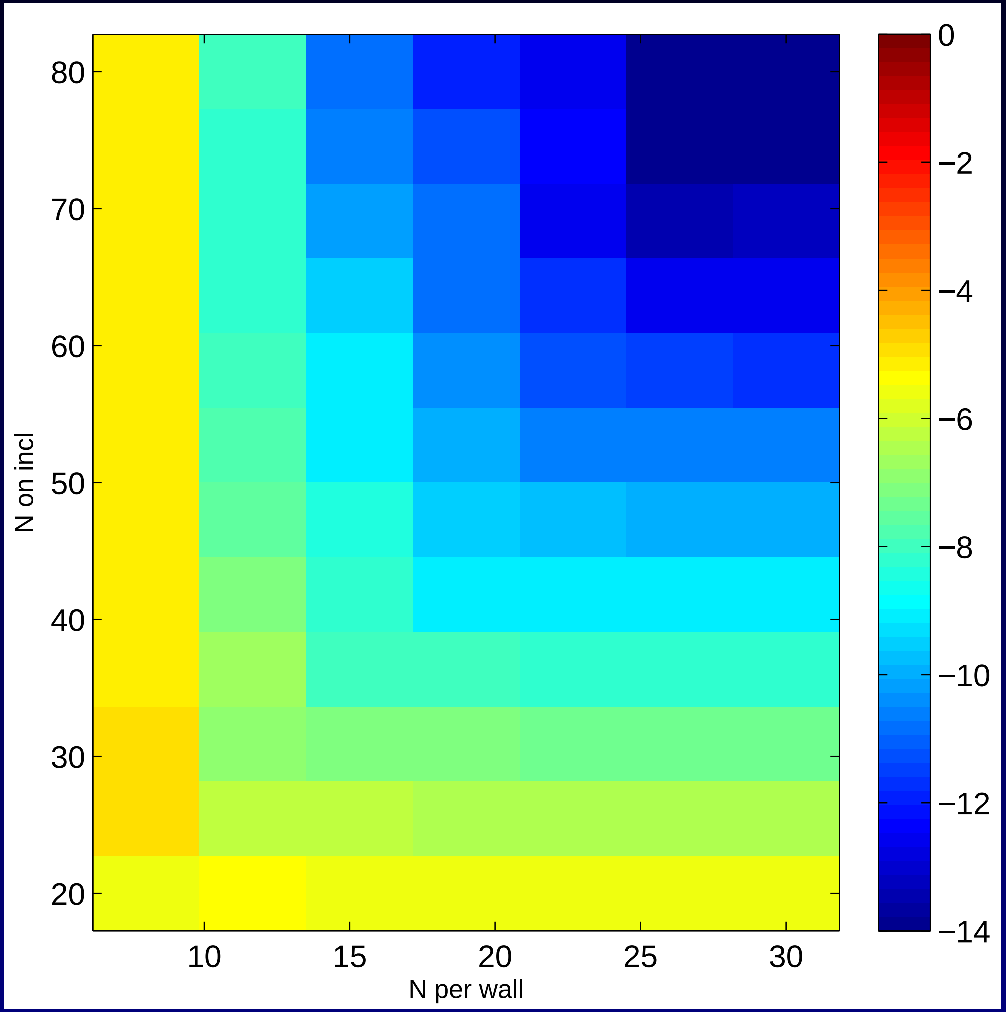


- Careful cancellations: B, C, Q have only interactions of distance ≥ 1
- Large dist increases convergence rate, i.e. large c in error = $O(e^{-cN})$

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

Error convergence

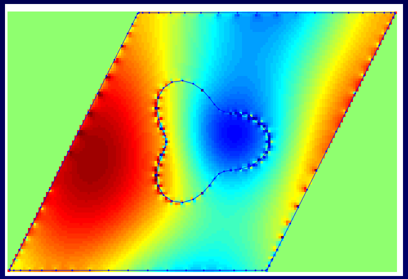
$\log_{10}$ min sing. val M for known Bloch eigenvalue (should be zero):



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

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

mode:



- spectral (exponential) convergence in inclusion & wall # dofs

Crude results: small inclusion

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

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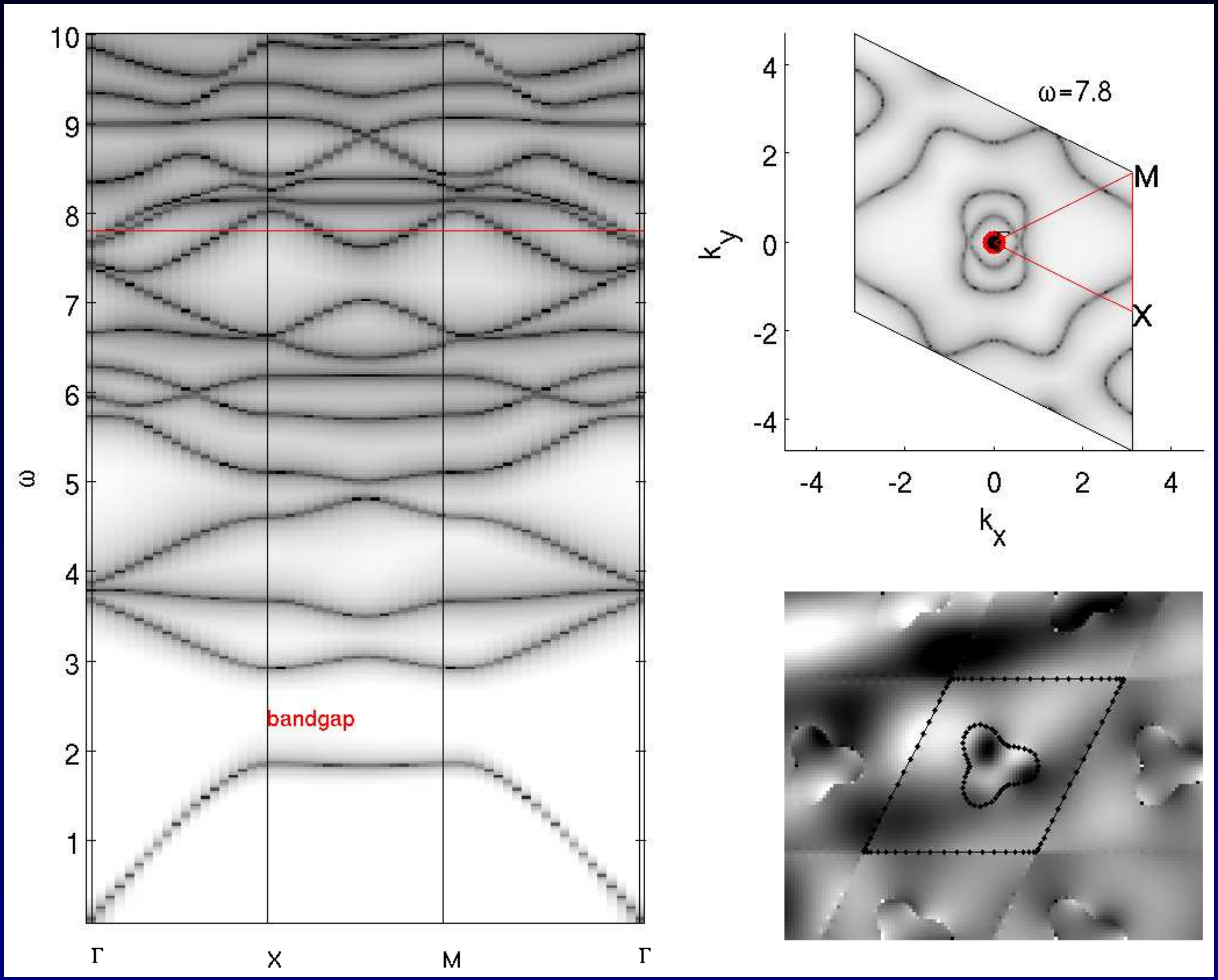


0.1 sec per eval

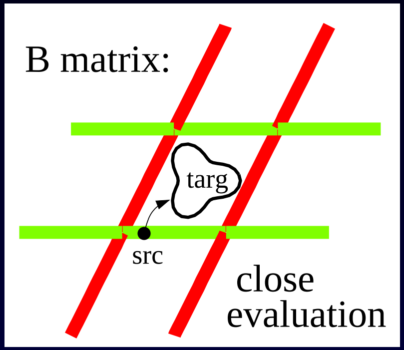
pre-store α, β coeffs

30 sec per const-ω slice

24×24 evals

- errors 10^{-9} for 40 pts on $\partial\Omega$, 20 on each wall (total $N = 160$)

Large inclusion passing through unit cell



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

- fix via adaptive quadrature of Lagrange interpolant?
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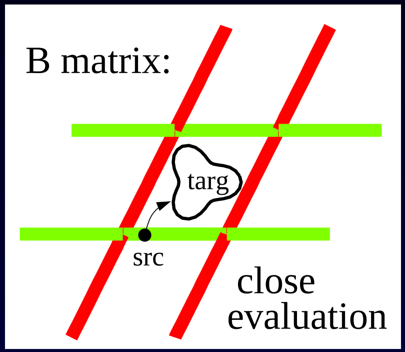

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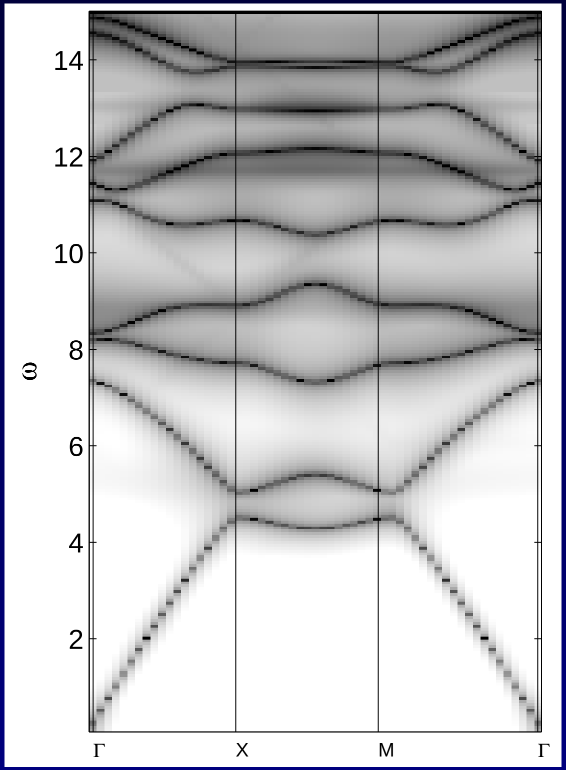

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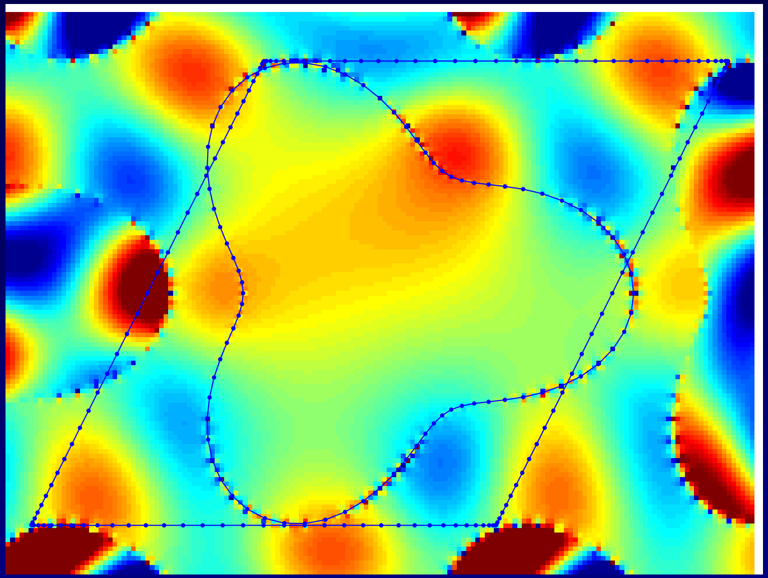

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$\mathbf{k} \approx (0.17, 2.11)$

$n{=}1$ inside

$n{=}3.3$ outside

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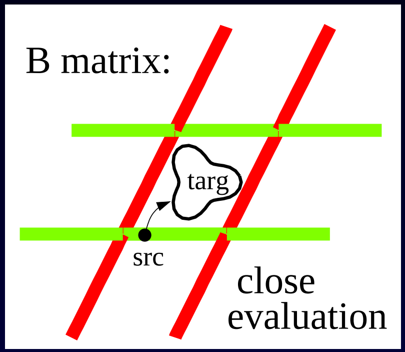

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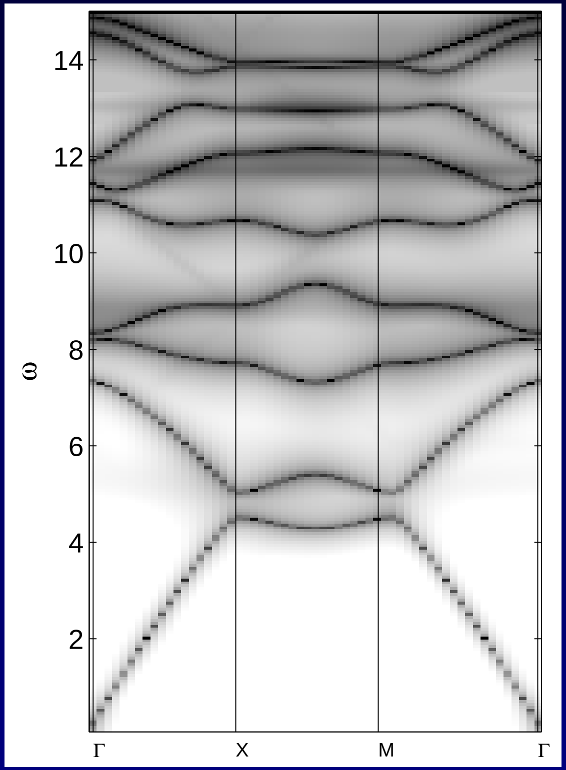

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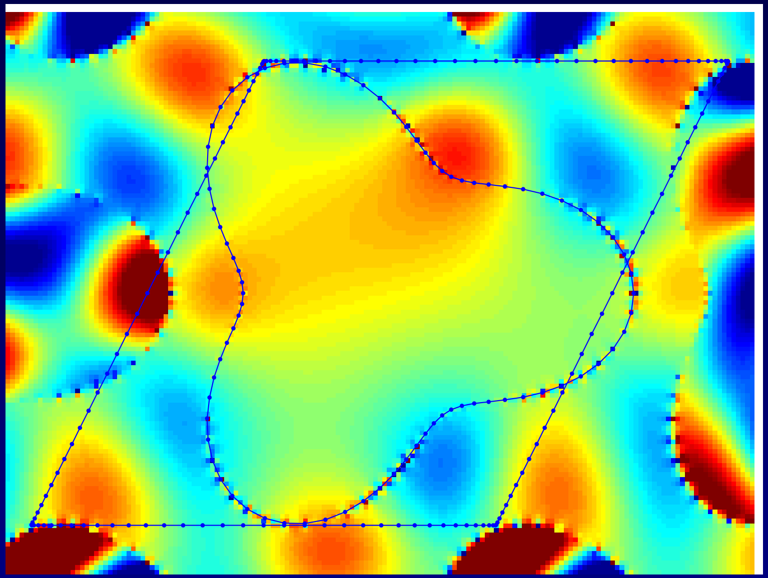

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Sampling fine 3D grid is crude & slow: how find bands to spectral acc?

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How find eigenvalue sheets in the volume $S^1 \times S^1 \times (0, \omega_{\text{max}})$?

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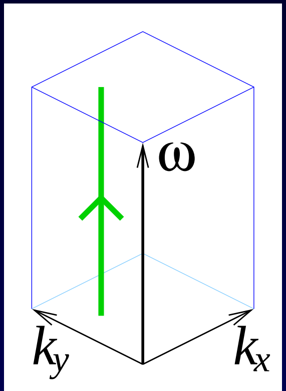

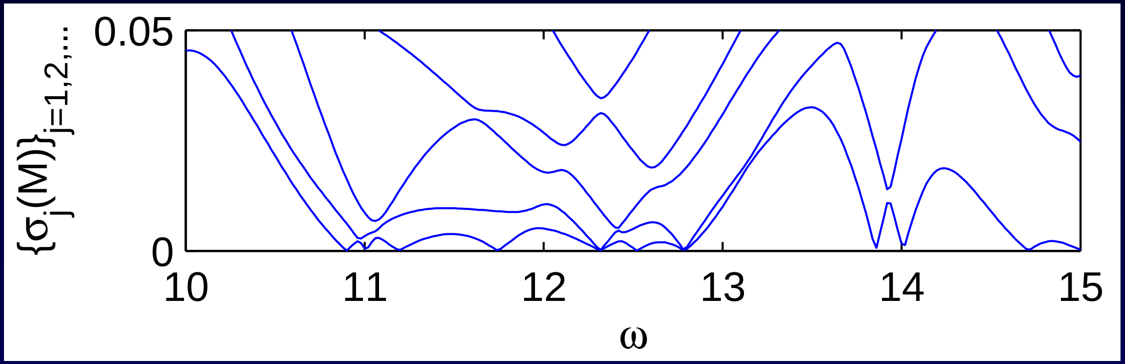

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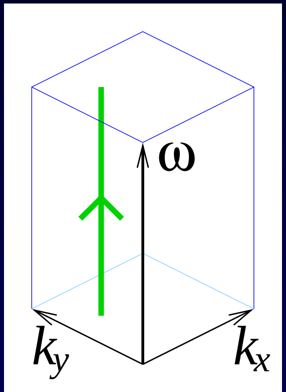

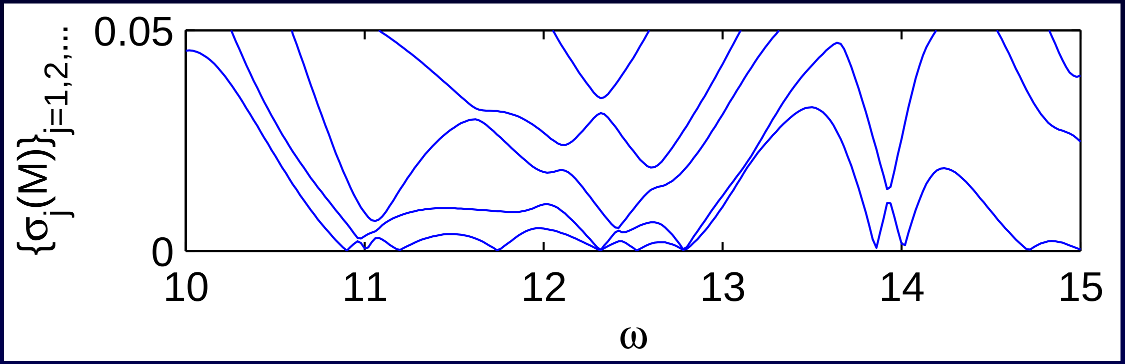

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Realize: $M = I +$ (cpt op-valued analytic func of ω, k_x and k_y)

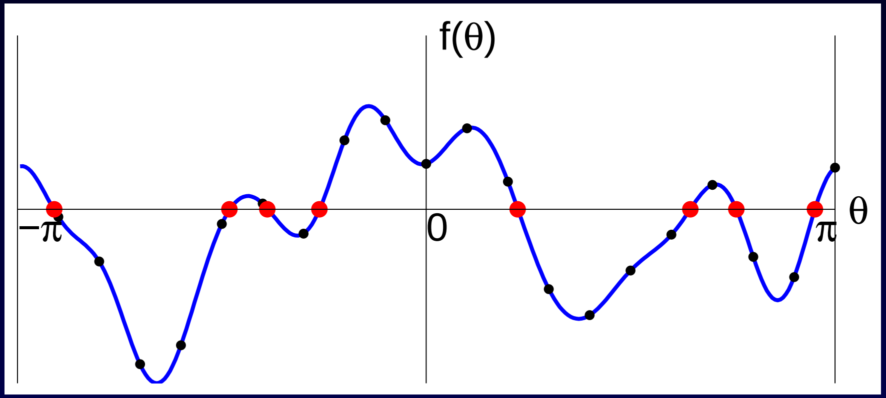
det M is a Fredholm determinant, also analytic

- rootfinding a real-analytic function is nice. . . (J. Boyd '02)

Spectral rootfinding of analytic functions

(Boyd '02)

$f : \mathbb{R} \to \mathbb{R}, \quad 2\pi$-periodic



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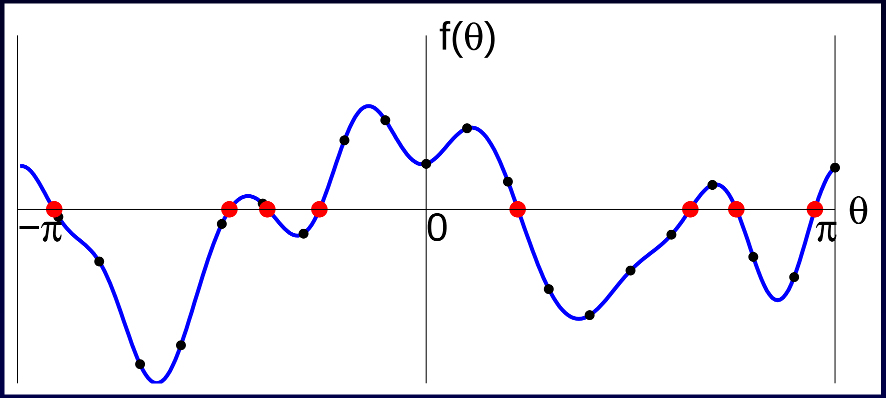

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$$f(\theta) \approx \sum_{n=-N}^{N} c_n e^{in\theta}$$

exponentially convergent in N

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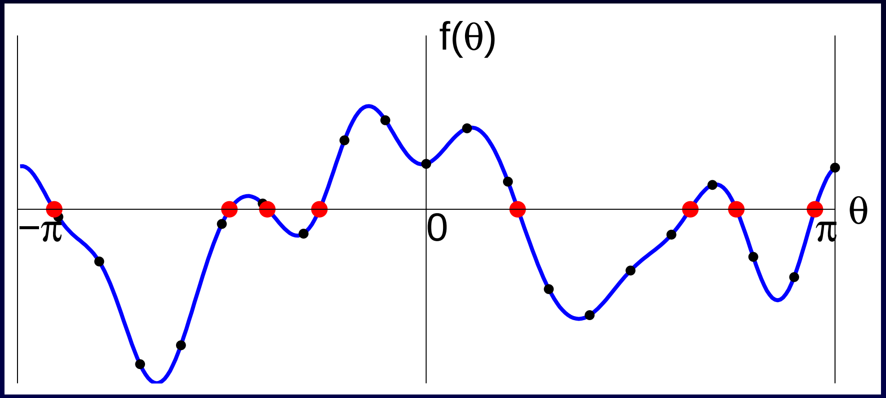

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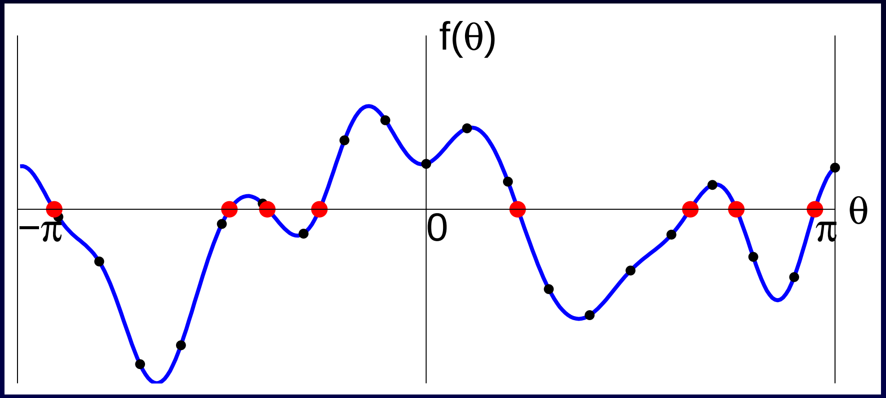

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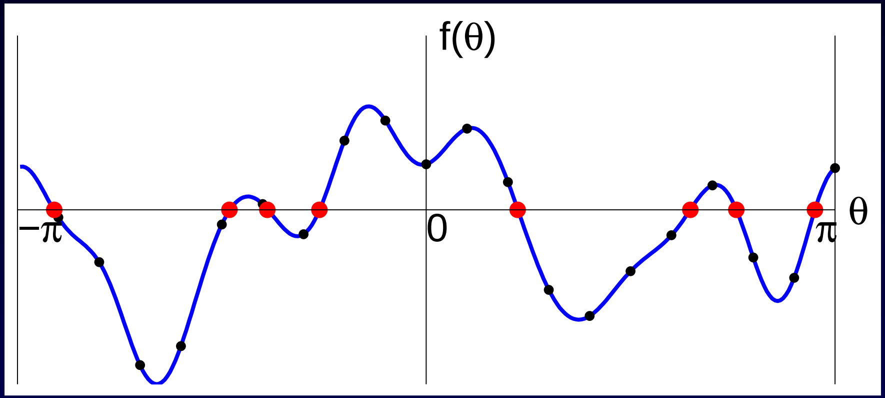

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"Degree doubling": $z^N q(z)$ is degree-$2N$ poly, so...

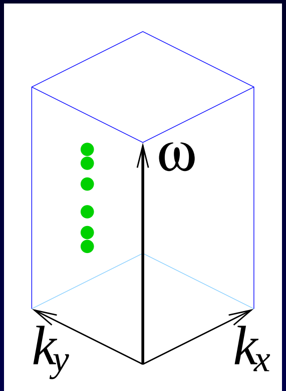
- use Matlab `roots` QR for eigvals of companion matrix, $O(N^3)$ but v. stable
- extract the angles θ of roots near unit circle

(Boyd nonlin EVP; Trefethen-Battles '06 `chebfun`)

Rootfinding det M in the ω direction

det $M(\omega, k_x, k_y)$ not periodic in ω: map $\omega = \omega_0 + a\cos\theta$ periodic θ

this is Chebyshev interpolation on interval $[\omega_0 - a, \omega_0 + a]$



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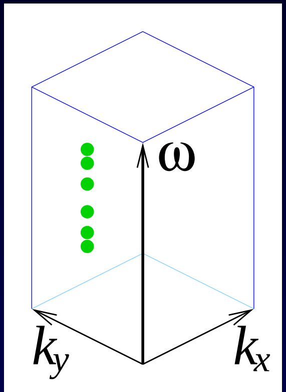

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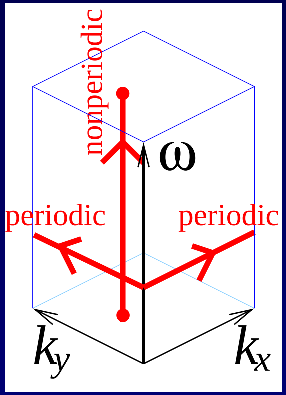
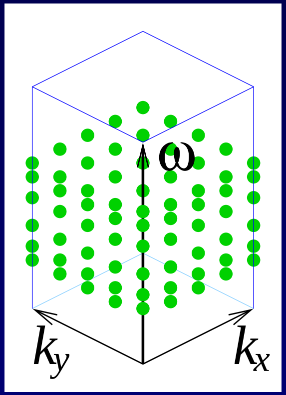


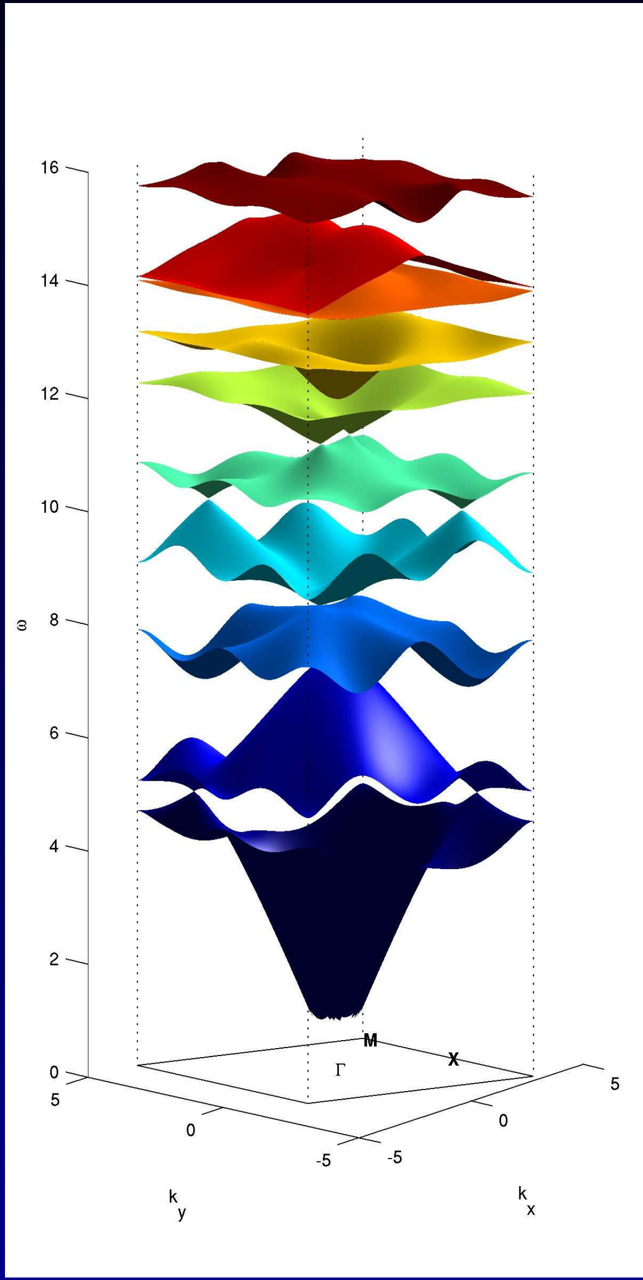
Also analytic in $k_x, k_y \Rightarrow$ interpolate in 3D!



Robust spectrally-accurate bands via small # grid evals

e.g. $25 \times 24 \times 24$ for $\omega \in [4, 6]$ and whole Brillouin zone, error 10^{-8}

Band structure to spectral accuracy



n=0.3 inside
n=1 outside
large inclusion

eval only 24×24 samples in $\mathbf{k}$
but contains much finer details
10^{-8} errors, 1 hour on laptop

- Note: eigenvalues $\omega_j(\mathbf{k})$ are not analytic!
  $\exists$ conical (diabolical) points ...interpolates poorly

- like level set method: handle smooth func

movie 1

Software environment (teaser)

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- implements above & more: Helmholtz, Laplace, scattering
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piecewise analytic curves

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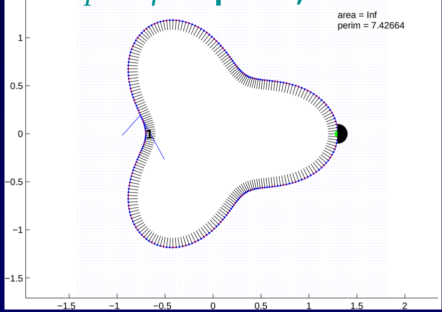
output of **`d.plot;`**

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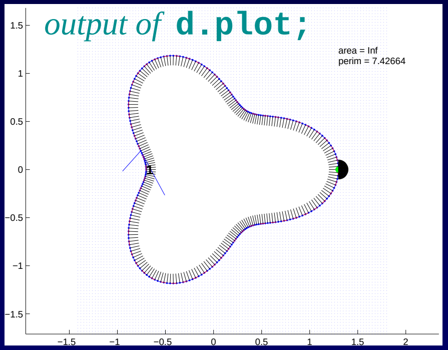


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```
d.setbc(1, ’N’, []);
```

Neumann BCs on exterior

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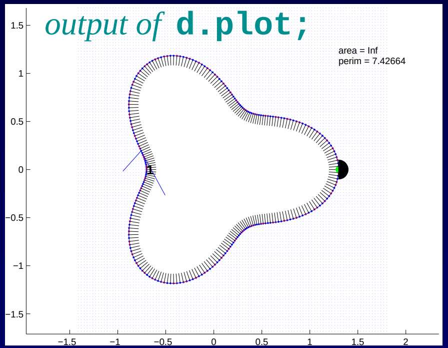


```
d = domain([], [], s, -1);
```

make exterior domain using segment

```
d.setbc(1, 'N', []);
```

Neumann BCs on exterior

```
d.addmfsbasis(s, 200, struct('tau',0.05));
```

choose basis set for solution

Software environment (teaser)

`MPSpack`: object-oriented 2D PDE toolbox in Matlab (B-Betcke '09)

- implements above & more: Helmholtz, Laplace, scattering
- intuitive interface: curves, domains, basis sets, problems, are objects

E.g.

```
s=segment.radialfunc(100,{@(q)1+.3*cos(3*q),@(q)-.9*sin(3*
```

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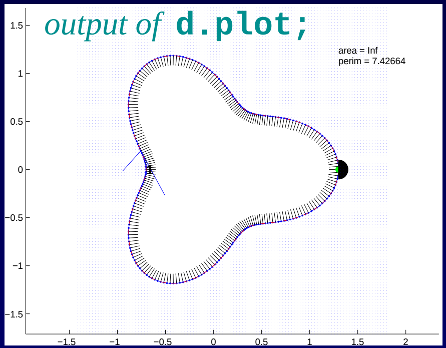

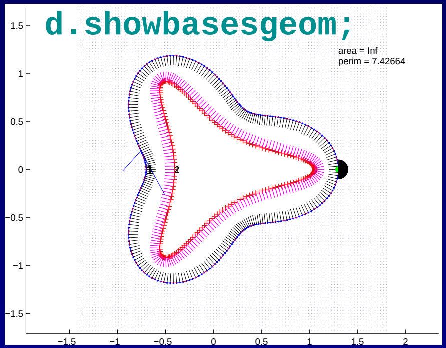

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make a scattering problem from domain `d`

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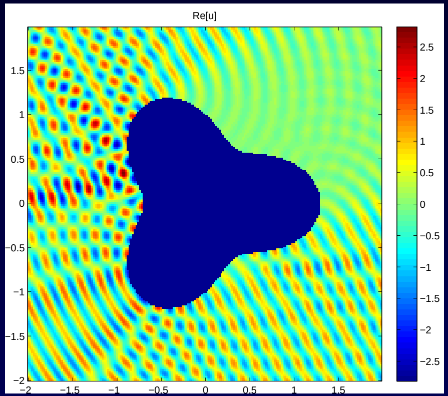

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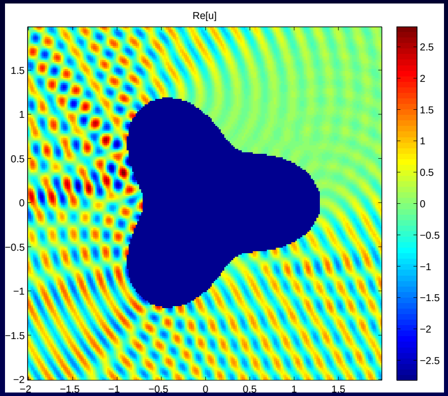
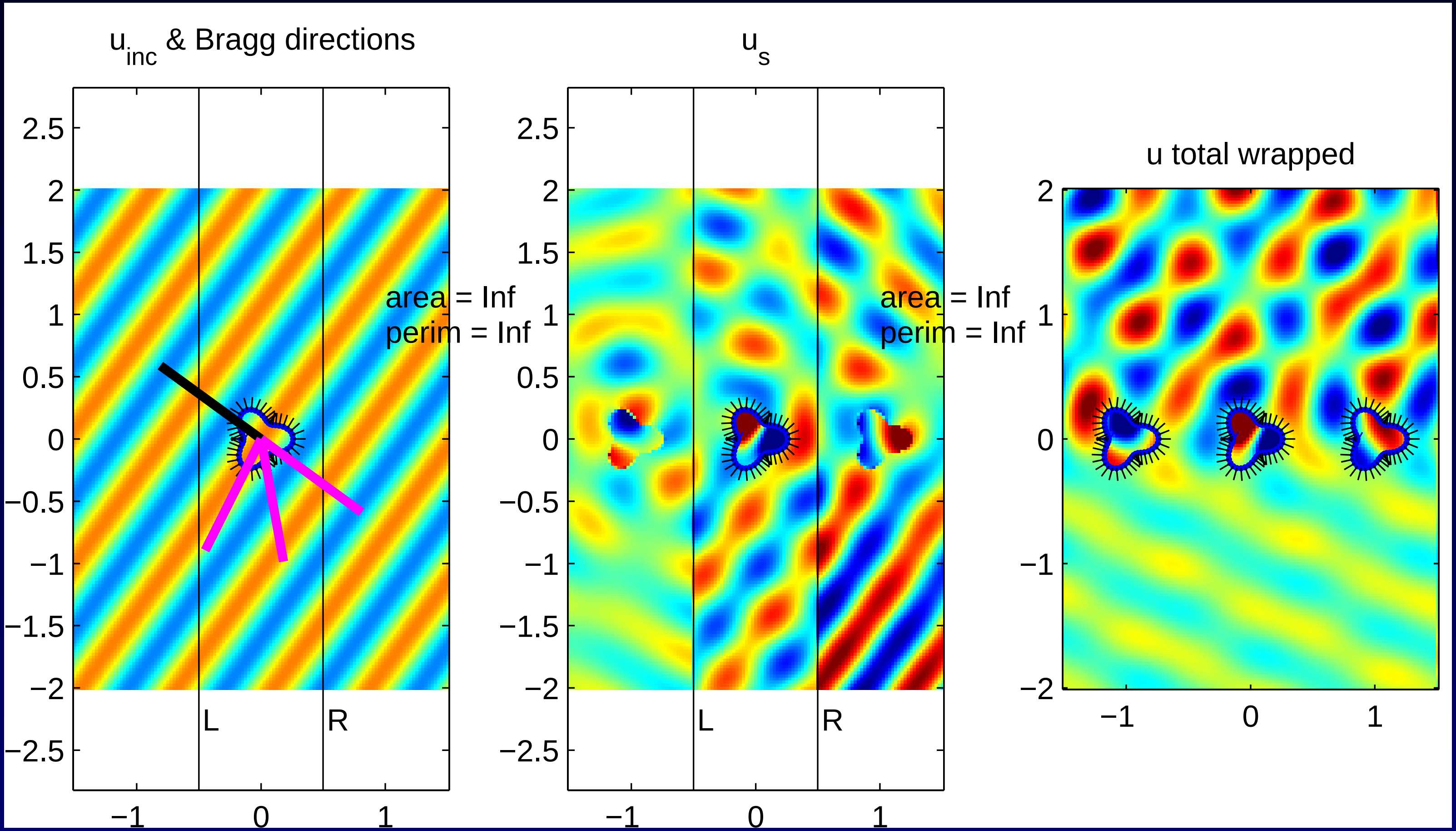


- was easy case: 8 lines (could have done in 80 lines of Matlab)
- multiple (sub)domains: basis, quadrature, bookkeeping hidden
  e.g. dielectric band structure still only 20 lines of code
- human-readable, rapid to code, sensible defaults (you can change)

To do: automatic meshing, Dirichlet EVP, …

Current work: grating scattering

Quasi-periodize in x-direction only: layer-potentials infinite in y …



- $N = 50$ unknowns on inclusion, $M = 200$ unknowns to periodize
- accuracy 10^{-13}

Conclusions

- efficient 2nd-kind integral equations 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 blow-up at empty resonances
  – extends simply to 3D (unlike lattice sums)
- interpolate Fredholm det, not Bloch eigenvalues themselves

Future:

- 3D; drop in FMM for inclusion; gratings with substrate …

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

funding: NSF DMS-0507614
DMS-0811005

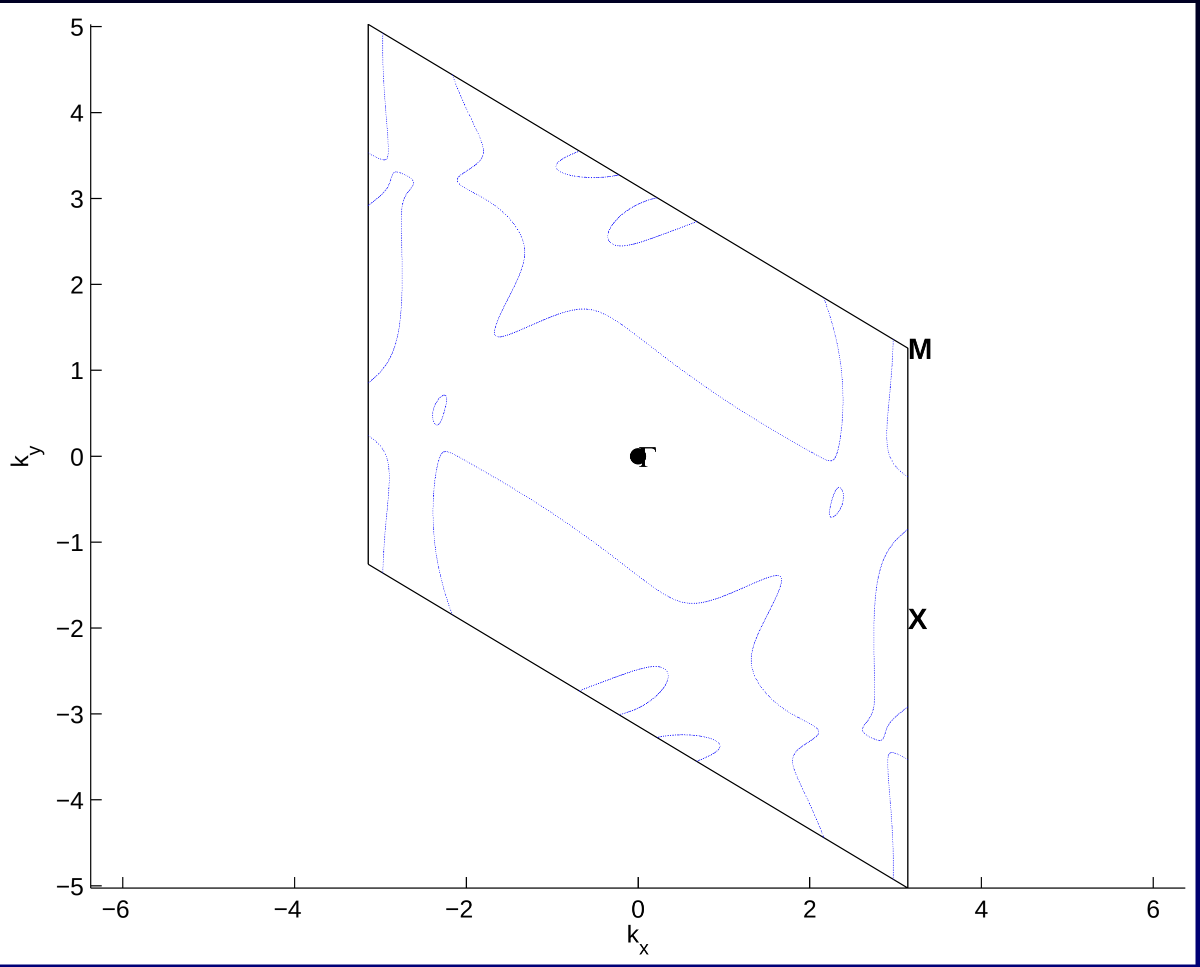
Preprints, talks, movies:
http://math.dartmouth.edu/∼ahb

made with: Linux, LaTeX, `Prosper`

EXTRA SLIDES

Equal-frequency curves

Complexity of const-ω slice across Brillouin zone:



- only 24×24 evaluations of det M, Boyd's spectral rootfinding
- Apps: Snell's Law for reflection off semi-∞ crystal