A new integral representation of quasi-periodic fields and its application to scattering and Bloch eigenvalue problems

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joint work with Leslie Greengard (Courant Institute, NYU)

Scattering in 2D from periodic grating

time-harmonic linear waves, obey $(\Delta + \omega^2)u = 0$ Helmholtz, freq ω

incident plane wave $u^i(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}}$ wavevector $\mathbf{k} = (\kappa^i, k^i)$ $|\mathbf{k}| = \omega$, unit speed

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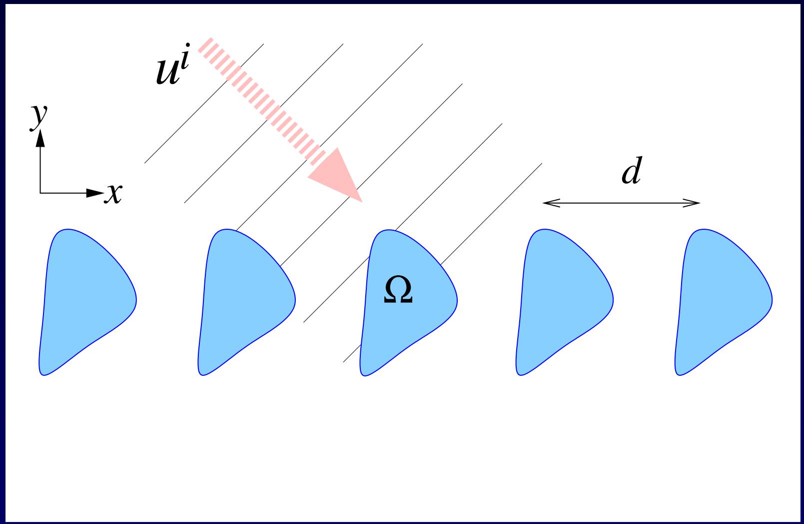

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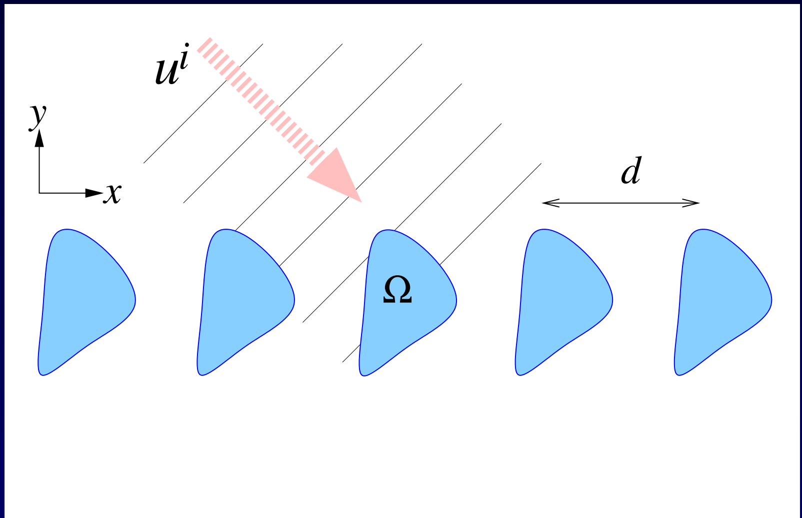

total field $u^t = u^i + u$, where

scattered field u solves BVP:

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(\Delta + \omega^2)u &= 0 && \text{in } \mathbb{R}^2 \setminus \overline{\Omega_\mathbb{Z}} \\
u &= -u^i && \text{on } \partial\Omega_\mathbb{Z} \quad \text{Dirichlet} \\
u & \text{ `radiative' as } y \to \pm\infty
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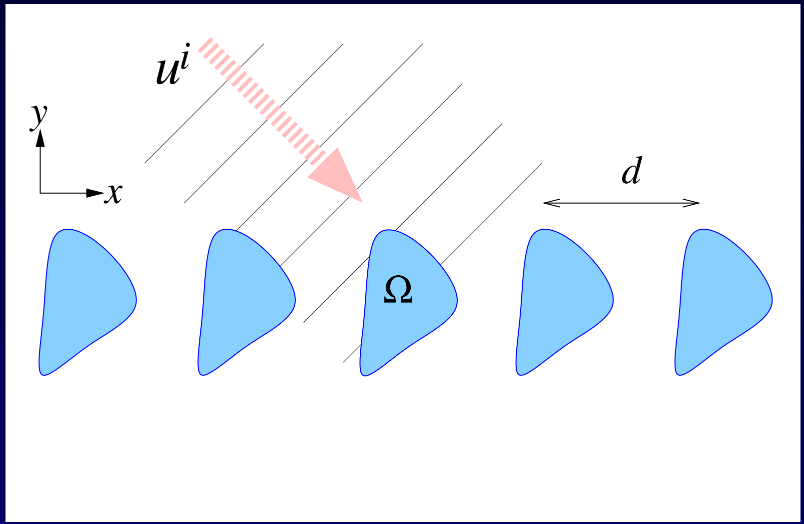

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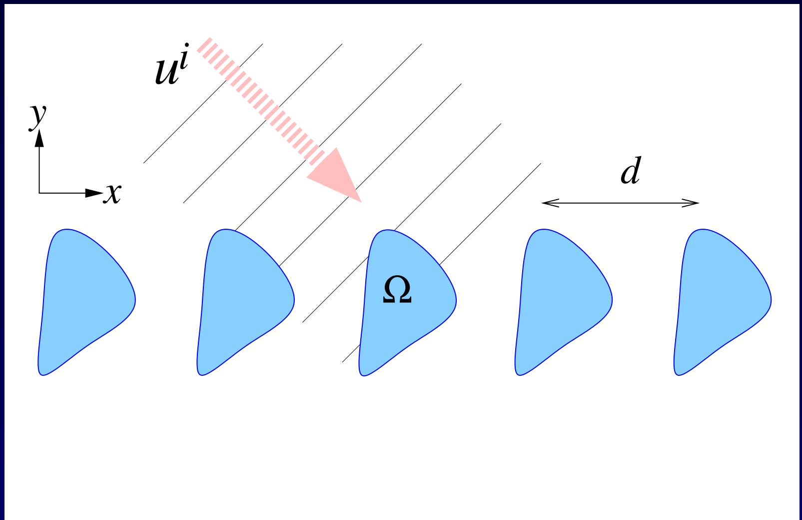

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- classical BVP: acoustics, z-invariant Maxwell (Rayleigh 1897,...)
- Apps: optics, filters, lithography, photonics, plasmons, surface meas...

Plane waves of same quasi-periodicity

u^i is QP, but so are other plane waves, wavevectors (κ_n, k_n):

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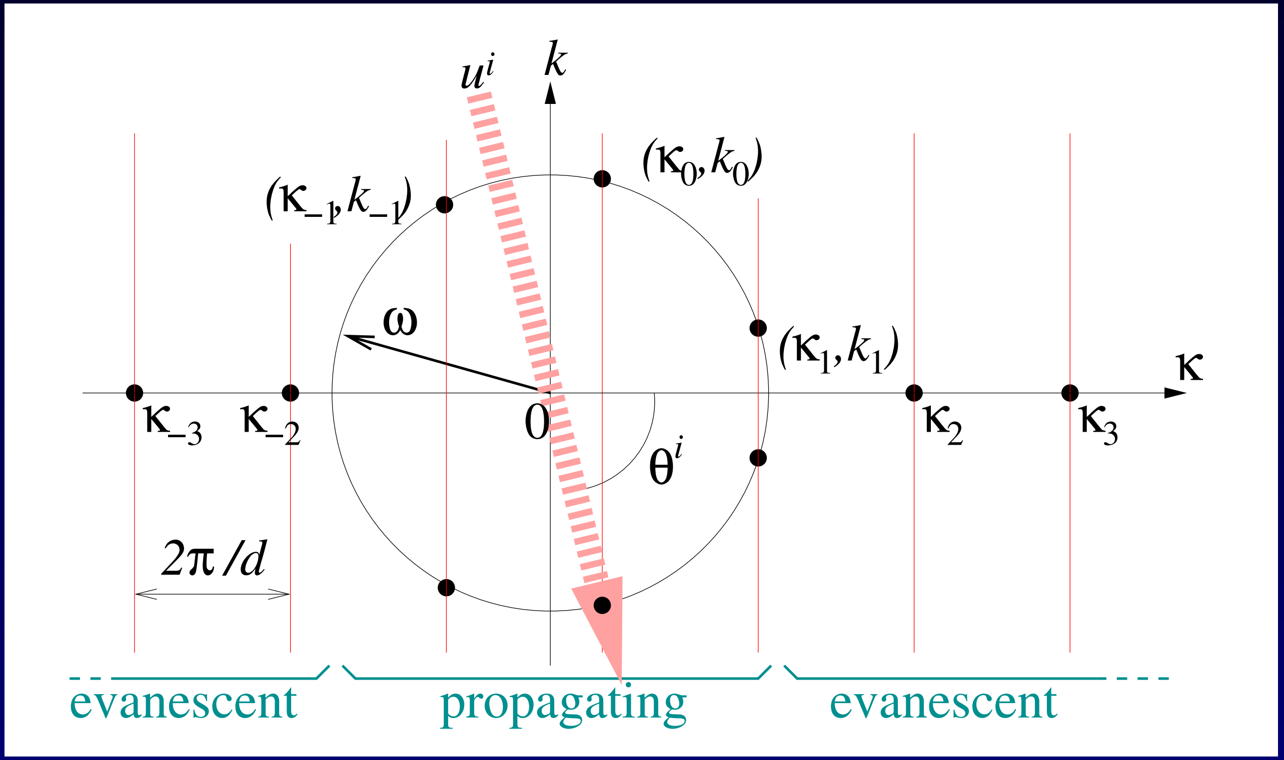

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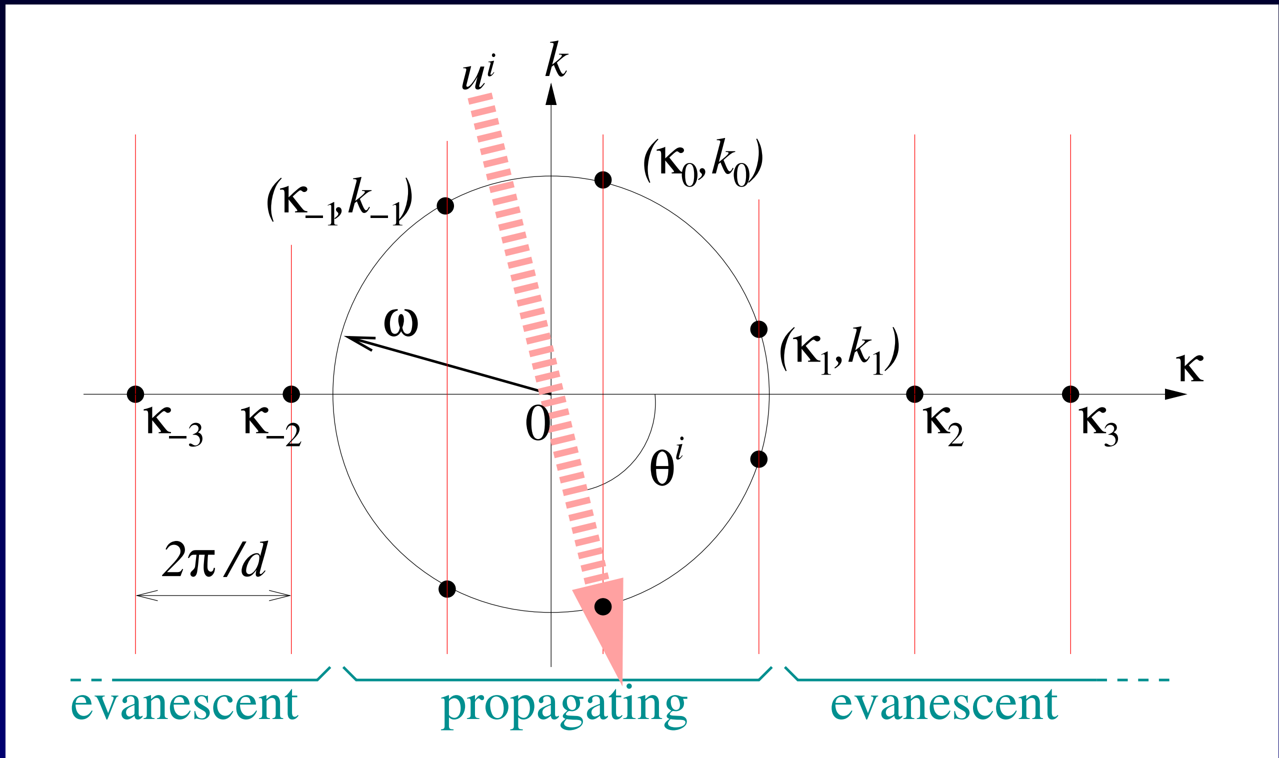

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k_n imag: evanescent (decaying or growing in y)

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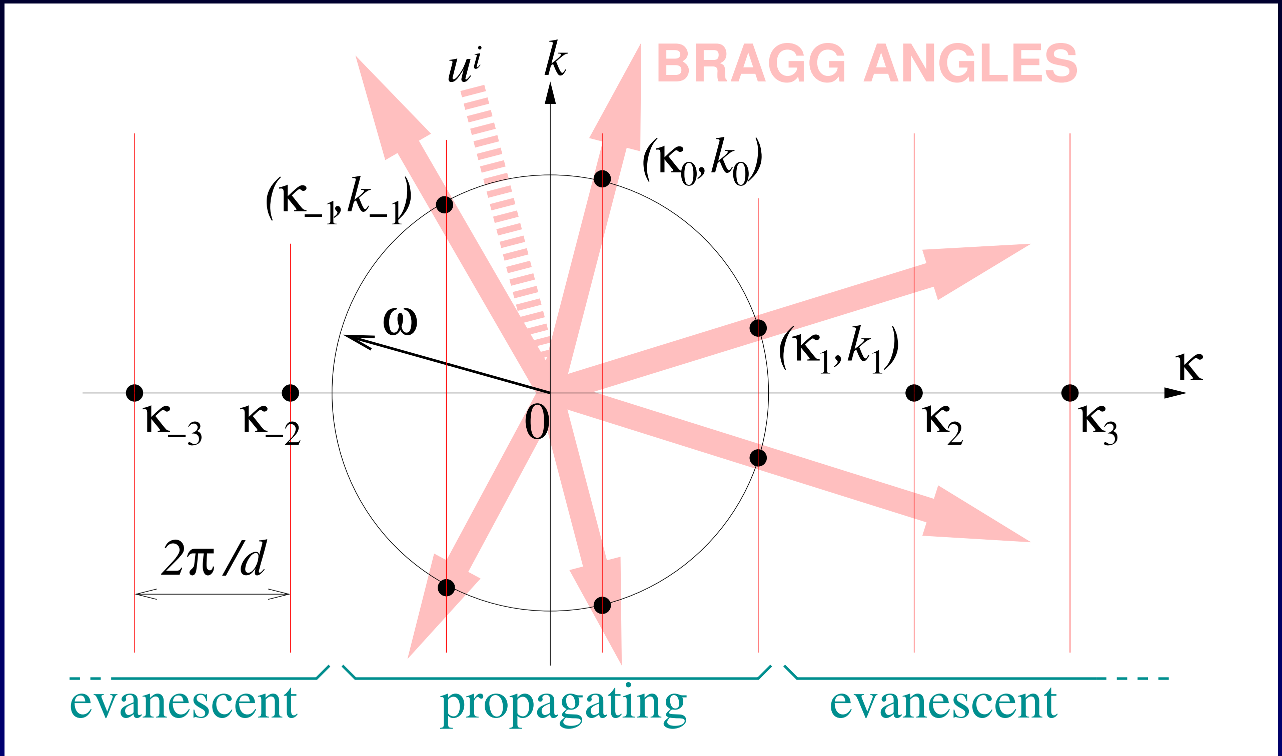

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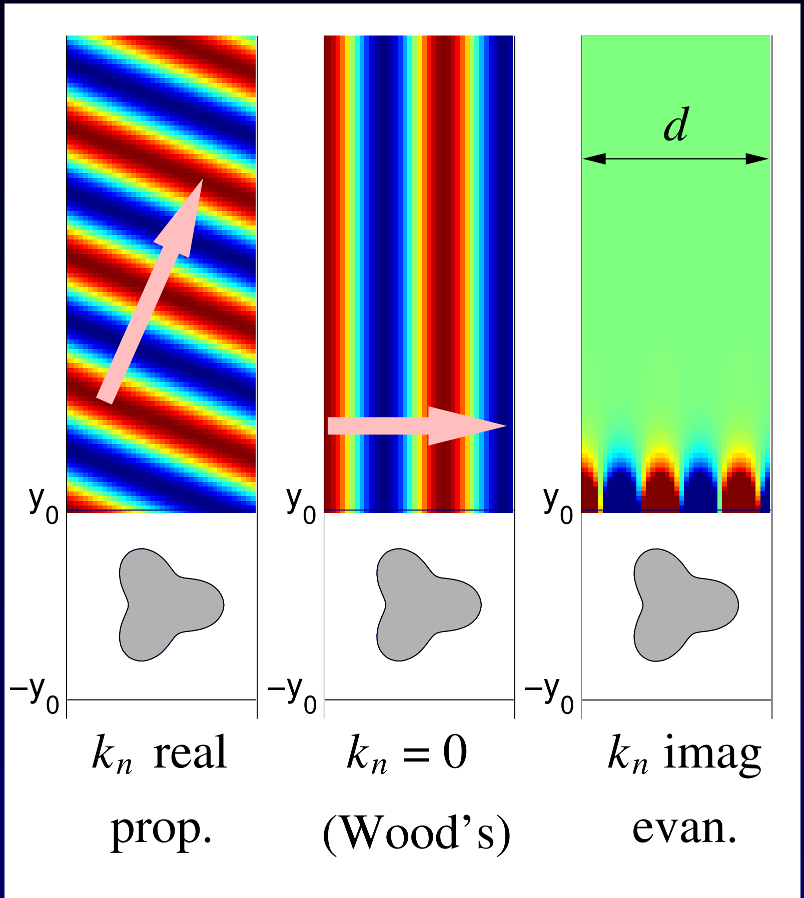

scattered u only outgoing or decaying channel modes:

$y > y_0$: upwards-prop. (or -decay)

$$u(x,y) = \sum_{n\in\mathbb{Z}} c_n e^{i\kappa_n x} e^{ik_n(y-y_0)}$$

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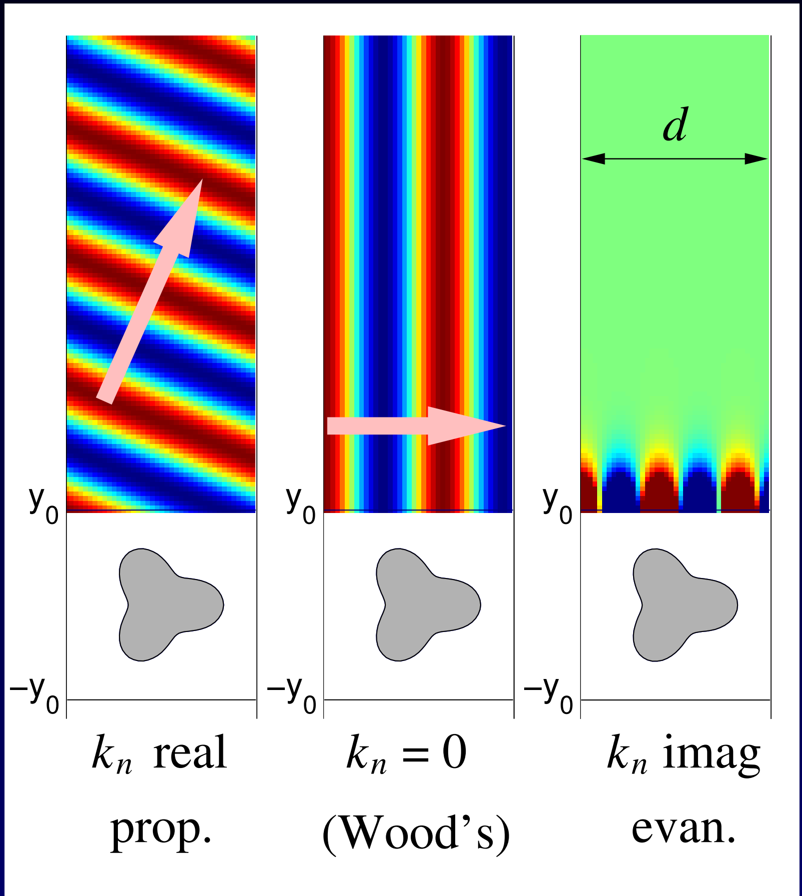

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vertical channel/waveguide with QP BC

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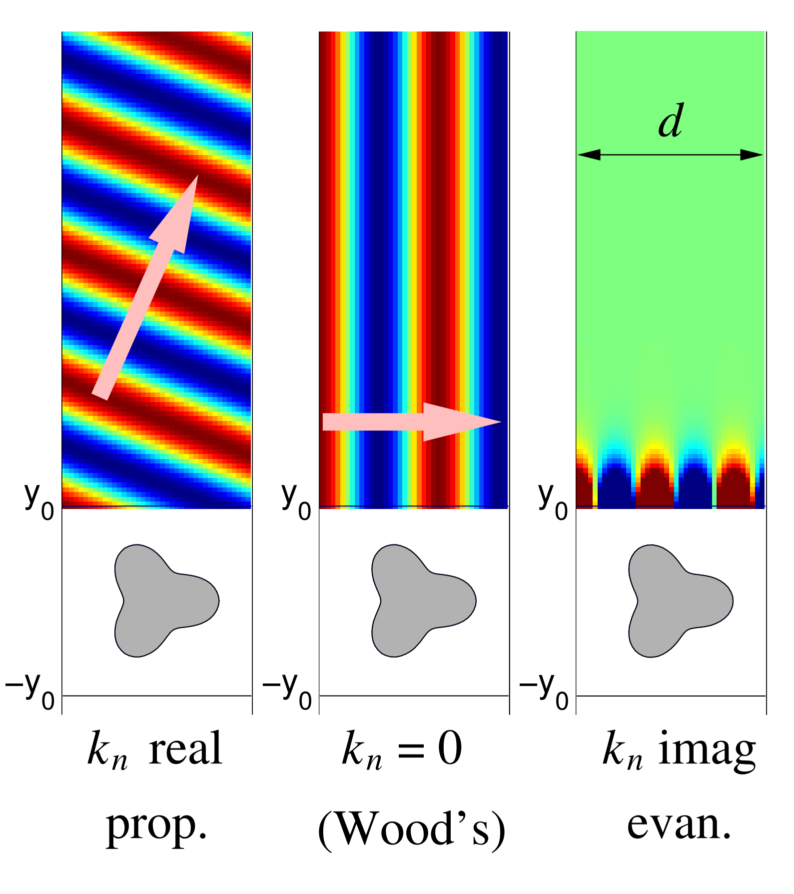

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Numerical PDE methods $\exists$ many: finite difference, finite elements. . .

Formulate BVP as integral equation on $\partial\Omega$ to solve numerically for u

adv: efficient rep (small # unknowns), rad. cond. for free, high-order accurate

Potential theory (review)

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

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

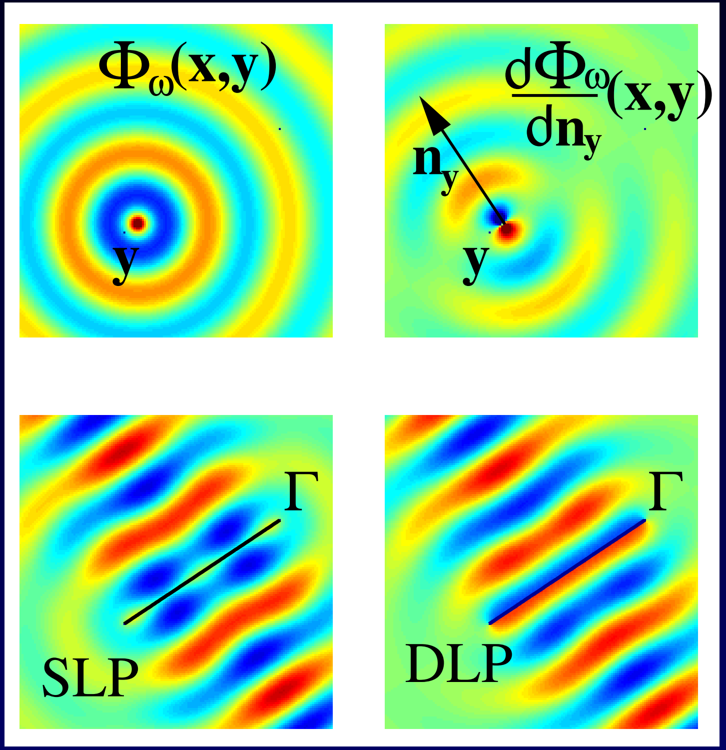
$$v(\mathbf{x}) = \int_\Gamma \Phi_\omega(\mathbf{x},\mathbf{y})\sigma(\mathbf{y})ds_\mathbf{y} := (\mathcal{S}\sigma)(\mathbf{x})$$

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

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

Helmholtz fundamental soln

a.k.a. free space Greens func



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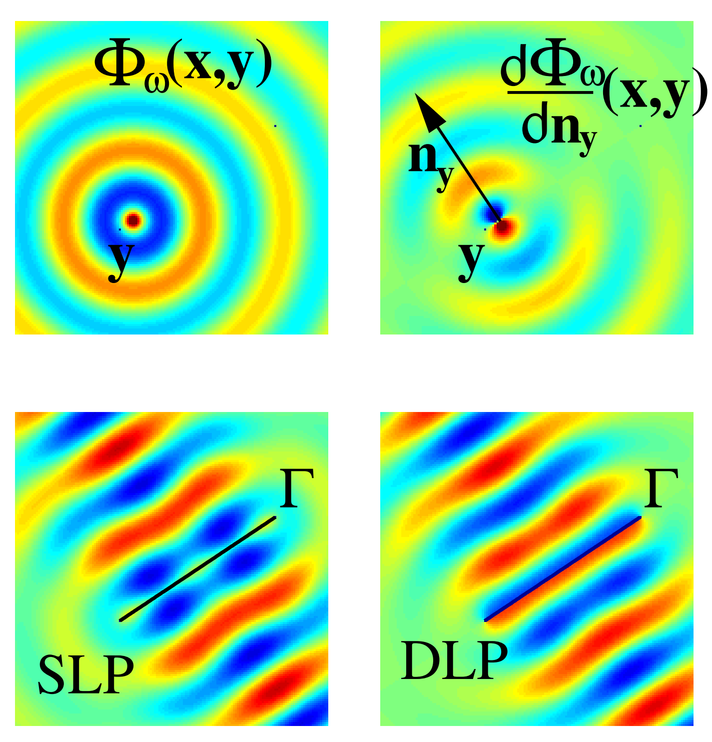

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Jump relations: limit as $\mathbf{x} \to \Gamma$ may depend on which side ($\pm$):

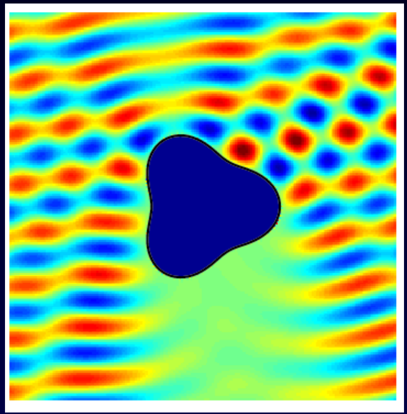
$$v^\pm = S\sigma$$
$$v_n^\pm = D^T\sigma \mp \tfrac{1}{2}\sigma$$
$$u^\pm = D\tau \pm \tfrac{1}{2}\tau$$
$$u_n^\pm = T\tau$$

S, D are integral ops with above kernels but defined on $C(\Gamma) \to C(\Gamma)$

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

Integral equations for scattering (sketch)

single Dirichlet obstacle: represent scattered $u = \mathcal{D}\tau$ DLP on $\partial\Omega$



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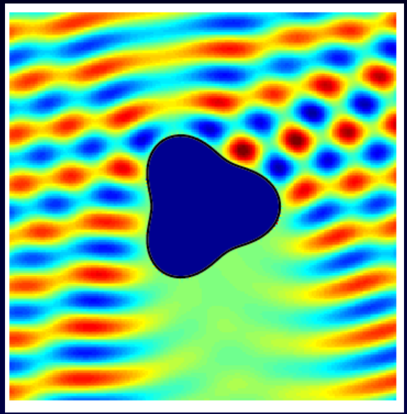

BC & JR3: $A\tau := (\frac{1}{2}I + D)\tau = -u^i$

2nd-kind IE on $\partial\Omega$, D compact so A sing. vals. $\not\to 0$

- why important? large scale problems…
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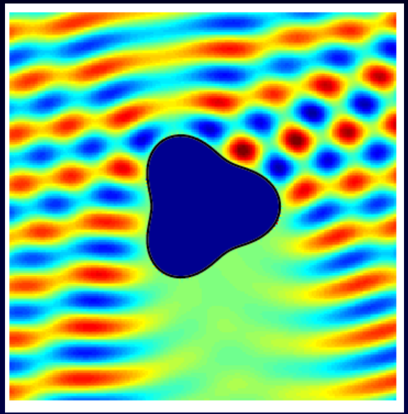

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Nyström discretization: N-by-N linear system for vector $\{\tau_j^{(N)}\}_{j=1}^N$

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

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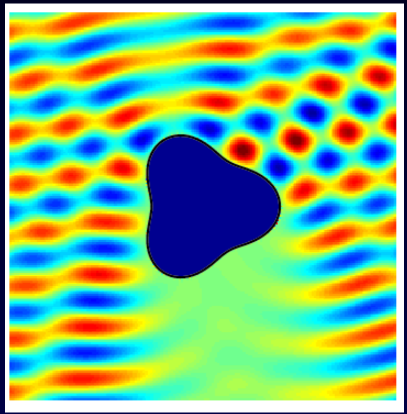

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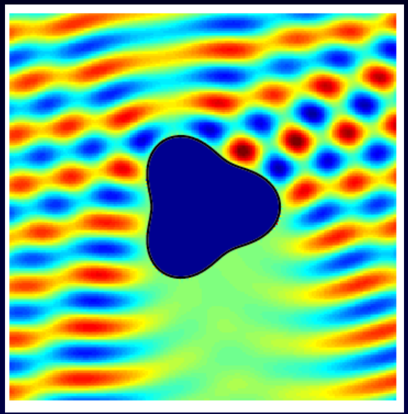

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- efficient (2D became 1D), $\exists$ fast $O(N \log N)$ schemes for $N > 10^4$
- in practice for unique solution $\forall\omega$: replace $\mathcal{D}$ by $\mathcal{D} - i\omega\mathcal{S}$

The standard way to periodize

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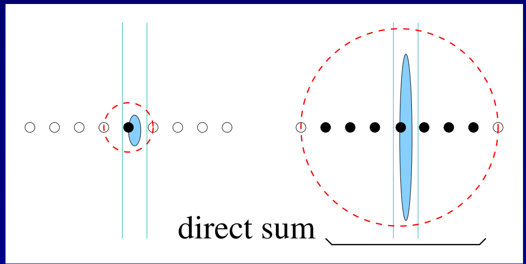
- $(*)$ converges in disc $\Rightarrow$ high aspect ratio Ω is bad:

  expand disc? sum near neighbors directly, needs large #



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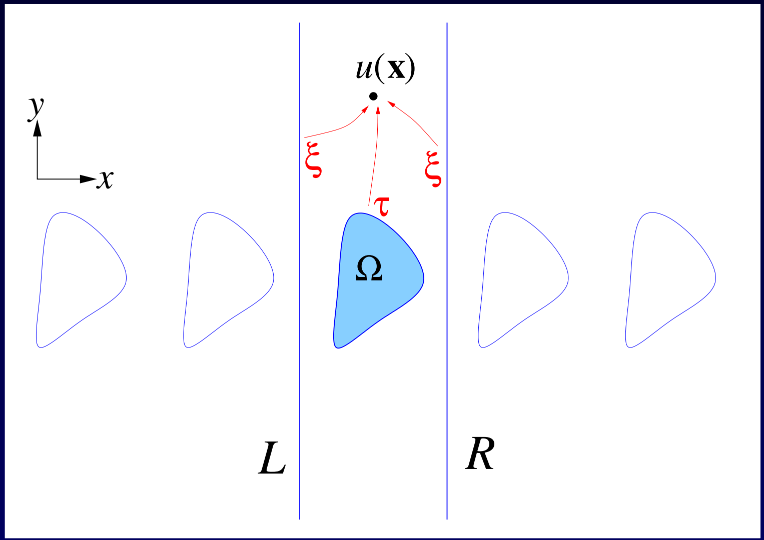

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as before — densities ξ on L and R

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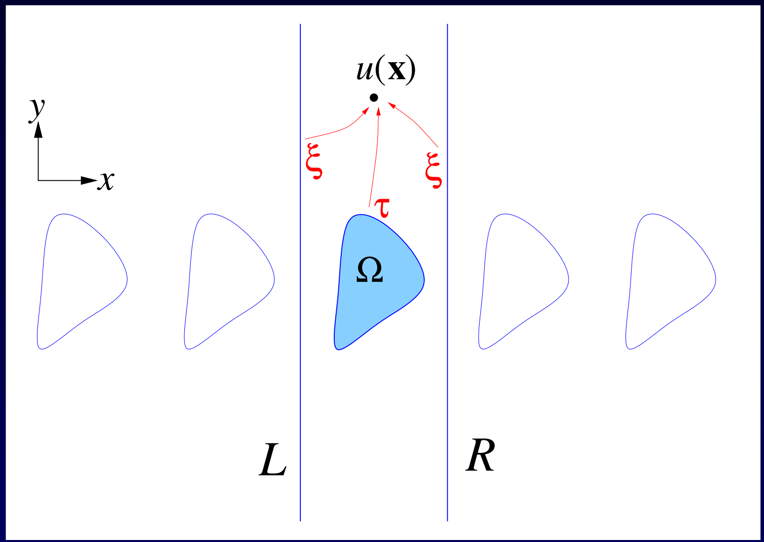

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new condition: vanishing 'discrepancy'

$$\forall y \quad \begin{cases} f & := \quad u_L - \alpha^{-1} u_R \; = \; 0 \\ f' & := \quad u_{nL} - \alpha^{-1} u_{nR} \; = \; 0 \end{cases}$$

2 unknowns $[\tau; \xi]$, 2 conditions $\Rightarrow$ solve 2×2 linear operator system

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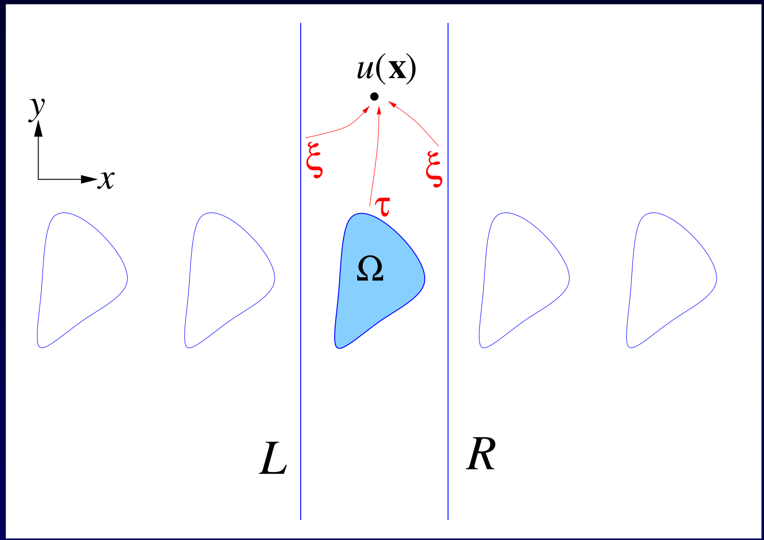

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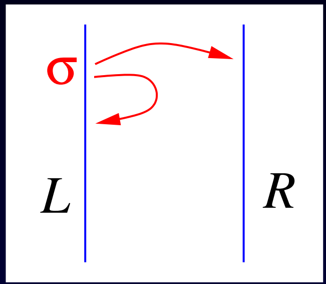
Major issues

(1) How choose rep $u_{\mathrm{QP}}[\xi]$ so effect of ξ on $[f; f']$ is ‘nice’ ? (2nd-kind)

(2) How handle densities on ∞-long L, R ? (no decay as $|y| \to \infty$)

Trick (1): choose a good $u_{\mathrm{QP}}[\xi]$ representation

Consider ξ one SLP:



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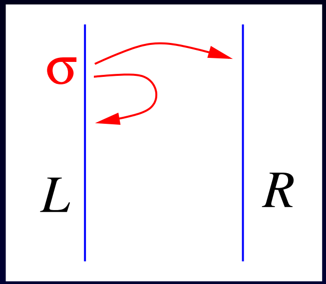

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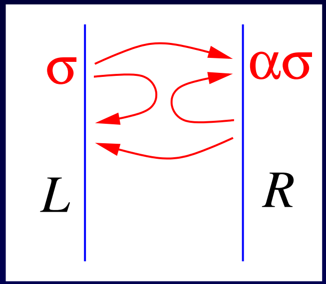

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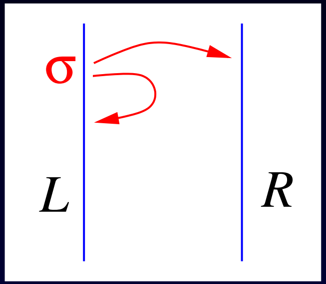
$$= (-\alpha^{-1} S_{RL} + \alpha S_{LR})\sigma \qquad \text{distant only}$$

Trick (1): choose a good $u_{\mathrm{QP}}[\xi]$ representation

Consider ξ one SLP:



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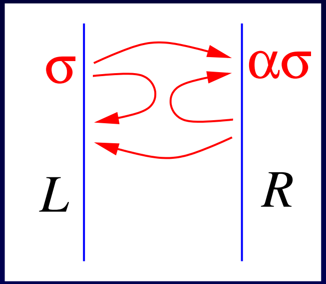

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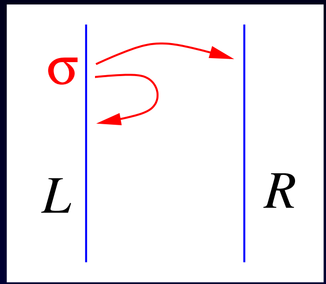

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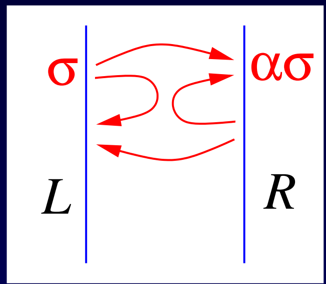

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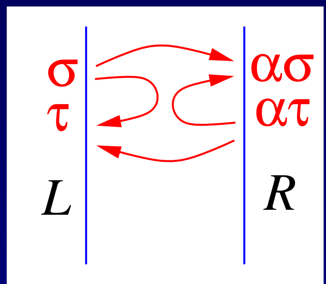
Similarly need to control f via JRs, so...

Add DLP τ on L, R,:



$$\begin{bmatrix} f \\ f' \end{bmatrix} = Q \begin{bmatrix} \tau \\ -\sigma \end{bmatrix} =: Q\xi$$

block operator $Q = I + (\text{interactions of distance} \geq d)$

- If L, R bounded segments: $Q\xi = g$ is 2nd kind, rapidly convergent

Trick (2): handle densities on $y \in (-\infty, \infty)$

Fourier transform in y-direction: work with $\hat{\sigma}$, $\hat{\tau}$, $\hat{f}$, $\hat{f}'$

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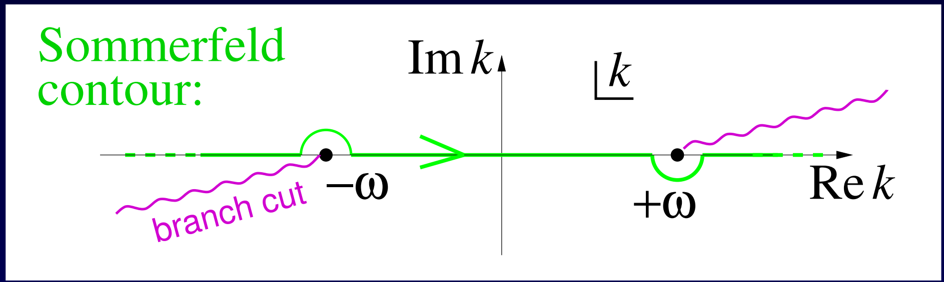
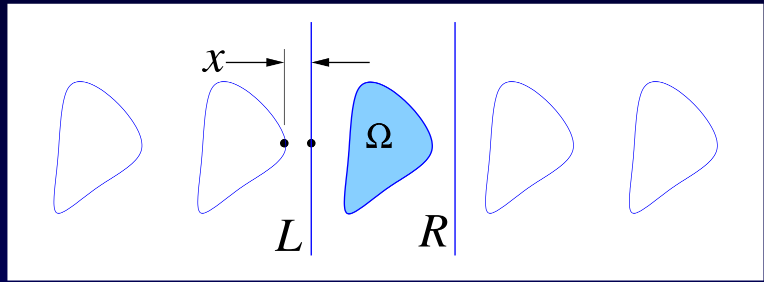
$$\Phi_\omega(x,y) \;=\; \frac{i}{4\pi}\int_{-\infty}^{\infty} e^{iky}\,\frac{e^{i\sqrt{\omega^2-k^2}\,|x|}}{\sqrt{\omega^2-k^2}}\,dk$$

exponential tails for $|k| > \omega$
decay rate prop. to $|x|$





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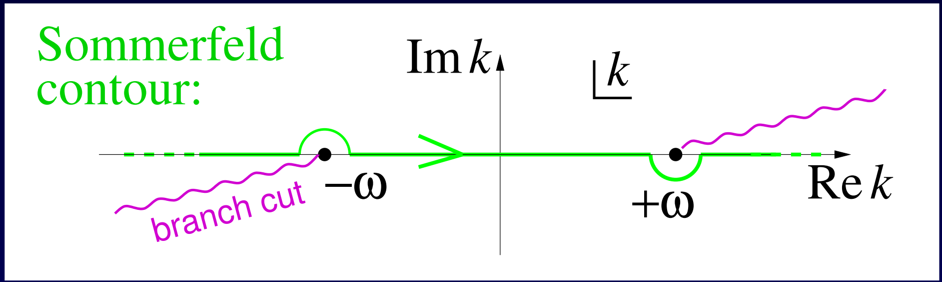
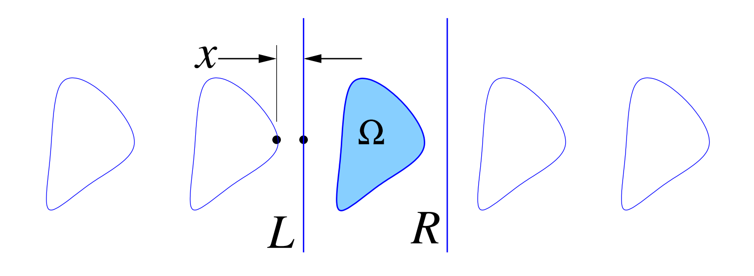




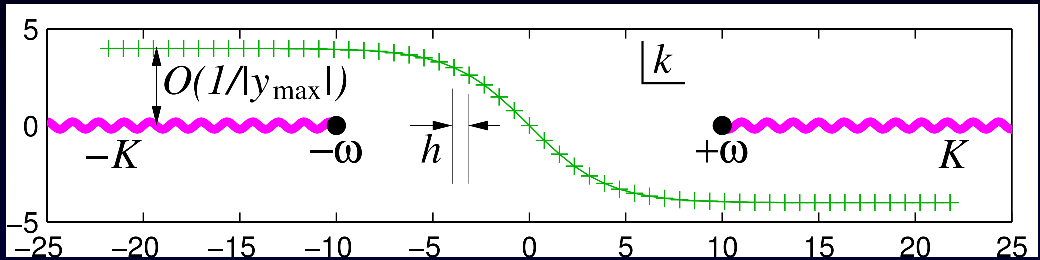
Use FT-y densities on L (or R) wall at x_0:

$$(\hat{\mathcal{S}}_L\hat\sigma)(x,y) = \frac{i}{2}\int_{-\infty}^{\infty} e^{iky}\,\frac{e^{i\sqrt{\omega^2-k^2}\,|x-x_0|}}{\sqrt{\omega^2-k^2}}\,\hat\sigma(k)\,dk$$

$$(\hat{\mathcal{D}}_L\hat\tau)(x,y) = \frac{\mathrm{sign}(x-x_0)}{2}\int_{-\infty}^{\infty} e^{iky}\,e^{i\sqrt{\omega^2-k^2}\,|x-x_0|}\,\hat\tau(k)\,dk$$

- same JRs as before; $\hat\sigma(k)$, $\hat\tau(k)$ affect only $\hat f(k)$, $\hat f'(k)$ diagonal in k

Quadrature on Sommerfeld contour



nodes k_j
weights w_j
$j = 1, \ldots, M$

Re k is periodic trapezoid rule, Im k is scaled tanh curve

- exponentially convergent as $h \to 0$, $K \to \infty$ beats nodes on real axis

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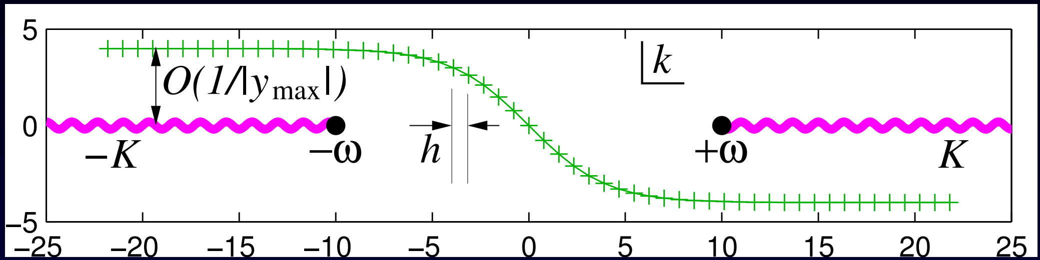

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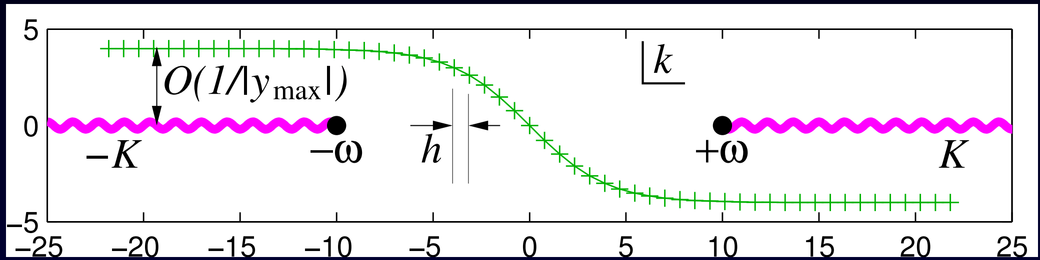

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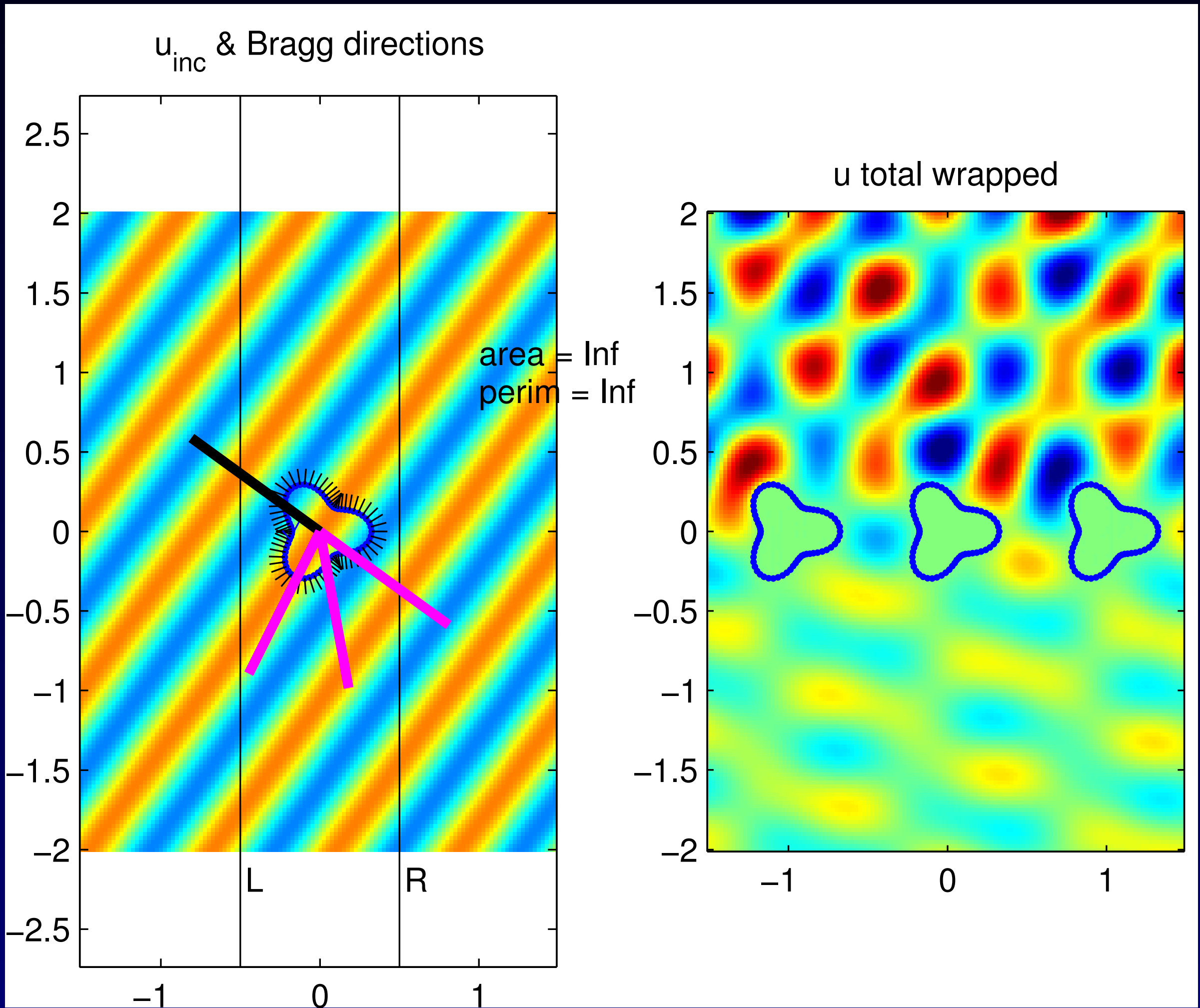
Solve full $(N+2M)$-by-$(N+2M)$ linear system:

$$\begin{bmatrix} A & B \\ C & \hat{Q} \end{bmatrix} \begin{bmatrix} \tau \\ \hat{\xi} \end{bmatrix} = \begin{bmatrix} -u^i \\ 0 \end{bmatrix} \quad \begin{matrix} \leftarrow \text{BC on } \partial\Omega \\ \leftarrow \text{FT-}y \text{ of discrep.} \end{matrix}$$

- fill B by evaluating $\hat{\mathcal{S}}$, $\hat{\mathcal{D}}$ Sommerfeld integrals at nodes $\mathbf{y}_j \in \partial\Omega$
- fill C by spectral rep. of each source $\mathbf{y}_j \in \partial\Omega$ at walls L, R

Results

(using Matlab toolbox `MPSpack` by B–Betcke '09)



$d = 1.6\lambda \quad N = 70 \quad M = 80 \quad \text{error } 10^{-14} \quad t_{\text{fill}} = 0.13\text{ s} \quad t_{\text{solve}} = 0.04\text{ s}$

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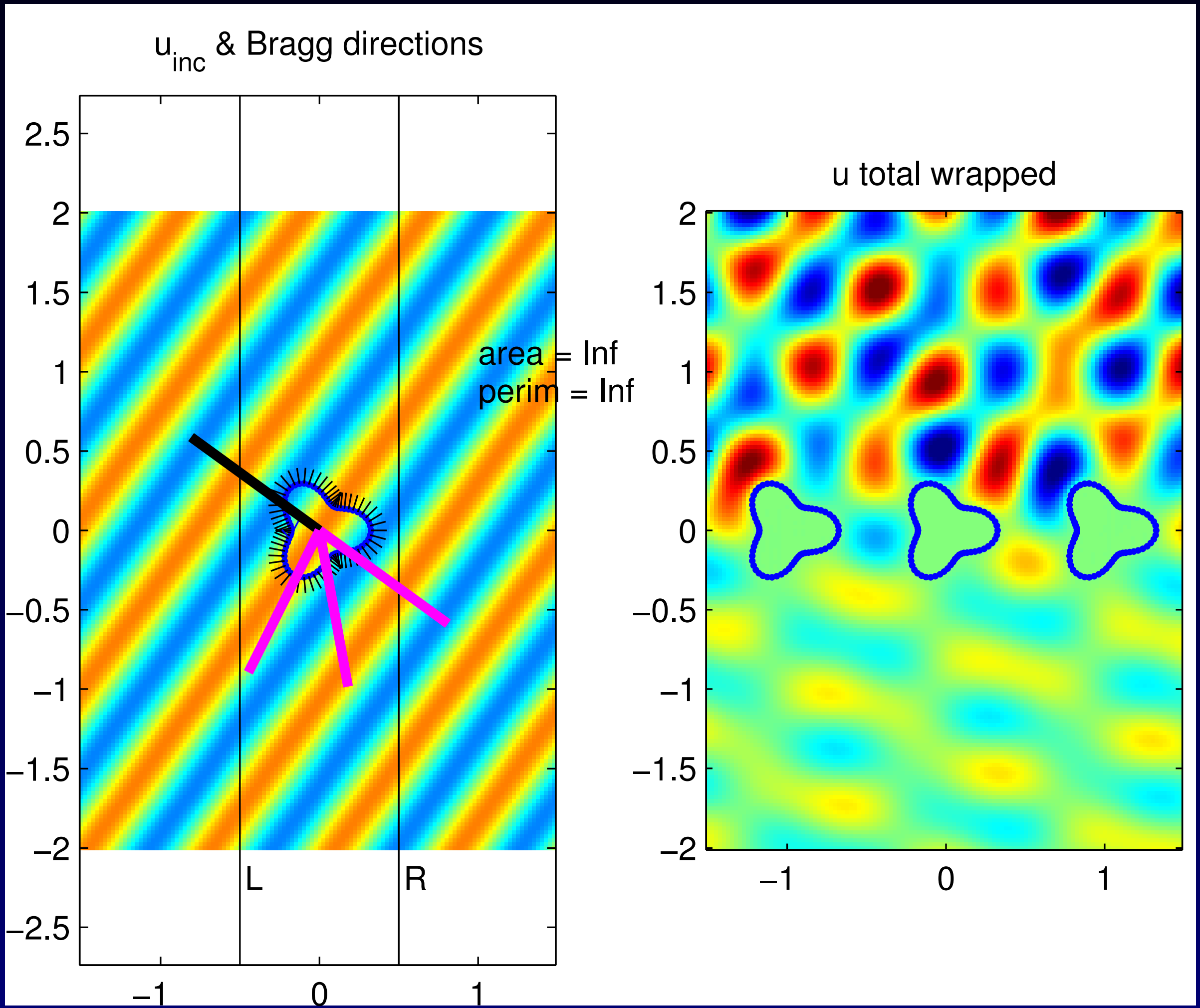

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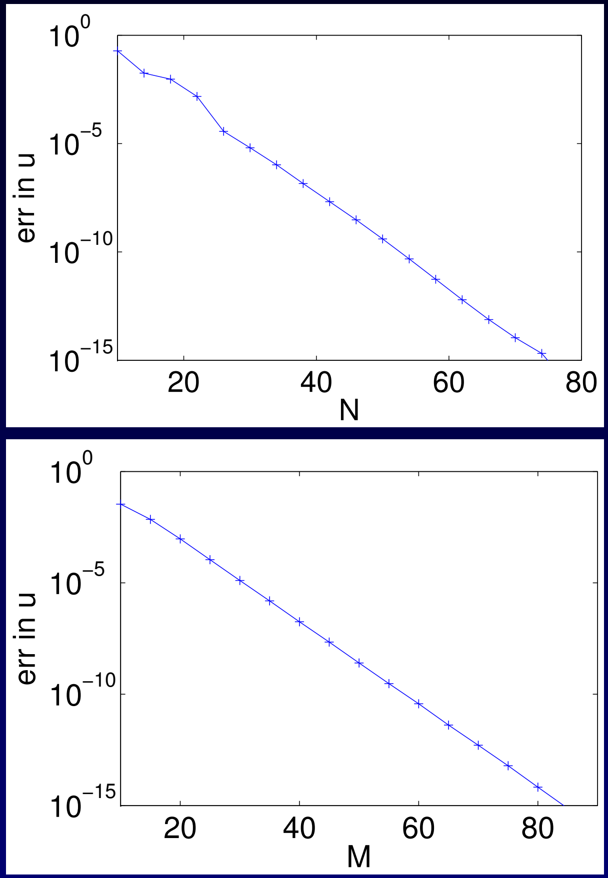

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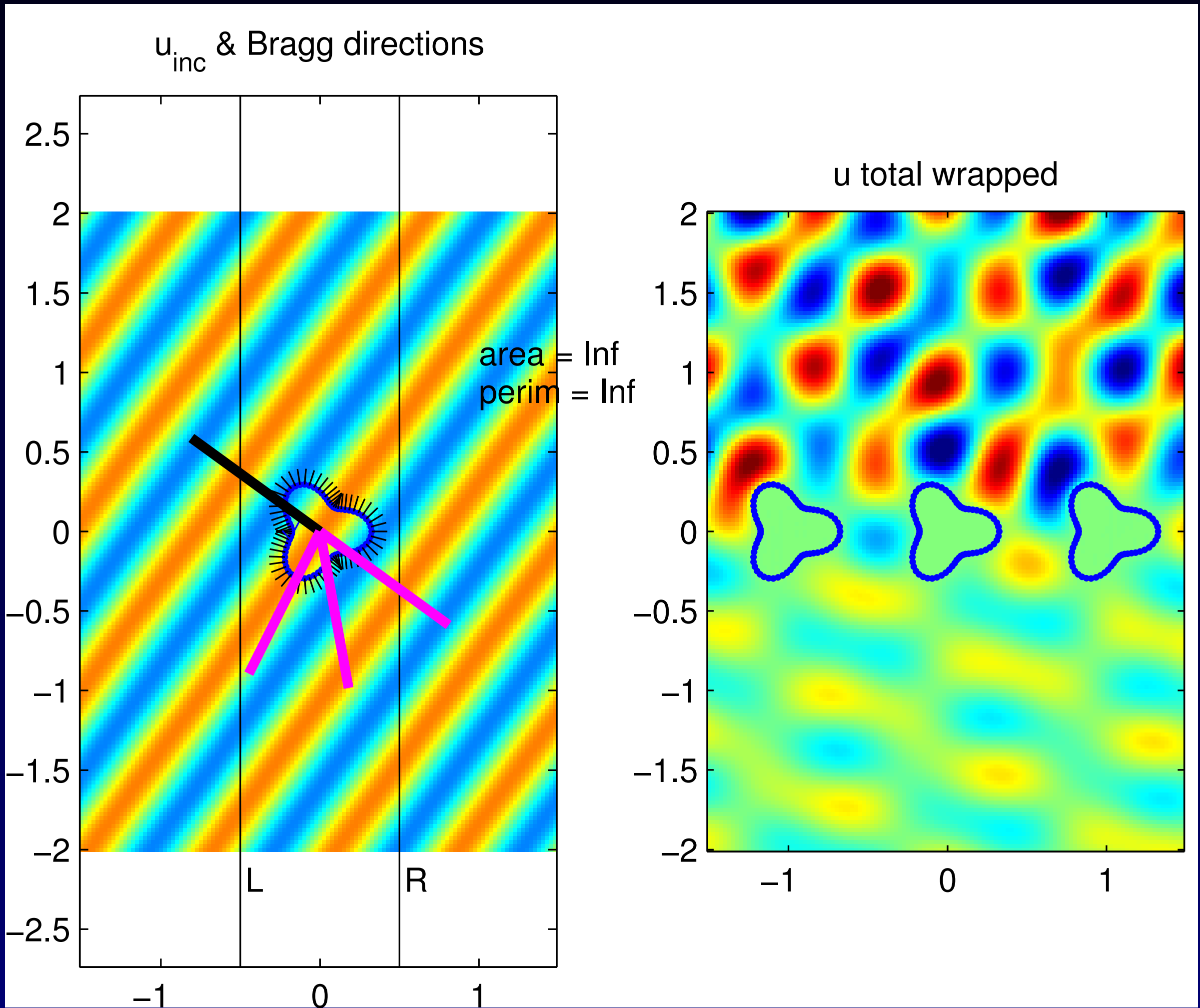

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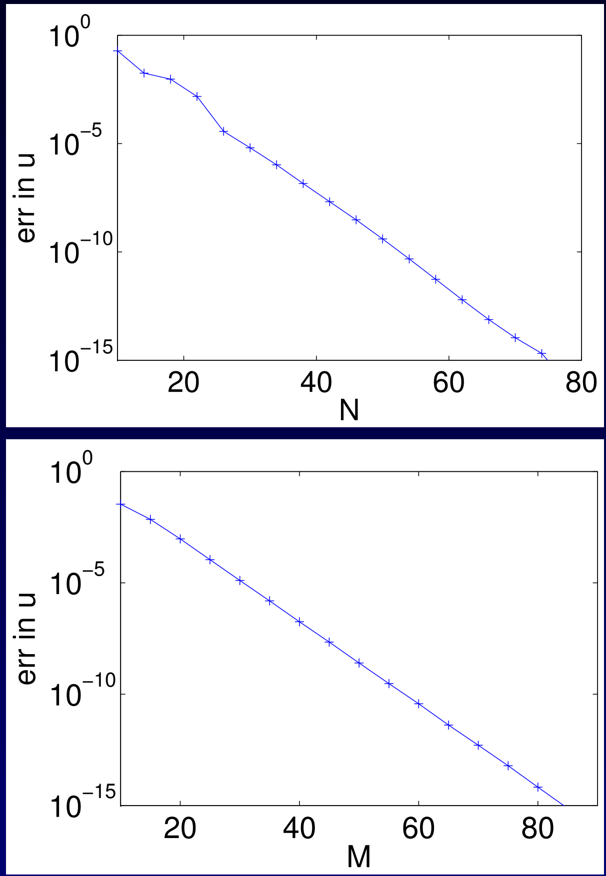
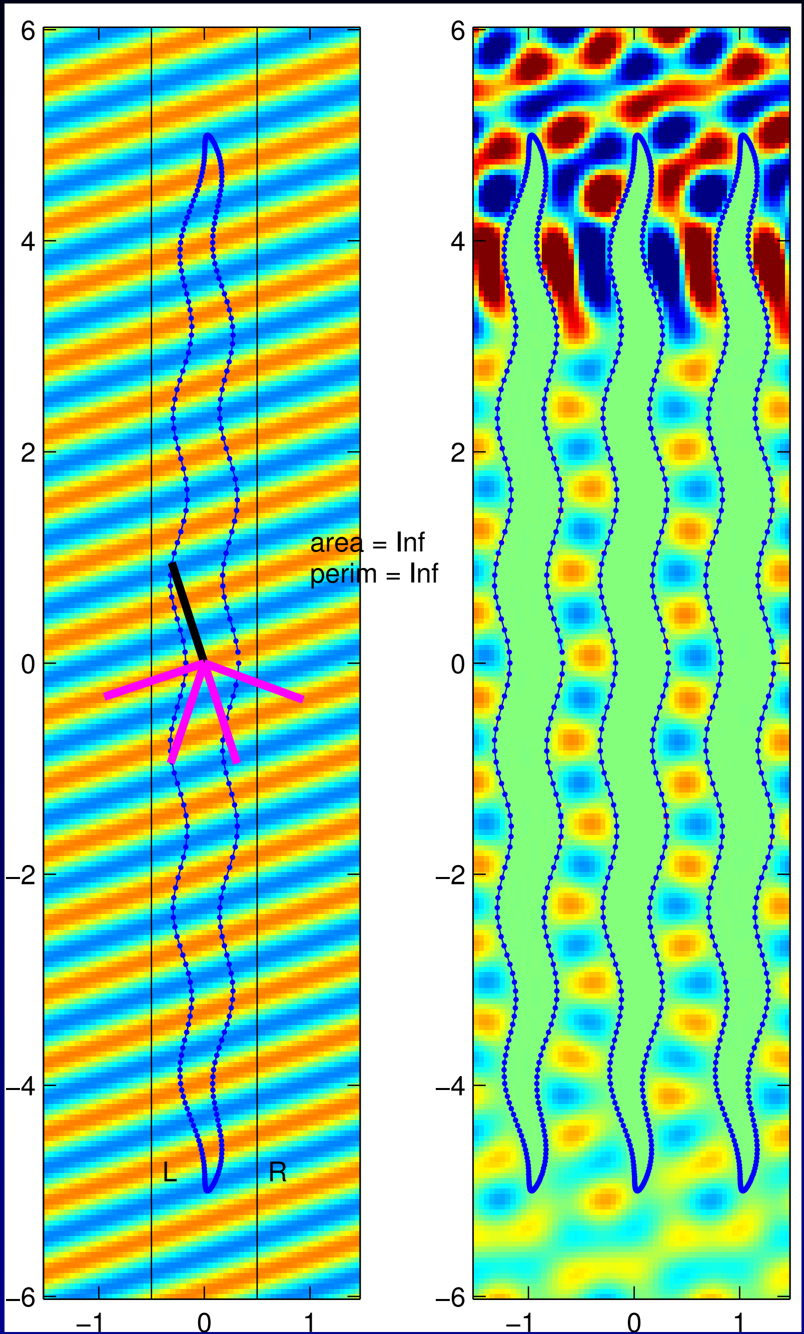


$d = 1.6\lambda$ $\quad N = 70$ $\quad M = 80$ $\quad$ error 10^{-14} $\quad t_{\text{fill}} = 0.13$ s $\quad t_{\text{solve}} = 0.04$ s

- improved convergence rate by summing 1 or 2 $\partial\Omega$ neighbors directly
- low condition # $\sim 10^2$: solved to 14 digits in 55 GMRES iters.

Results: high aspect ratio



height = 10 periods

if lattice sums were used:
would need >20 neighbor copies of $\partial\Omega$
to be summed directly (slow)

$d = 1.6\lambda \quad N = 300 \quad M = 250$

error 10^{-10} $\quad t_{\text{fill}} = 1$ s $\quad t_{\text{solve}} = 0.5$ s

- Note, cond. # $\sim 10^6$: close-to-resonant BVP (not caused by scheme)

Handling Wood's anomalies ($k_n \to 0$)

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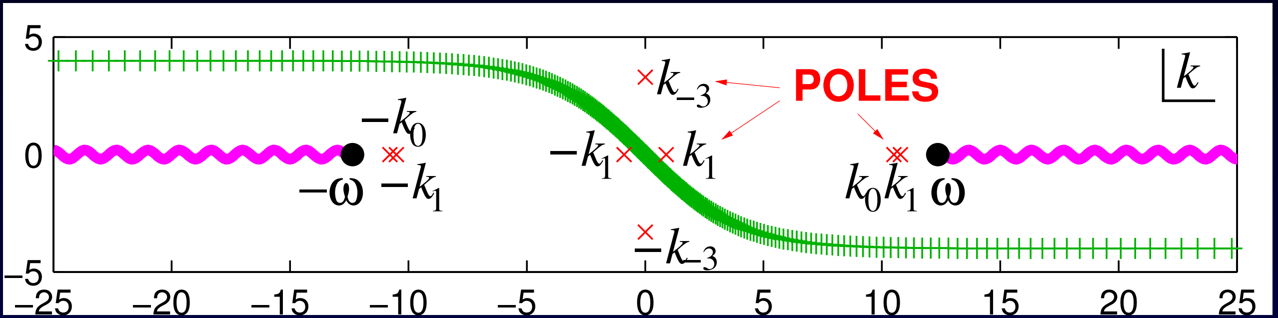

Why?

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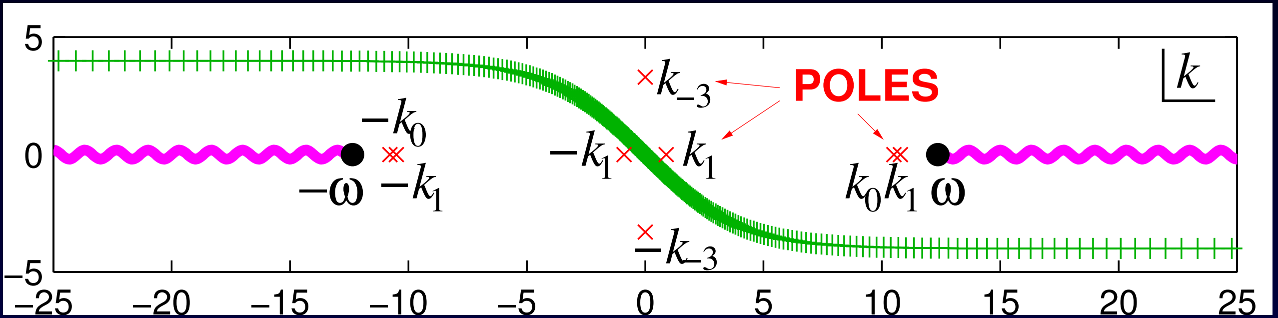

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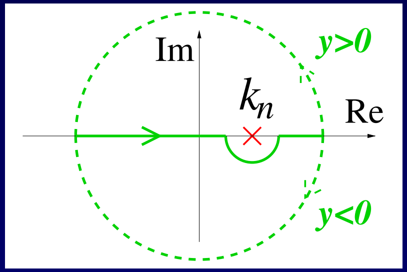

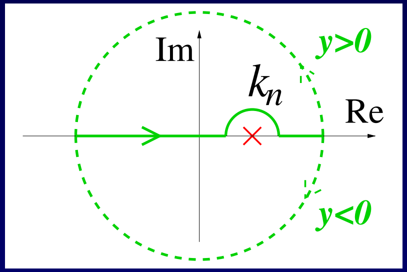

interpretation for $k_n > 0$: R–B outgoing above incoming below

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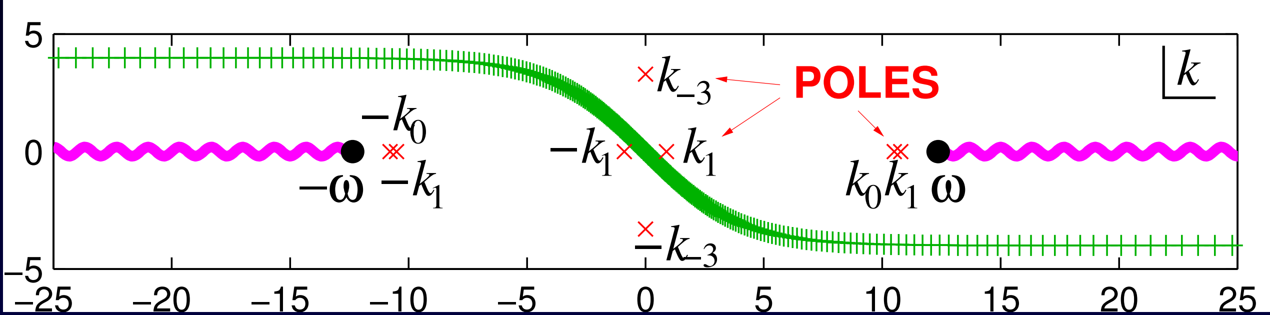

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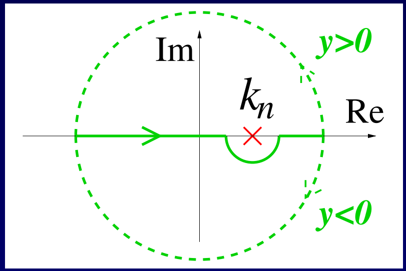
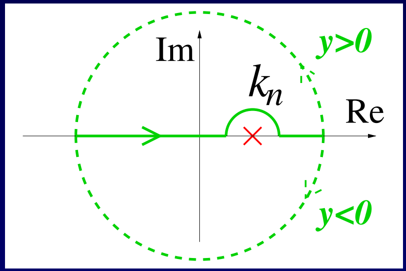




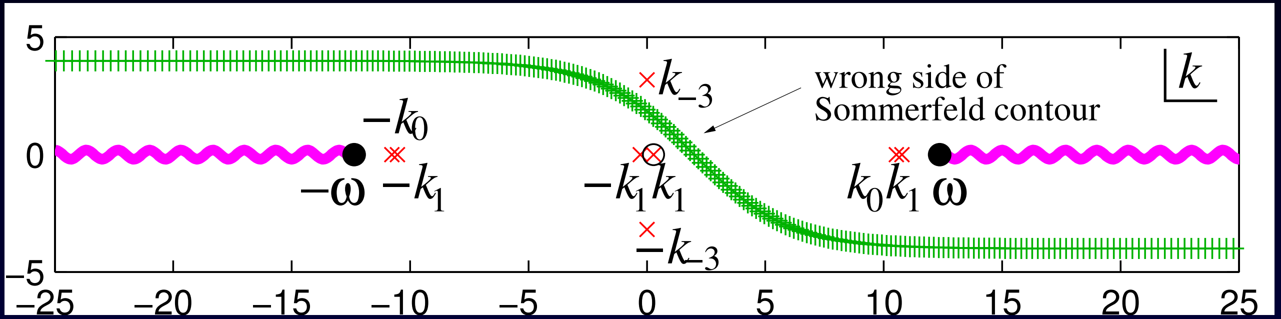
interpretation for $k_n > 0$: R–B outgoing above incoming below

Numerically: as $k_n \to 0$, grade nodes geometrically (sinh map) near 0

- works (10^{-9}), but: log blow-up of M, cond. # and $\|\hat{\xi}\|$ diverge (bad)

Well-conditioned handling of Wood's

deform contour to be safe dist $O(1)$ from all poles:



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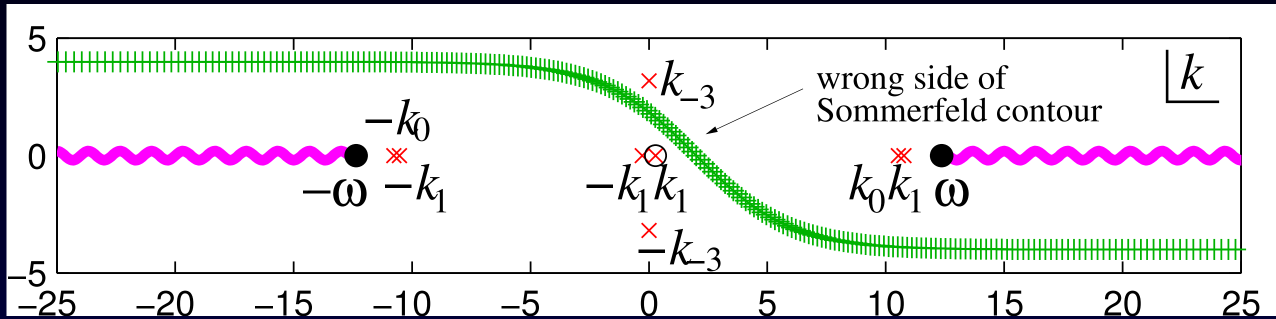

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The fix:

- add plane-wave $ae^{i\kappa_n x}e^{ik_n y}$, unknown a, to the $u(x,y)$ rep.
- add new linear condition: n^{th} amplitude incoming below = 0

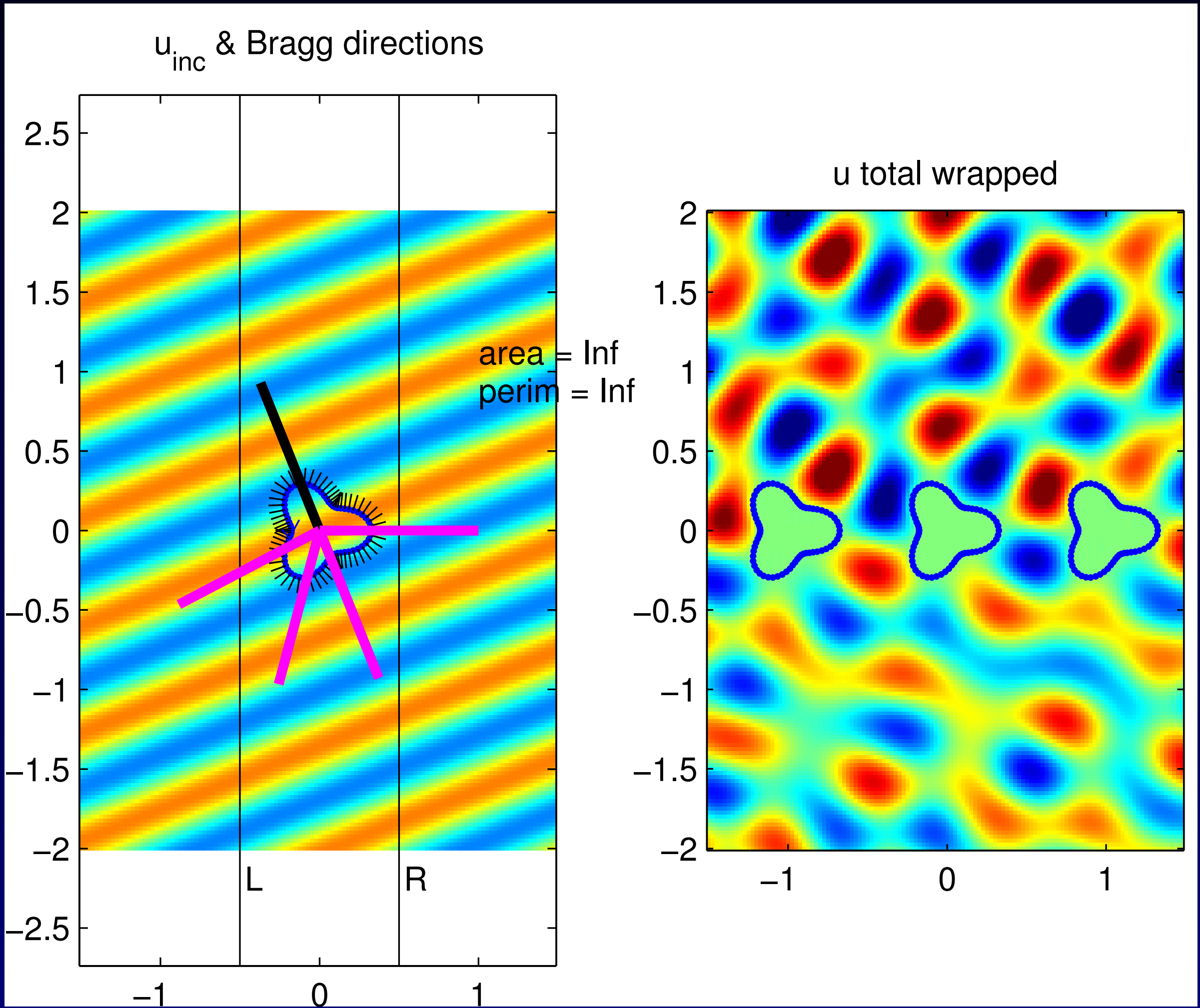
project evaluation of $u(\cdot, -y_0)$ onto n^{th} Fourier mode

matrix now has 1 row and 1 column extra, solve for unknowns $[\tau; \hat{\xi}; a]$

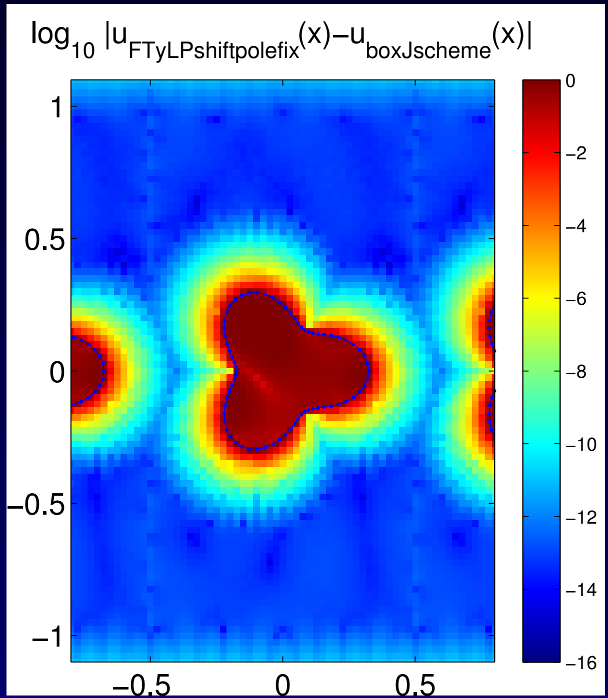
at Wood $k_n = 0$: replace $\{e^{ik_n y}, e^{-ik_n y}\}$ by $\{1, y\}$, enforce "y" amplitude = 0

Works: cond. # and error bounded uniformly in params (ω, θ^i) ...

Results precisely at Wood's anomaly



Pointwise error:
compared to indep. scheme



10^{-13} unless close to $\partial\Omega$

$d = 1.6\lambda$ $N = 70$ $M = 150$ error 10^{-14} $t_{\text{fill}} = 0.16$ s $t_{\text{solve}} = 0.1$ s

- cond # $< 10^4$, 150 GMRES iters. for 14 digits accuracy

MOVIES

Similar story for 2D Bloch eigenvalues (taste)

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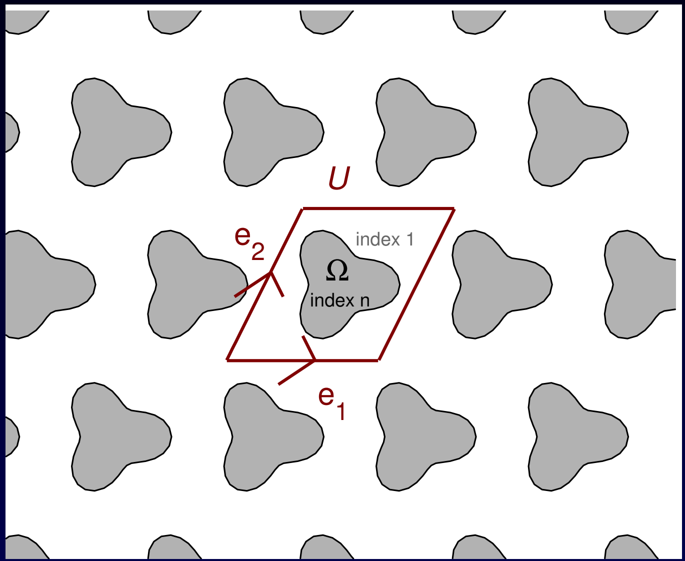

Lattice of inclusions, index n in index 1

PDE EVP: u, u_n continuous across $\partial\Omega$

$$\begin{aligned}(\Delta + n^2\omega^2)u &= 0 \text{ in } \Omega \\ (\Delta + \omega^2)u &= 0 \text{ in } U \setminus \overline{\Omega}\end{aligned}$$

u QP in both directions phases (α, β)

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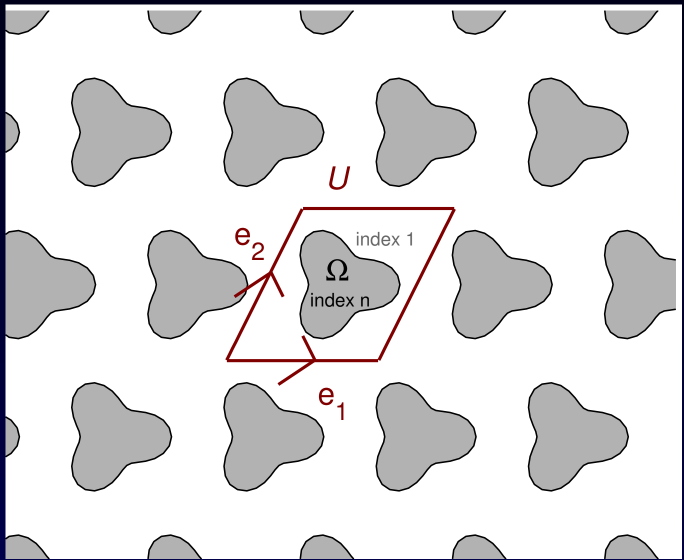

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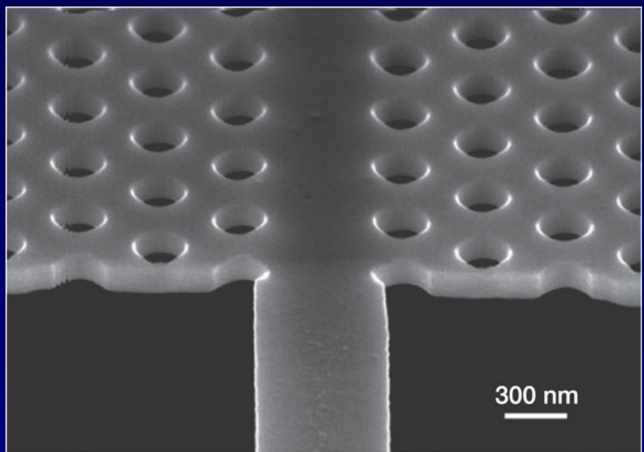
Photonic crystals: devices with period $\approx$ wavelength of light



- control of propagation: bandgaps, dispersion, density of states
- filters, couplers, integrated optical computing, meta-materials, solar cells

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

Need Bloch eigenvalues ('band structure'): are sheets in (ω, α, β)

Periodizing robustly

Single inclusion: use SLP+DLP densities η to rep fields in Ω and $\mathbb{R}^2 \setminus \overline{\Omega}$

integral op. $A\eta = [u^+ - u^-; u_n^+ - u_n^-]$, can make $A = I+$ cpt (Rokhlin '83)

As before, may periodize by replacing Φ_ω by $\Phi_{\omega,\text{QP}}$, A becomes A_{QP}

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Fix: use only free-space Φ_ω, add new densities on cell walls, enforce QP

$$\begin{bmatrix} A & B \\ C & Q \end{bmatrix} \begin{bmatrix} \eta \\ \xi \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \qquad \begin{array}{l} \longleftarrow \text{ matching conds. on } \partial\Omega \\ \longleftarrow \text{ discrep. in QP conds: } f, f', g, g' \end{array}$$

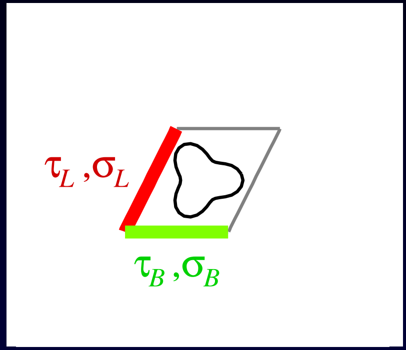
- Robust (no spurious resonances), 2nd-kind sys, rapid convergence

How choose new densities on unit cell walls?

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

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

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



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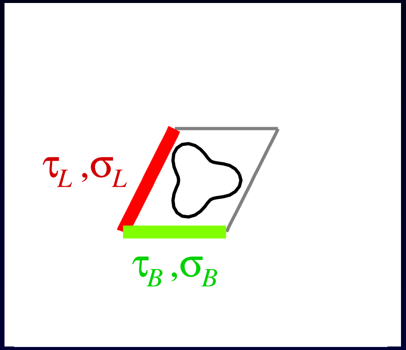
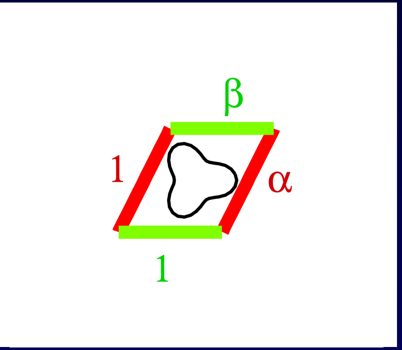


$Q = \frac{1}{2}\mathrm{Id}$ + (self-interactions) + (other interactions)

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

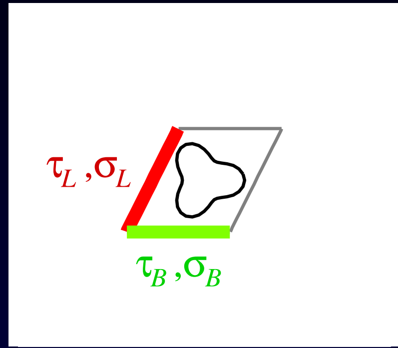
- add phased ghost copies on other 2 walls

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



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

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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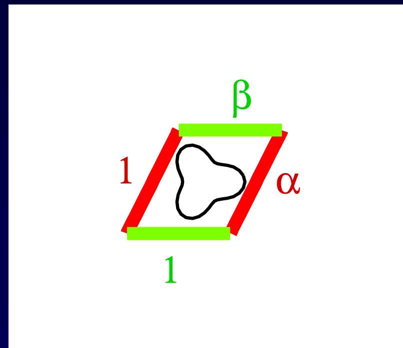

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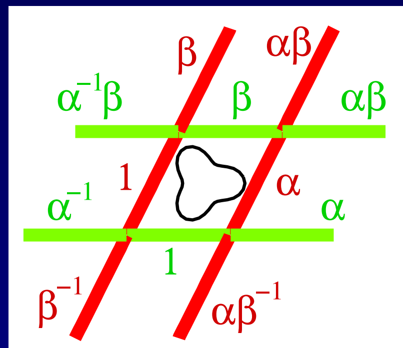
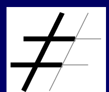
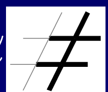


- add more 'sticking-out' ghost images

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!

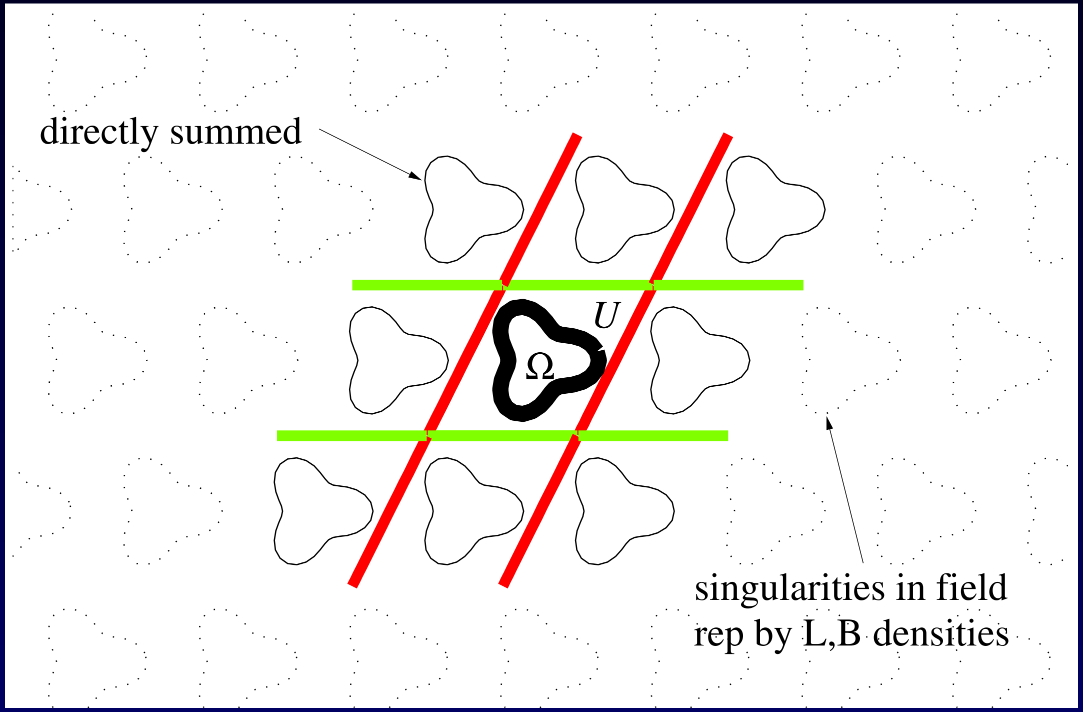
- result: $\quad Q = I +$ (interactions of distance ≥ 1)

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

Full Bloch solver scheme

(B–Greengard, JCP, *subm.*)

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



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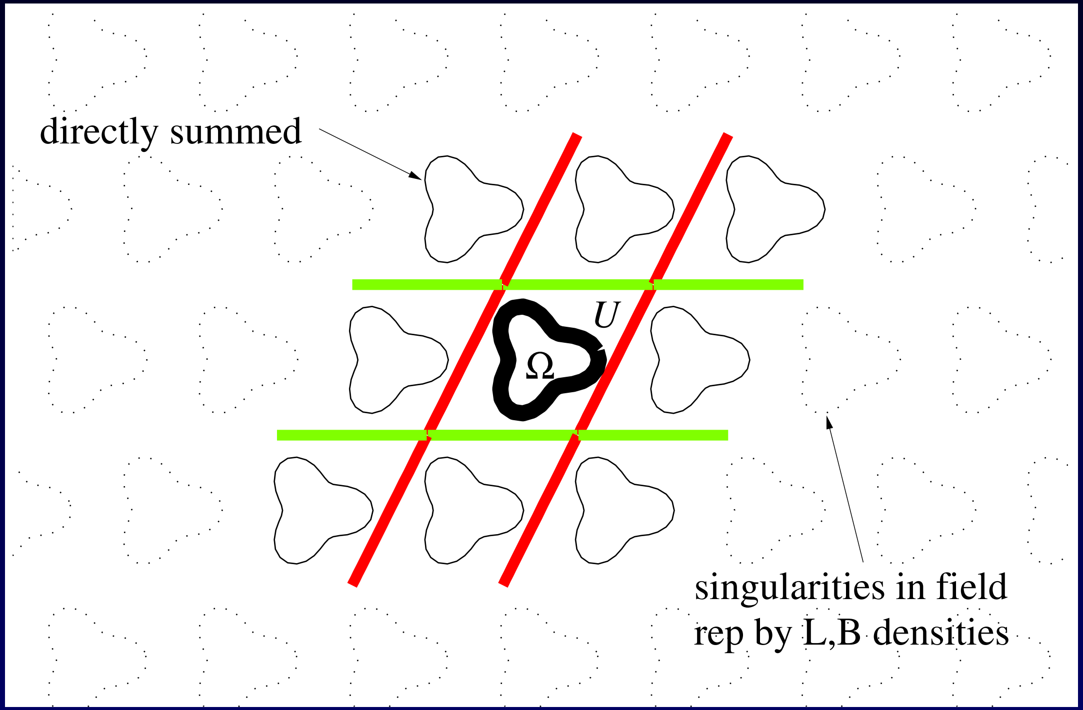

- Careful cancellations: B, C, Q have only interactions of distance ≥ 1
- Large dist increases convergence rate, i.e. large c in error = $O(e^{-cN})$

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

Results: small inclusion

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

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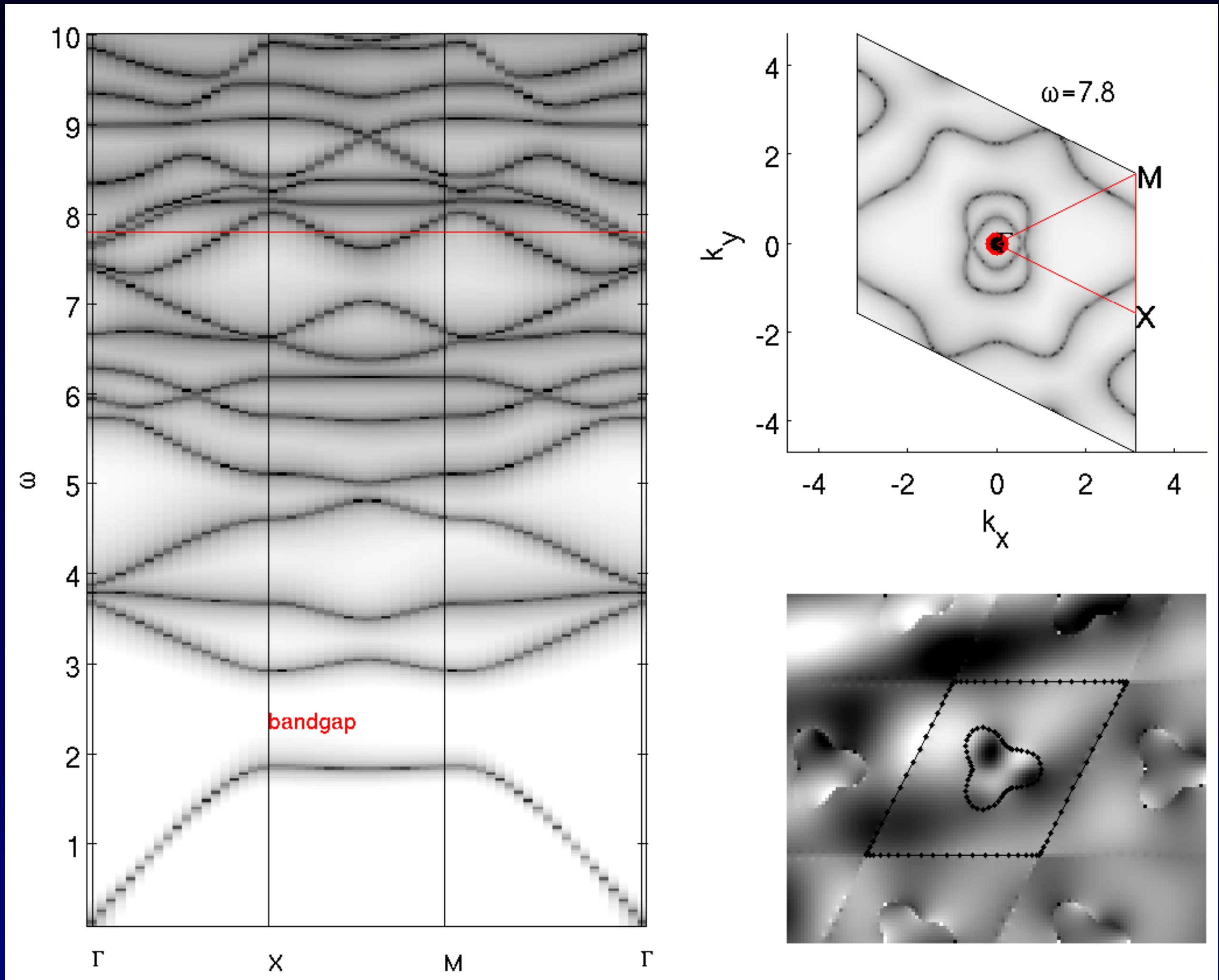

0.1 sec per eval

pre-store α, β coeffs

30 sec per const-ω slice

24×24 evals

$N = 40$ $M = 20$ (160 unknowns total) err 10^{-9}

MOVIE

Conclusions

- efficient 2nd-kind integral equations for 2D periodic problems
- periodize via small # extra degrees of freedom on cell walls
  – scattering: densities on unbounded walls via Fourier rep.
  – Bloch eigenvalue: kill corner singularities w/ tic-tac-toe
- more robust and flexible than quasi-periodic Greens function:
  – well-behaved at Wood's anomaly or spurious resonances
  – high aspect-ratios, extends simply to 3D, unlike lattice sums

Future:

- multi-layer; 3D; insert fast multipole methods for inclusion . . .

code: http://code.google.com/p/mpspack
(B–Betcke, SIAM J. Sci. Comp. '10)

funding: NSF DMS-0507614
DMS-0811005

B–Greengard, J. Comput. Phys., *subm.*
B–Greengard, BIT, *to be subm.*

http://math.dartmouth.edu/∼ahb
made with: Linux, LaTeX, Prosper

EXTRA SLIDES

Main numerical approaches

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

low order (inaccurate); close freqs $\longrightarrow$ need large t (inefficent)

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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)

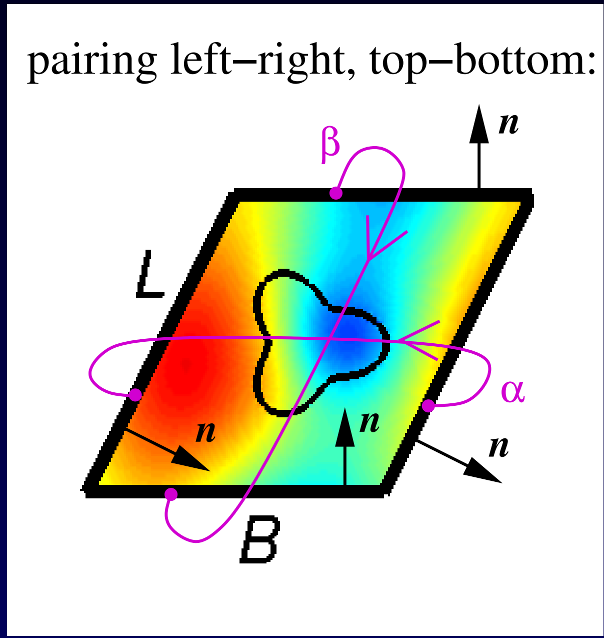
scarcely used for band structure (Yuan '08)

Recast problem on compact domain (torus)

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

Require vanishing unit cell discrepancy:

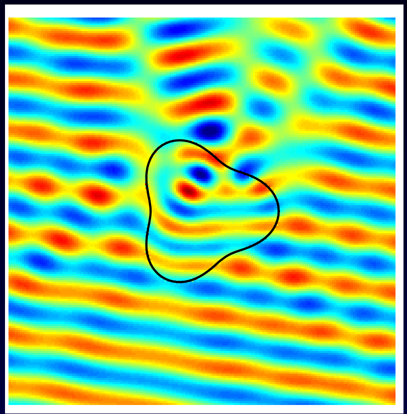
$$\begin{aligned} f &:= u|_L - \alpha^{-1} u|_{L+\mathbf{e}_1} = 0 \\ f' &:= u_n|_L - \alpha^{-1} u_n|_{L+\mathbf{e}_1} = 0 \\ g &:= u|_B - \beta^{-1} u|_{B+\mathbf{e}_2} = 0 \\ g' &:= u_n|_B - \beta^{-1} u_n|_{B+\mathbf{e}_2} = 0 \end{aligned}$$



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)

BIE for transmission scattering



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

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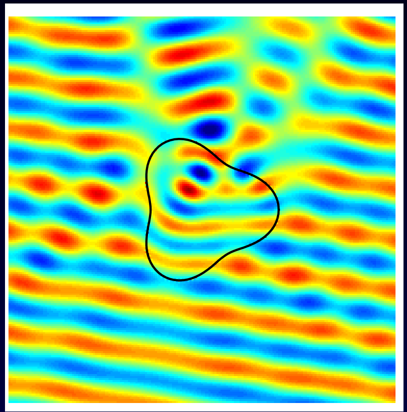

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mismatch on $\partial\Omega$: $h := u^+ - u^-$, $h' := u_n^+ - u_n^-$

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

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

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)

The standard way to periodize

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

as before, integral operator A becomes A_{QP}

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

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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

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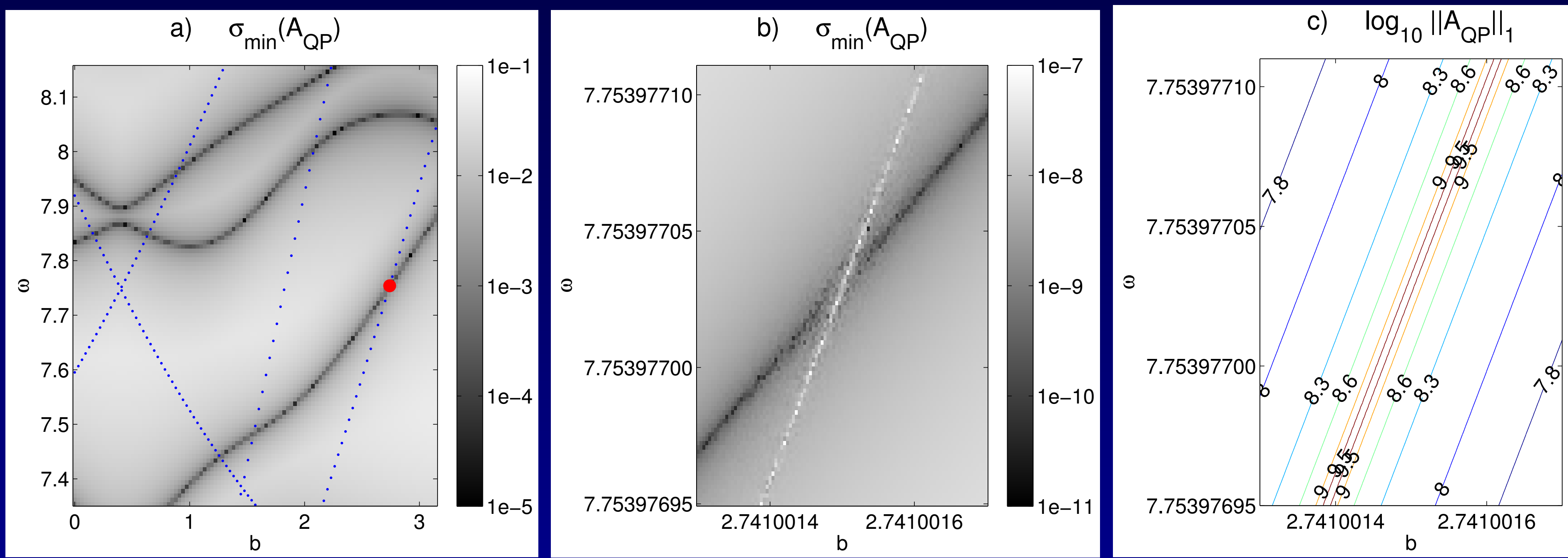

Robust way to periodize: back to free-space Φ_ω

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

$\uparrow$ can enforce mismatch $m = 0$

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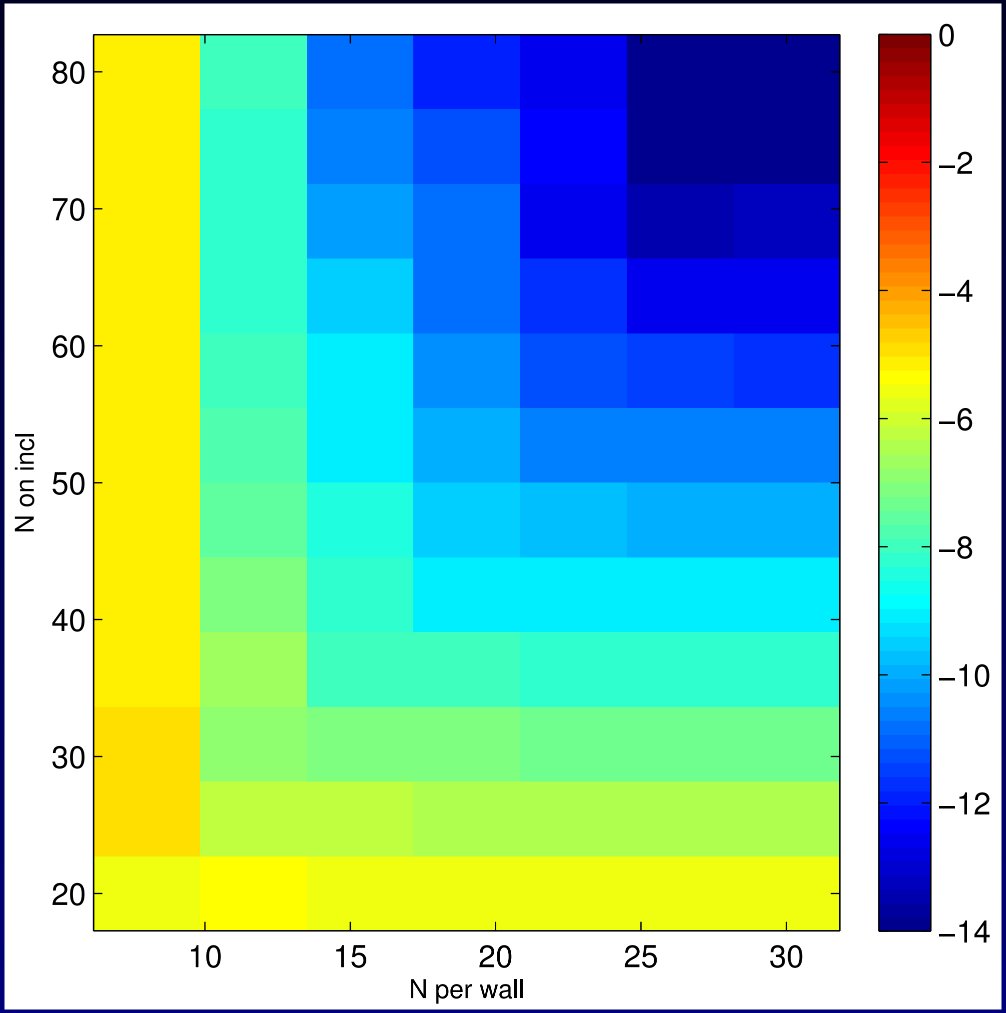
- added extra degrees of freedom (a small #, indep. of complexity of Ω)
- gain robustness: no matrix element blow-up at spurious resonances

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

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

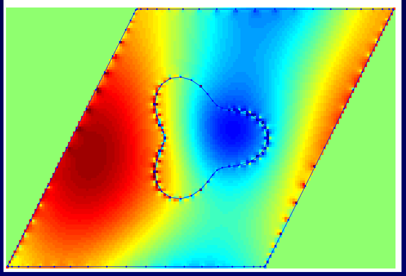
Error convergence

$\log_{10}$ 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

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

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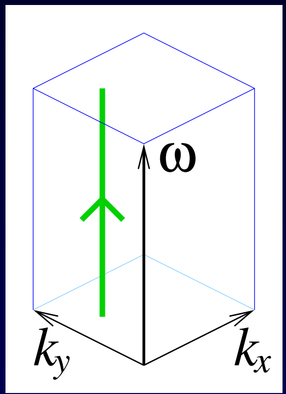

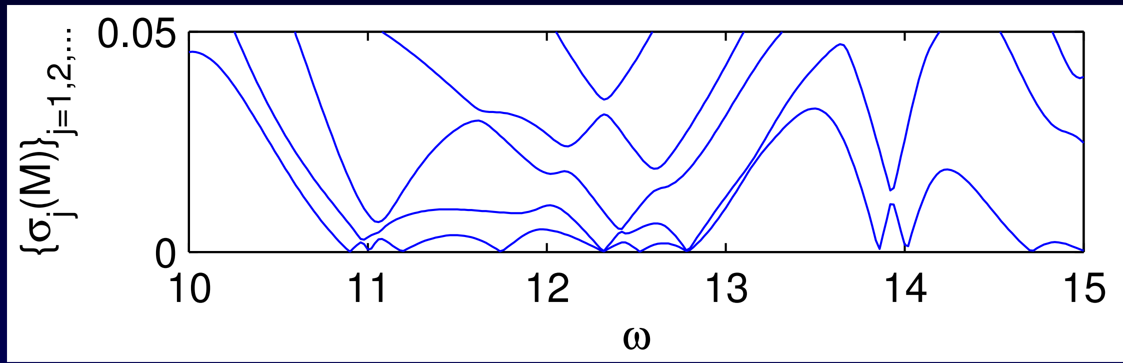

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(α, β fixed)

- slow (20 its per root), unreliable (misses nearby roots)

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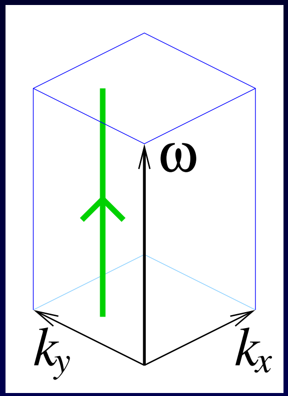

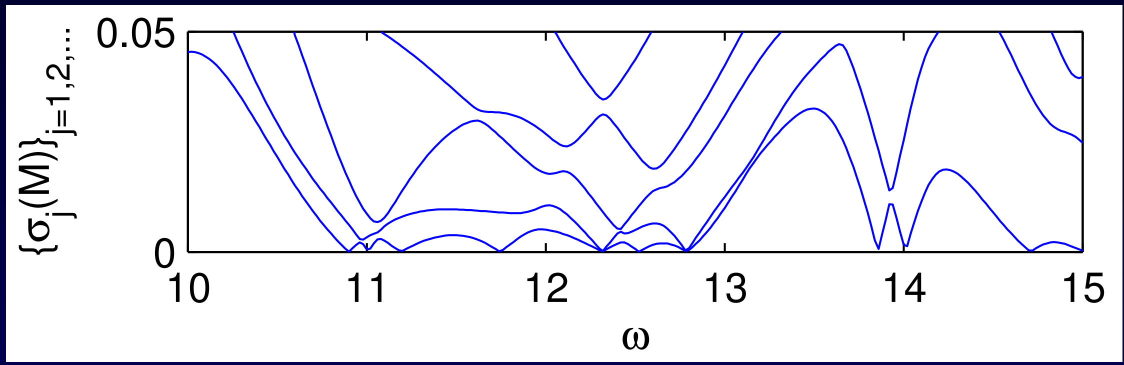

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Realize: $M = I +$ (cpt op-valued analytic func of ω, k_x and k_y)

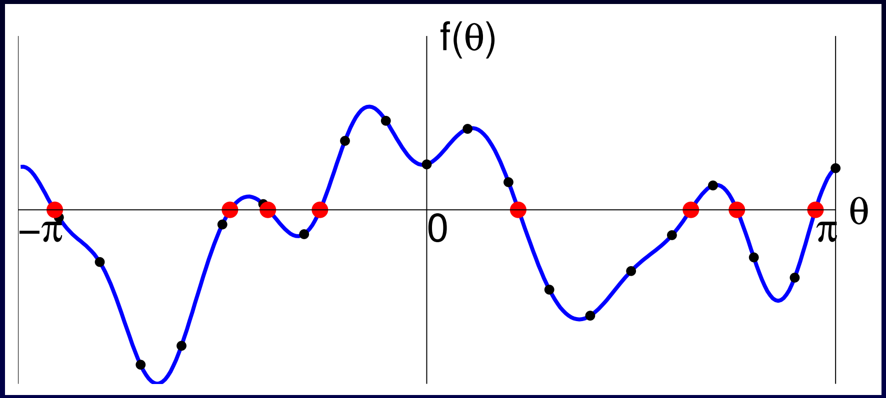
det M is a Fredholm determinant, also analytic

- 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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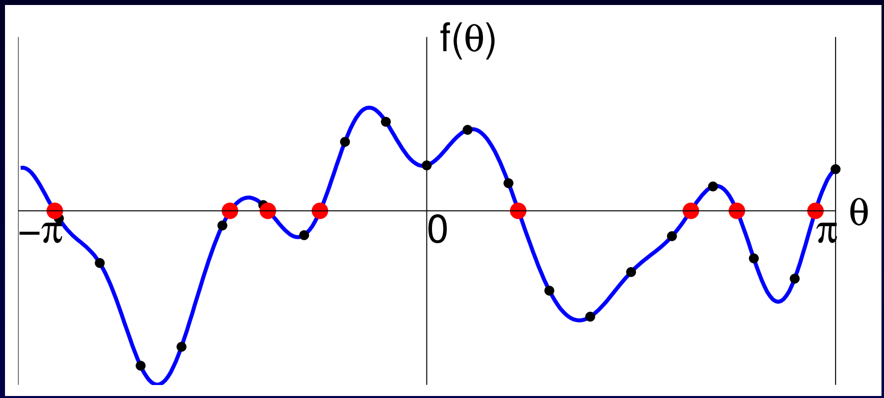

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$$f(\theta) \approx \sum_{n=-N}^{N} c_n e^{in\theta}$$

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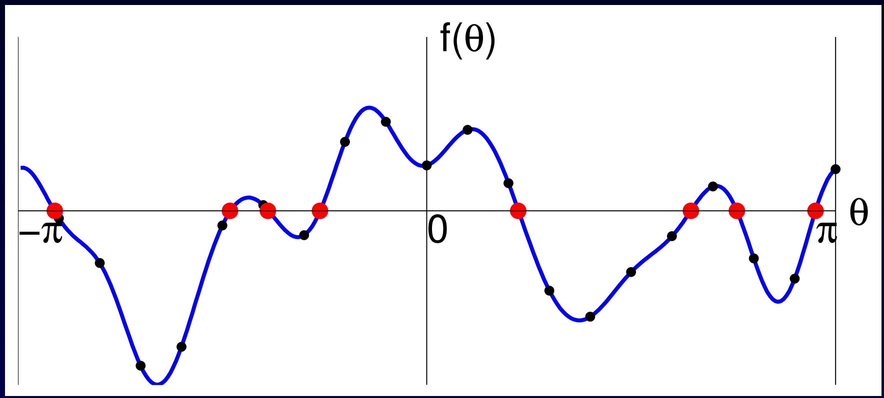

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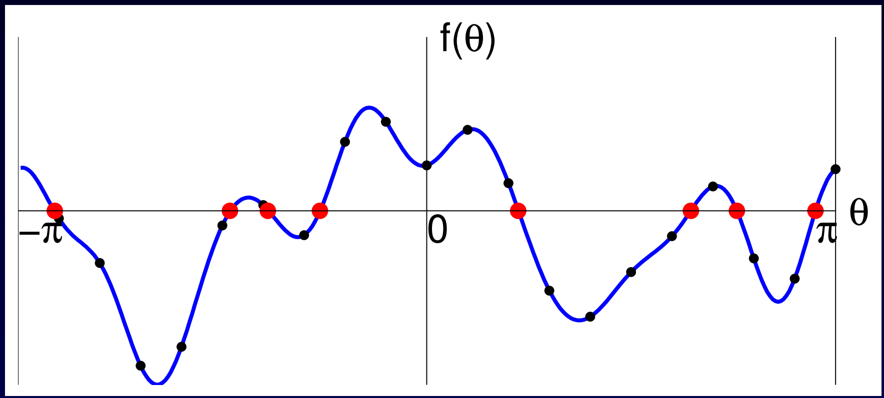

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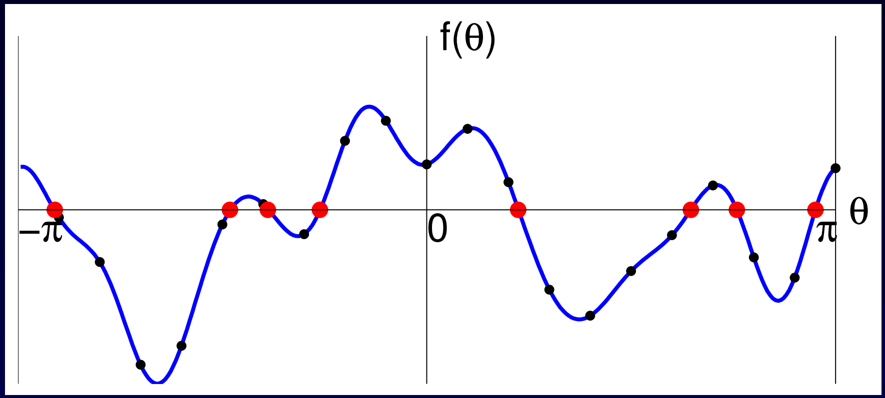

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“Degree doubling”: $z^N q(z)$ is degree-$2N$ poly, so...

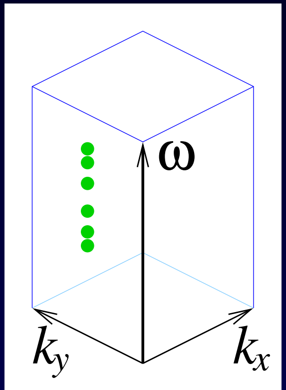
- use Matlab `roots` QR for eigvals of companion matrix, $O(N^3)$ but v. stable
- extract the angles θ of roots near unit circle

(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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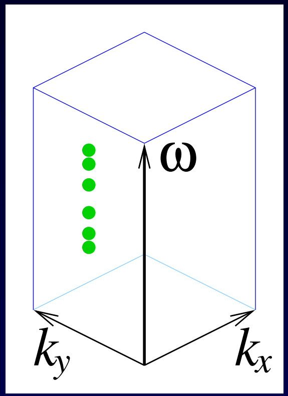

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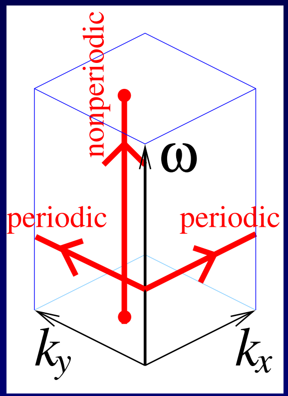
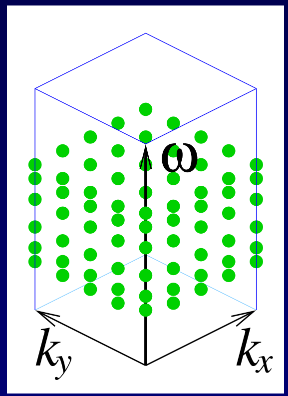


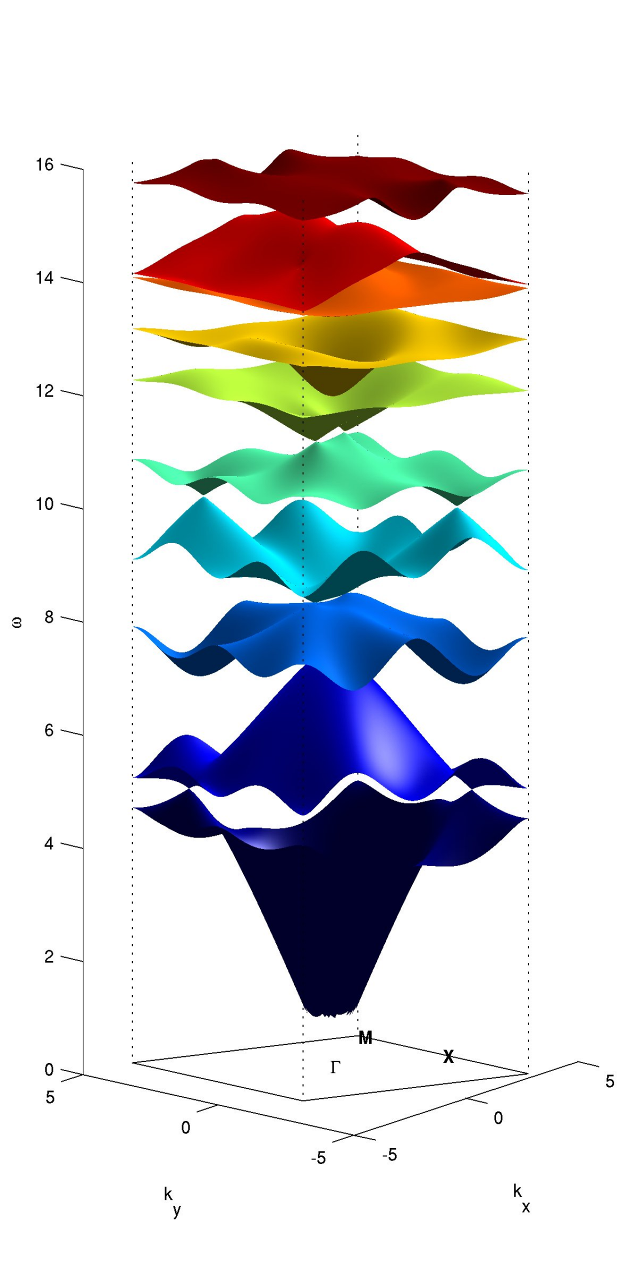
Also analytic in $k_x, k_y \Rightarrow$ interpolate in 3D!



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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`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

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E.g.

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

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make exterior domain using segment

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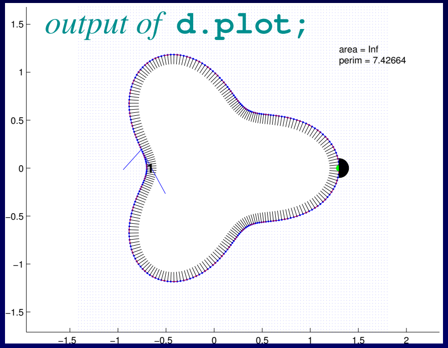


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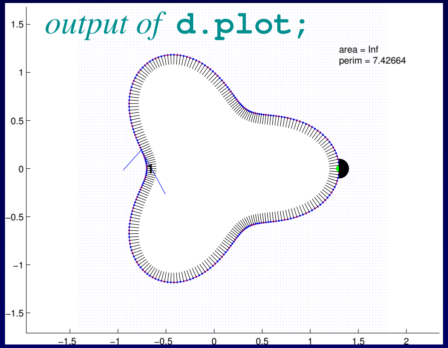


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```
d.setbc(1, 'N', []);
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Neumann BCs on exterior

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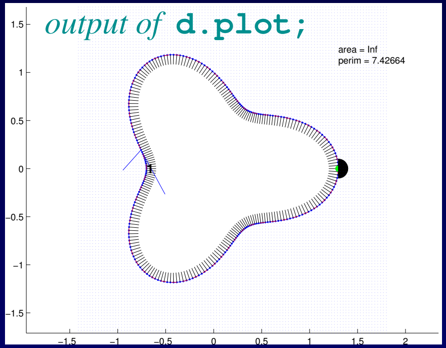


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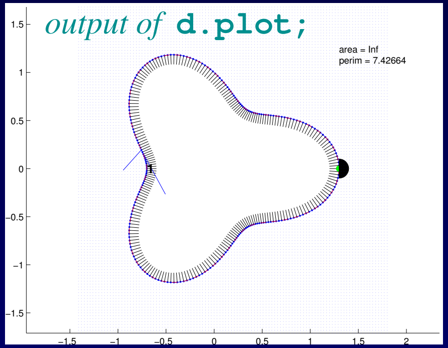


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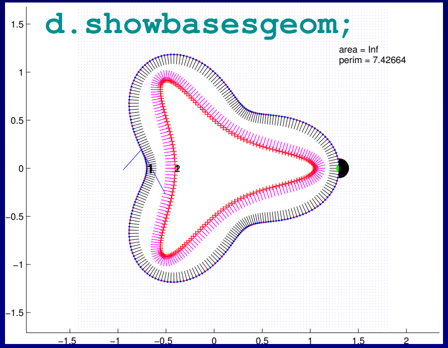


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p.showfullfield(struct('bb',[-2 2 -2 2]));
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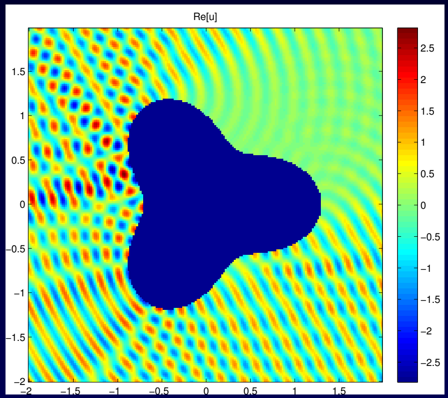

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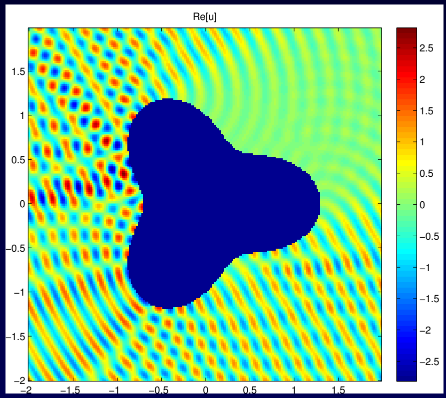

- was easy case: 8 lines (could have done in 80 lines of Matlab)
- multiple (sub)domains: basis, quadrature, bookkeeping hidden
  e.g. dielectric band structure still only 20 lines of code
- human-readable, rapid to code, sensible defaults (you can change)

To do: document periodic BVPs, meshing, Dirichlet EVP, ...