A new integral representation for quasi-periodic scattering problems in two dimensions

IMA workshop, Aug 4, 2010

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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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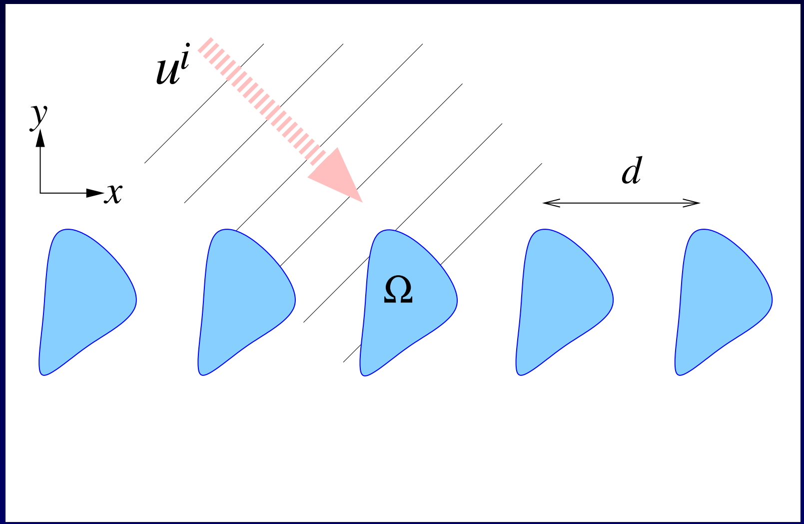

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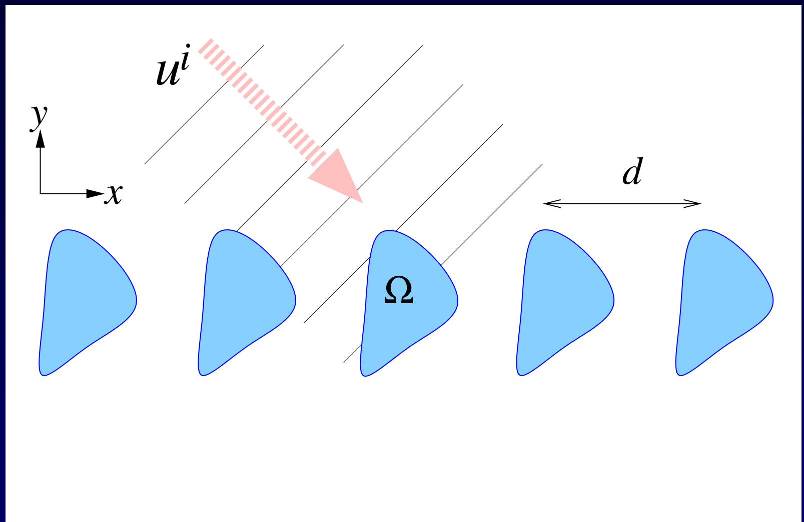

total field $u^t = u^i + u$, where

scattered field u solves BVP:

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\begin{aligned}
(\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} \\
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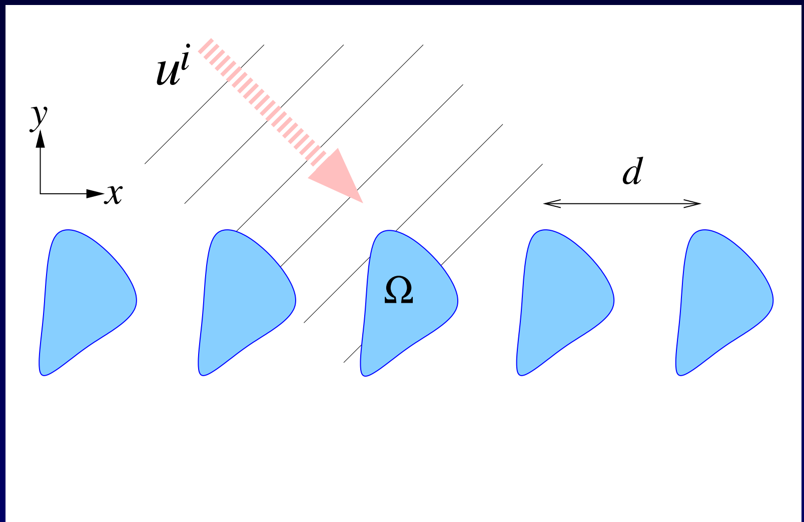

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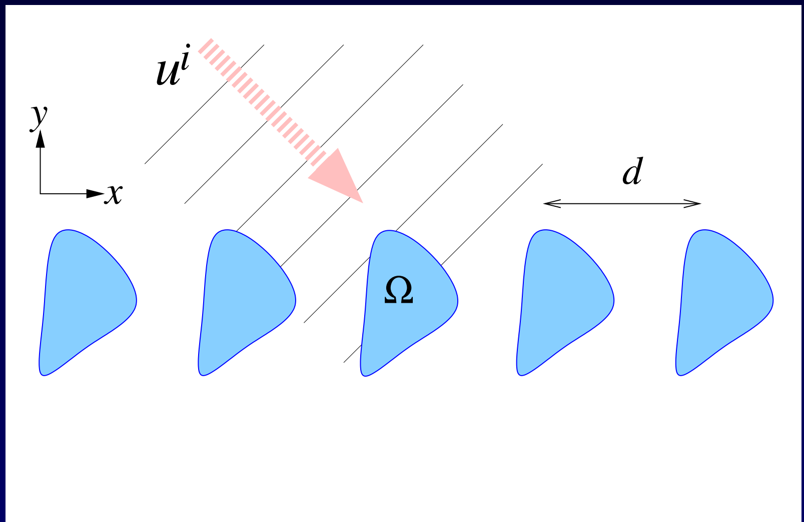

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- classical BVP: acoustics, z-invariant Maxwell (Rayleigh 1907,...)

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Gratings, filters, antennae, photonic crystals, meta-materials, solar…

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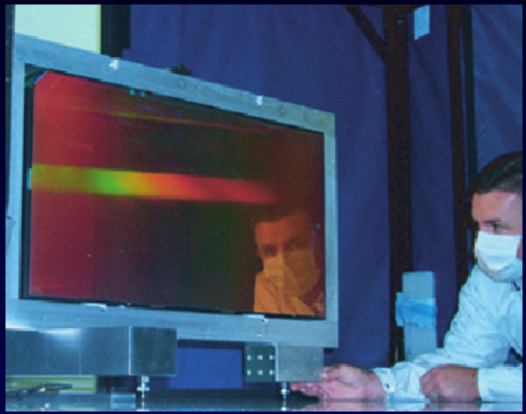

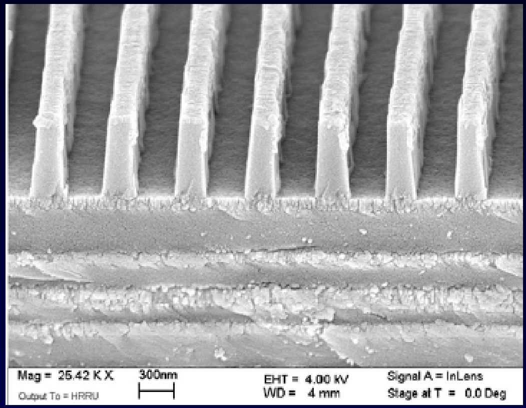

multi-layer dielectric diffraction grating, NIF lasers (LLNL)

2×10^6 periods! (Barty '04)

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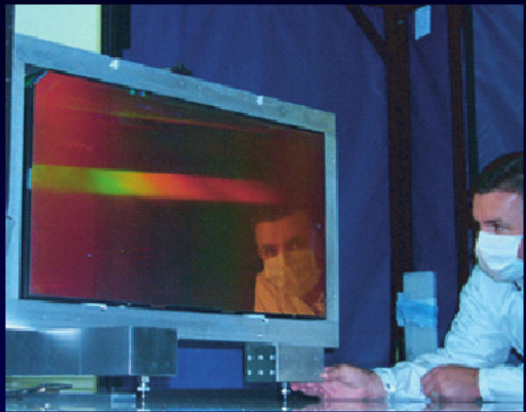

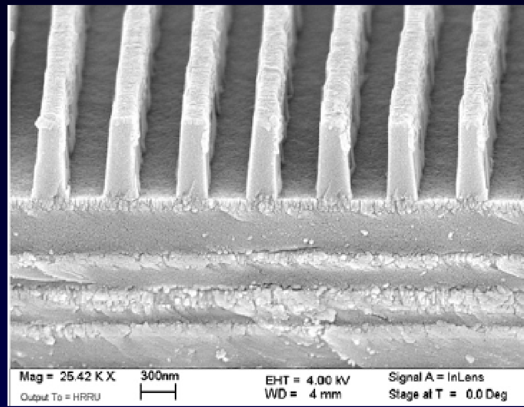

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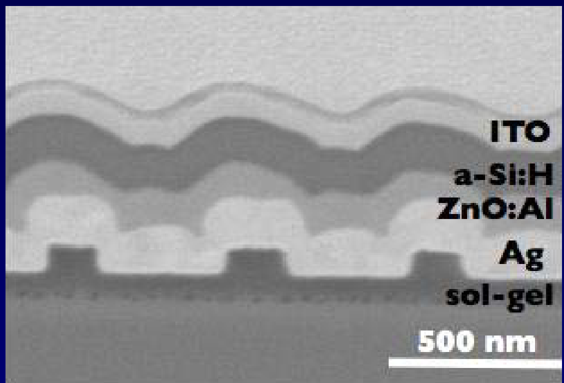
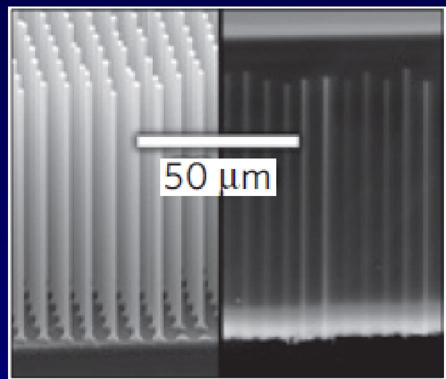


plasmonic solar cell (Atwater '10)



↕ high aspect ratio

Si microwires absorber (Kelzenberg '10)

- Design optimization
- Simulation at $>10^3$ inc. angles, frequencies

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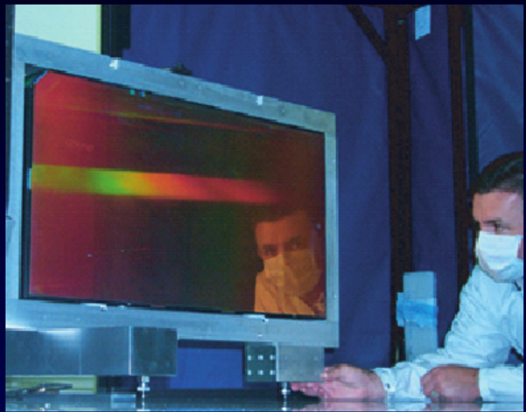

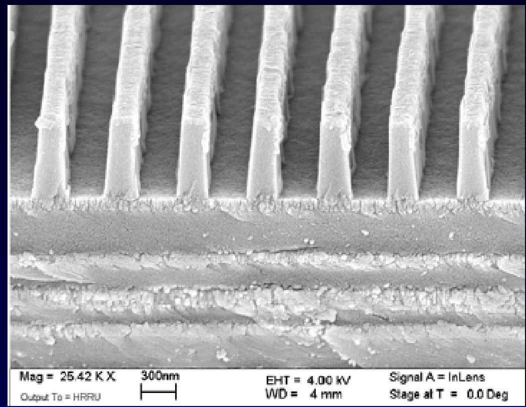

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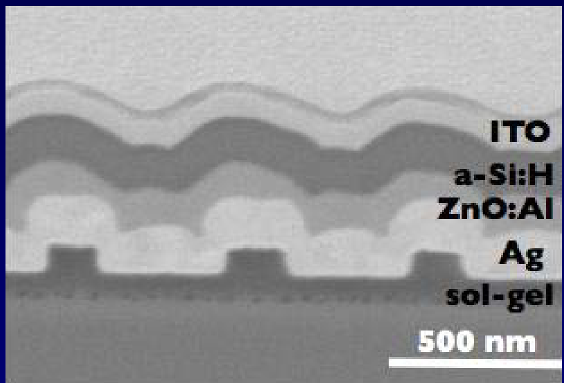

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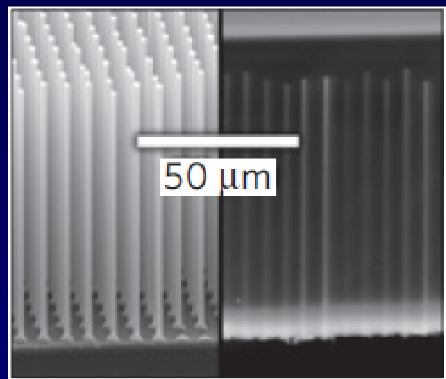

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First step is our paradigm problem: 2D grating of isolated obstacles…

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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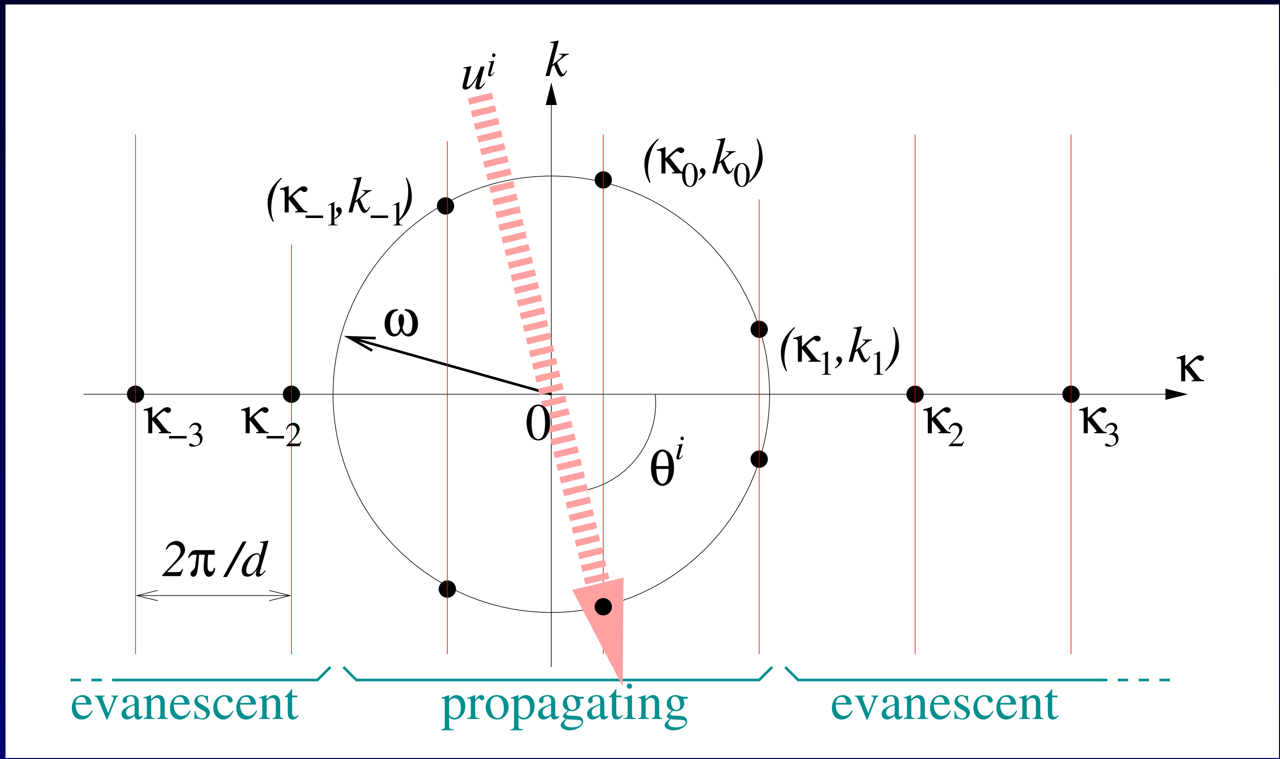

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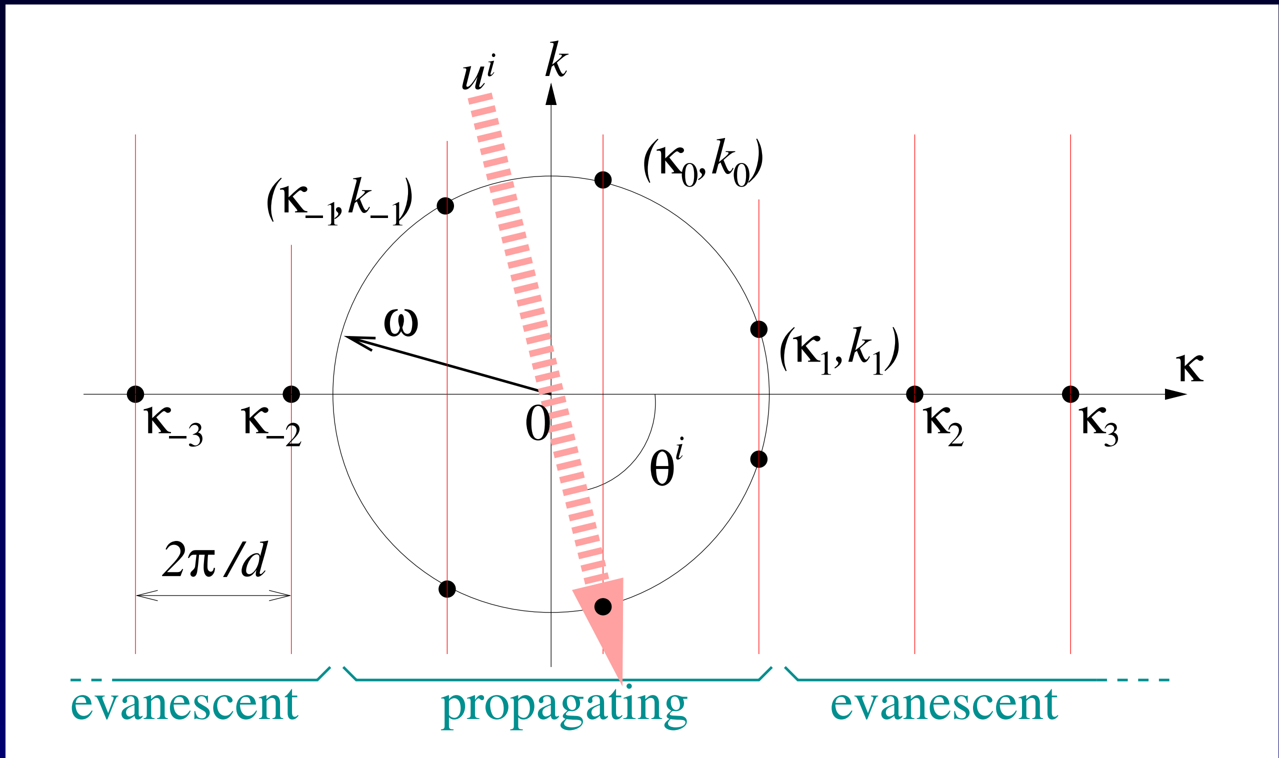

k_n real: propagating

k_n imag: evanescent (decaying or growing in y)

$k_n = 0$: Wood's anomaly rapid change wrt ω, inc. angle θ^i (Wood 1902)

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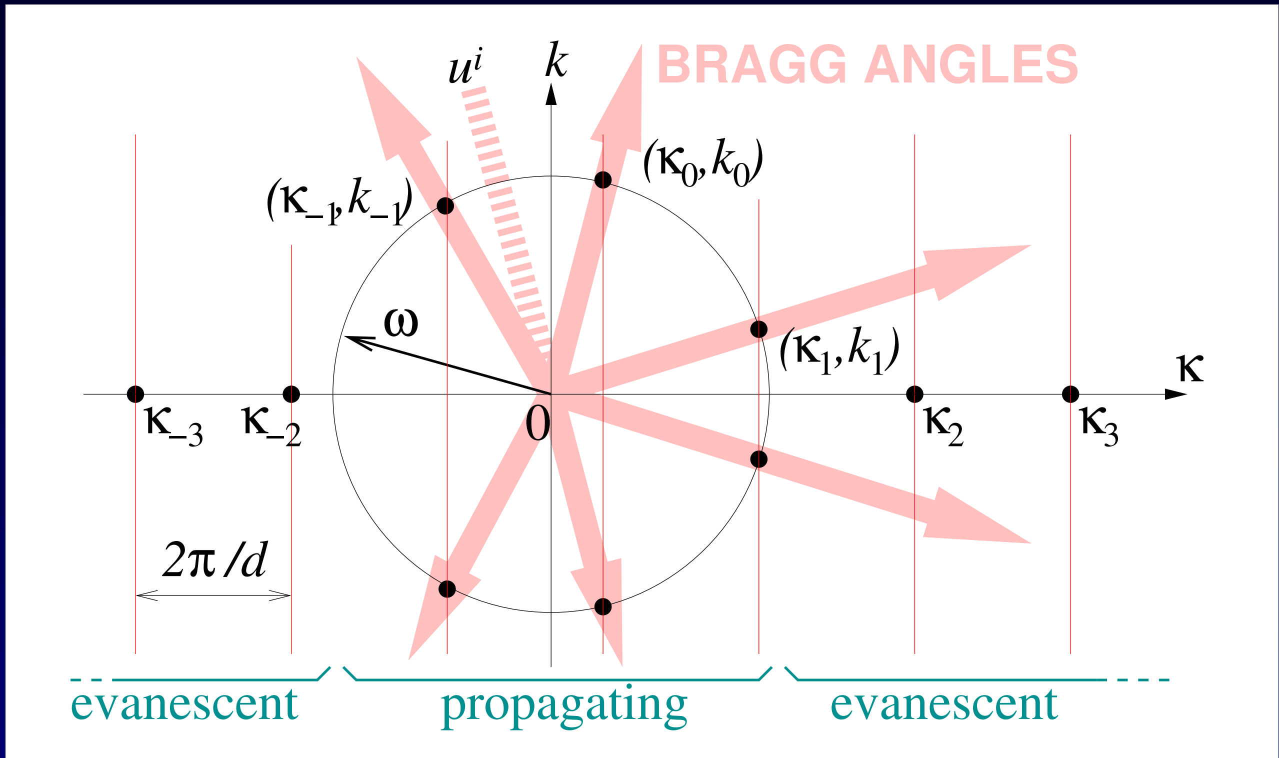

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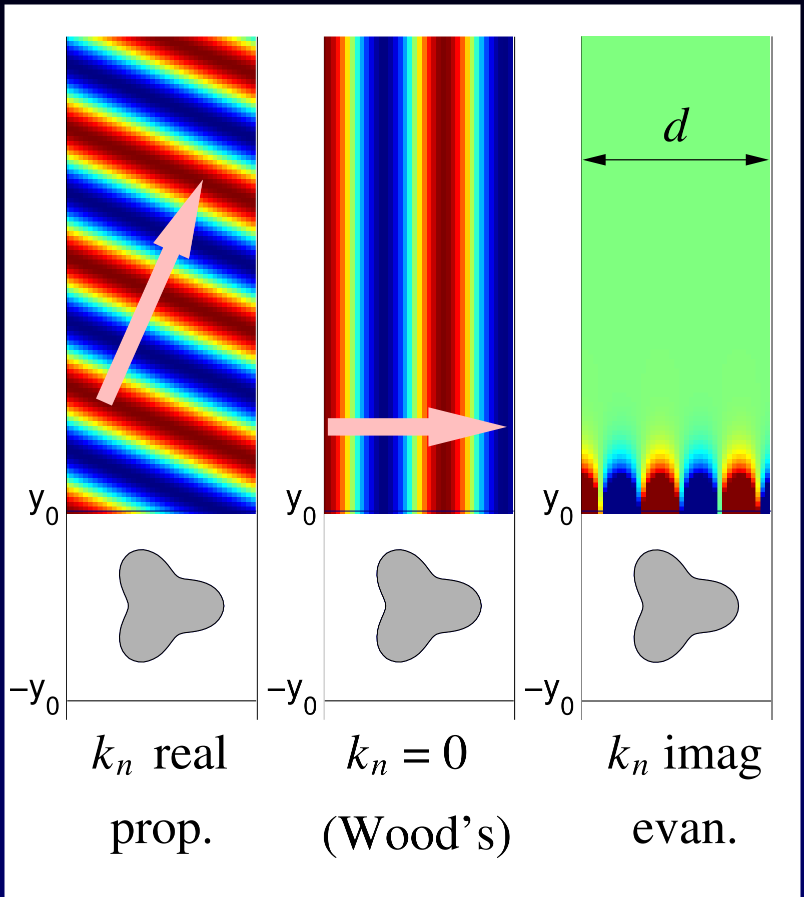
Rayleigh–Bloch radiation conditions



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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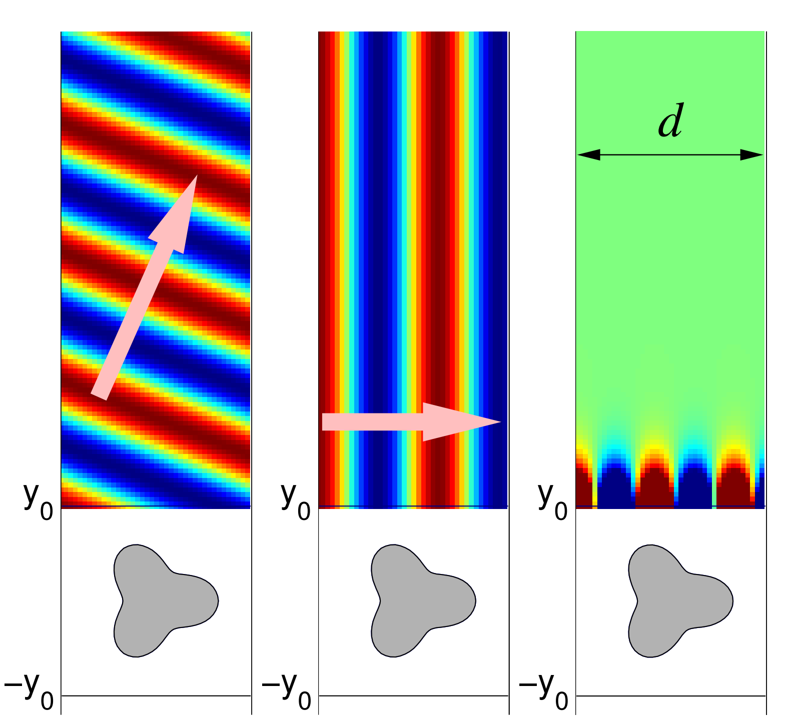

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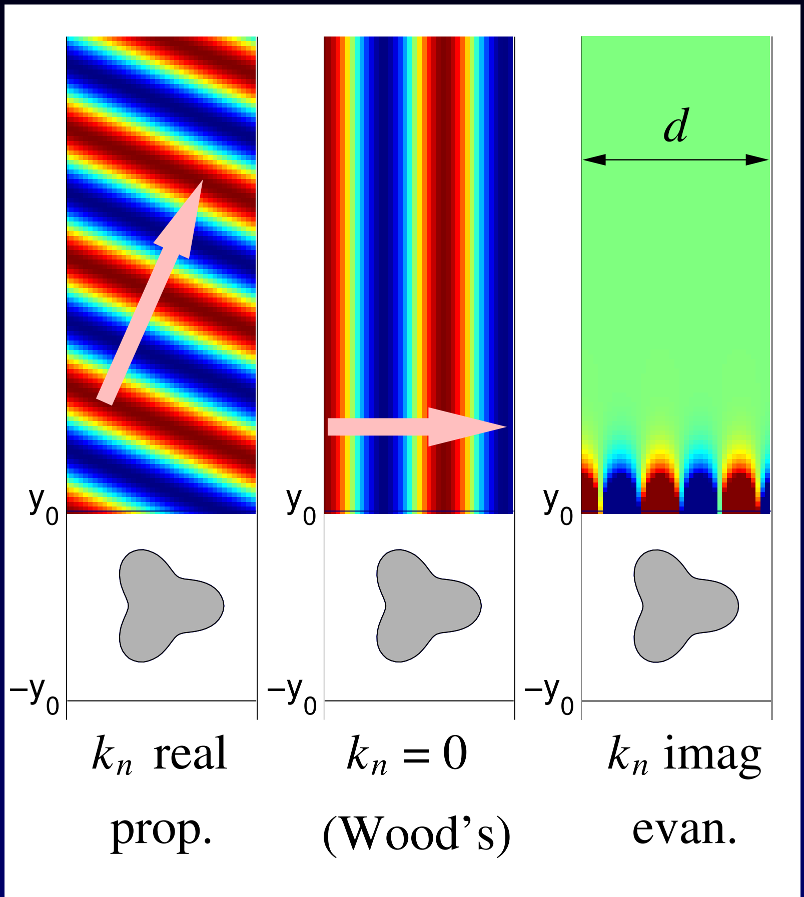

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Numerical methods for BVP   FDTD, FEM, C-method, coupled-wave,…

Piecewise homogeneous → integral equations: discretize only interface $\partial\Omega$

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

Potential theory (review)

Single-, double-layer, $\mathbf{x} \in \mathbb{R}^2$, curve Γ:

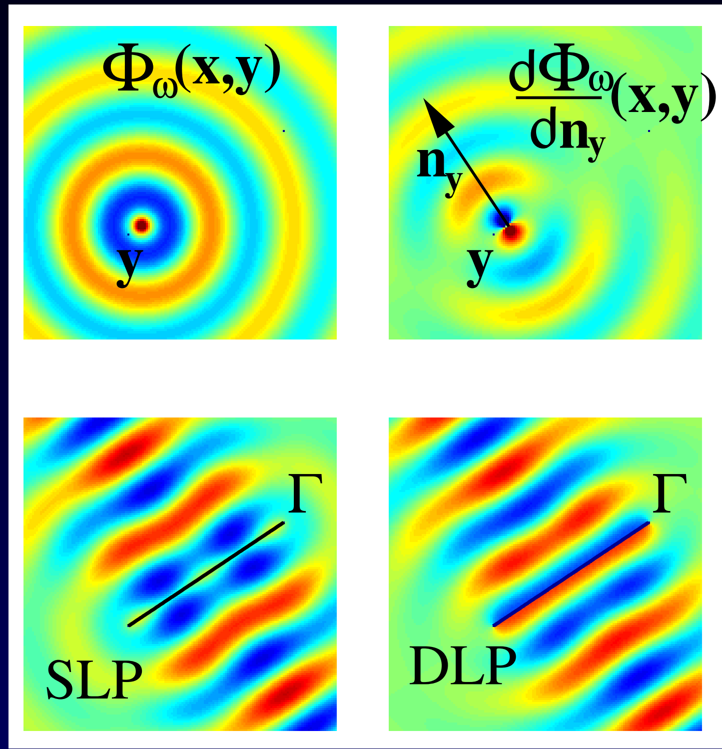
$v(\mathbf{x}) = \int_\Gamma \Phi_\omega(\mathbf{x},\mathbf{y})\sigma(\mathbf{y})ds_\mathbf{y} := (\mathcal{S}\sigma)(\mathbf{x})$

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

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

Helmholtz fundamental soln

a.k.a. free space Greens func



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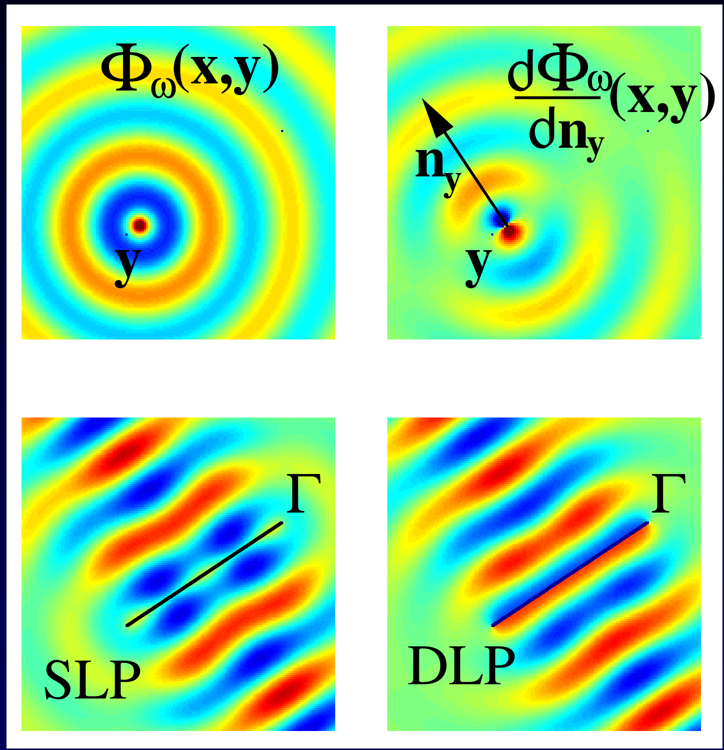


Jump relations: limit as $\mathbf{x} \to \Gamma$ may depend on which side ($\pm$):

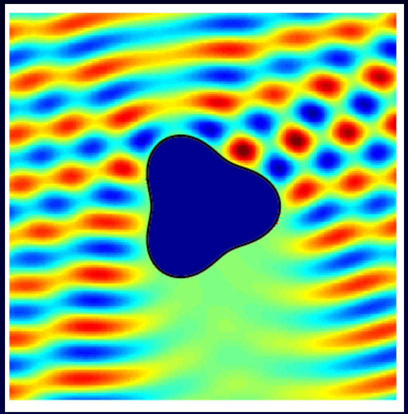
$$v^\pm = S\sigma$$
$$v_n^\pm = D^*\sigma \mp \tfrac{1}{2}\sigma$$
$$u^\pm = D\tau \pm \tfrac{1}{2}\tau$$
$$u_n^\pm = T\tau$$

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

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

Single Dirichlet obstacle scattering (review)

represent scattered field $u = (\mathcal{D} - i\omega\mathcal{S})\tau$ indirect CFIE on $\partial\Omega$



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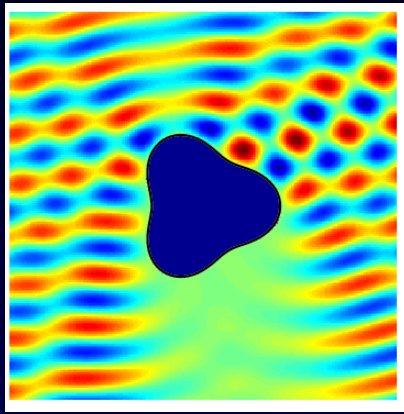

BC & JR1,3: $A\tau := (\frac{1}{2}I + D - i\omega S)\tau = -u^i|_{\partial\Omega}$

2nd-kind IE on $\partial\Omega$, D, S cpt so A sing. vals. $\nrightarrow 0$

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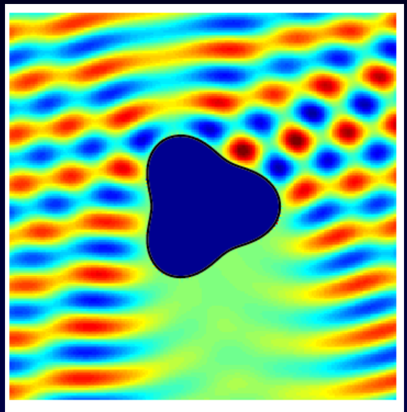

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Quadrature: nodes $\mathbf{y}_j \in \partial\Omega$, weights w_j, $j = 1, \ldots, N$
Nyström discretization: N-by-N linear system,

$$\boldsymbol{A\tau} = \boldsymbol{b} \qquad \text{unknown density vector } \boldsymbol{\tau} \approx \{\tau(\mathbf{y}_j)\}_{j=1}^N$$

- kernel weakly singular. E.g. for $\partial\Omega$ analytic, have spectral scheme for $f(s) + \log(4\sin^2\frac{s}{2})g(s)$, f, g analytic 2π-periodic (Kress '91)

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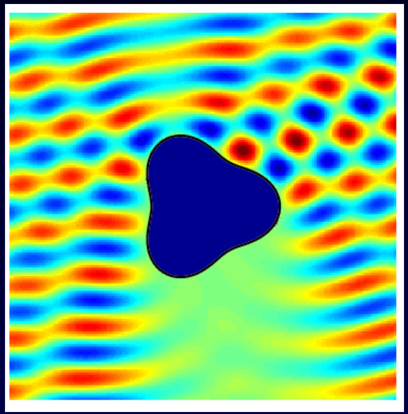

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How turn this into a *periodic* solver, compatible with modern IE tools?

- large-scale technology: corner and 3D quadratures, FMM accel...

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replace kernel $\Phi_\omega(\mathbf{x})$ by $\Phi_{\omega,\mathrm{QP}}(\mathbf{x}) := \sum_{m\in\mathbb{Z}} \alpha^m \Phi_\omega(\mathbf{x} - m\boldsymbol{d})$

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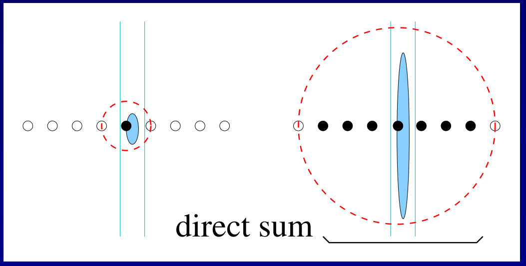
- $(*)$ converges in disc $\Rightarrow$ high aspect ratio Ω is bad:

  FMM based on cubes, tricky (Otani–Nishimura '08)



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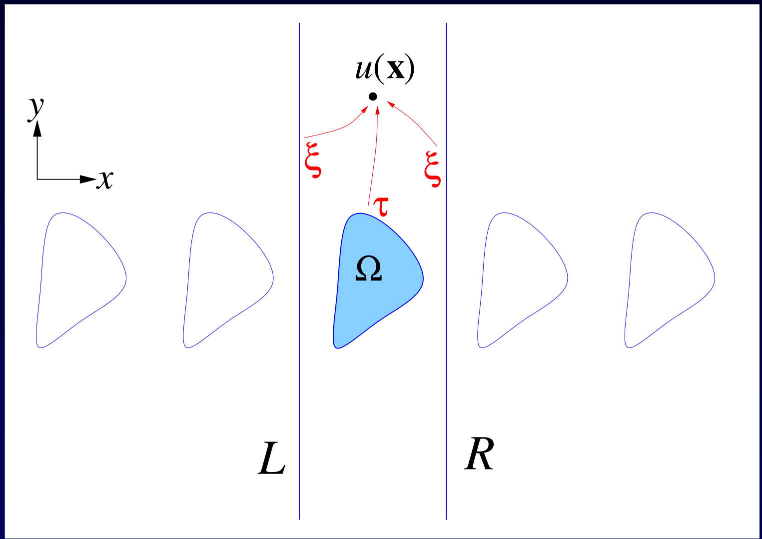

$$u \quad = \quad (\mathcal{D} - i\omega\mathcal{S})\tau \quad + \quad u_{\text{QP}}[\xi]$$

as before — densities ξ on L and R

BC $\quad u = -u^i \quad$ on $\partial\Omega$ $\quad$ as before

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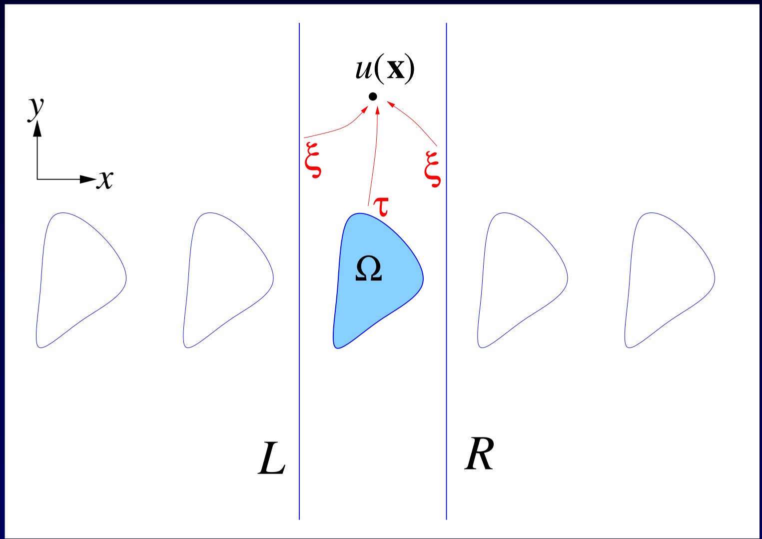

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BC $\quad u = -u^i \quad$ on $\partial\Omega$ $\quad$ as before

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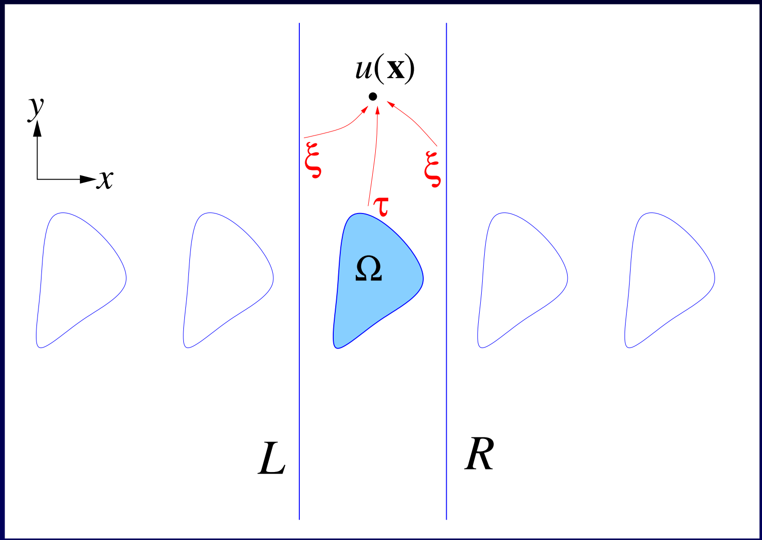

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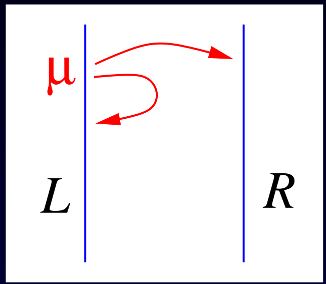
Major issues

(1) How choose rep. $u_{\rm QP}[\xi]$ so effect of ξ on $[f; f_n]$ 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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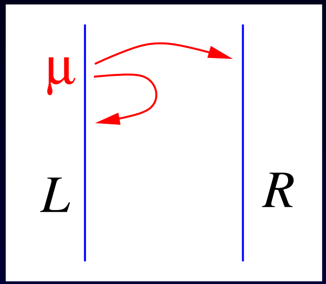

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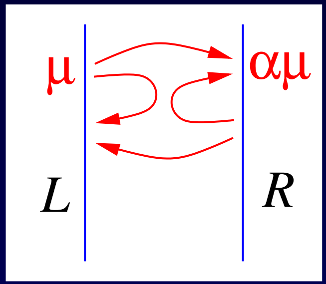

$$f = (S_{LL} - \alpha^{-1} S_{RL})\mu + \alpha(S_{LR} - \alpha^{-1} S_{RR})\mu$$
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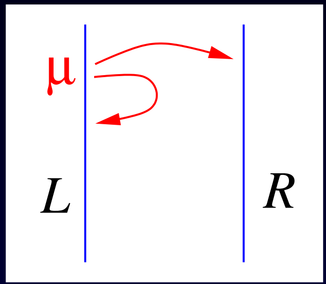

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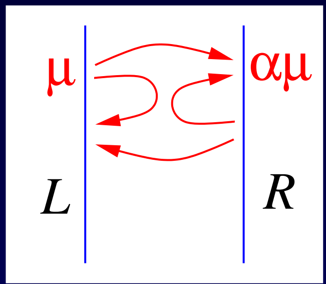

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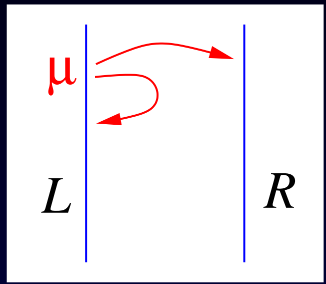

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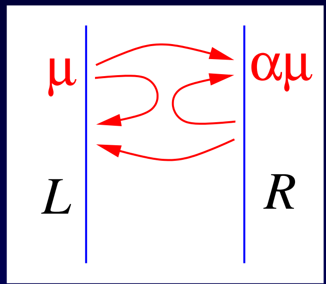

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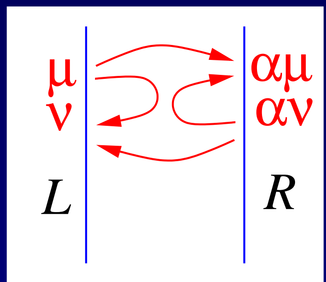
Similarly need to control f via JRs, so...

Add DLP ν on L, R,:



$$\begin{bmatrix} f \\ f_n \end{bmatrix} = Q \begin{bmatrix} \nu \\ -\mu \end{bmatrix} =: Q\xi$$

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

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

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Fourier transform in y-direction: handle $\hat{\mu}$, $\hat{\nu}$, $\hat{f}$, $\hat{f}_n$

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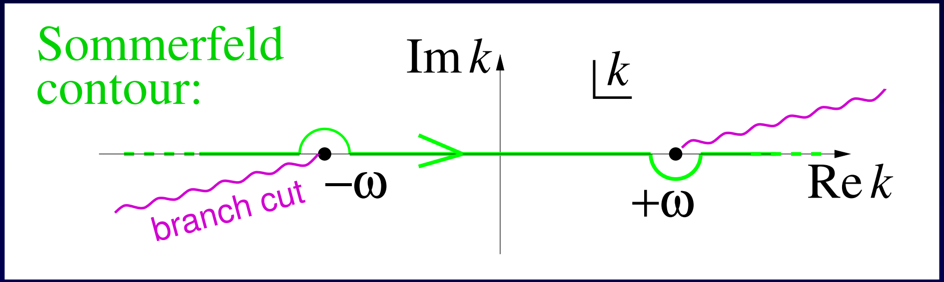
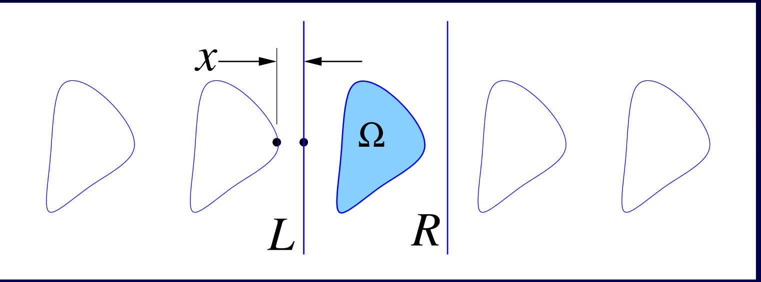
exponential tails for $|k| > \omega$
decay rate prop. to $|x|$





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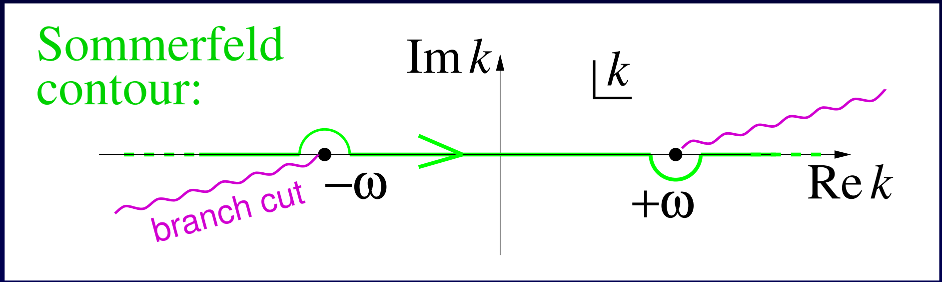
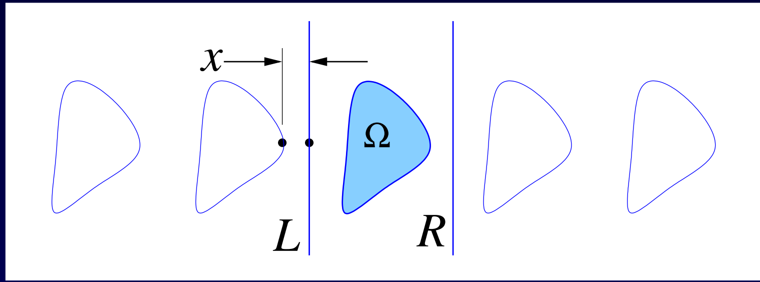




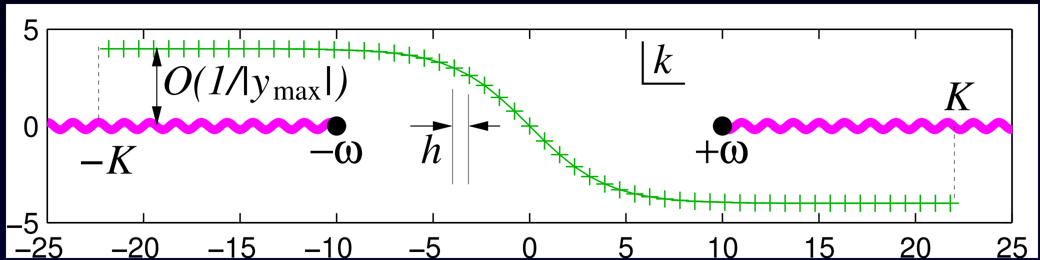
Gives FT-y densities on L (or R) wall at $x = x_0$:

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

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

- same JRs as before; $\hat{\mu}(k)$, $\hat{\nu}(k)$ affect only $\hat{f}(k)$, $\hat{f}_n(k)$ diagonal in k

k-space quadrature on Sommerfeld contour



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

sample Re k with 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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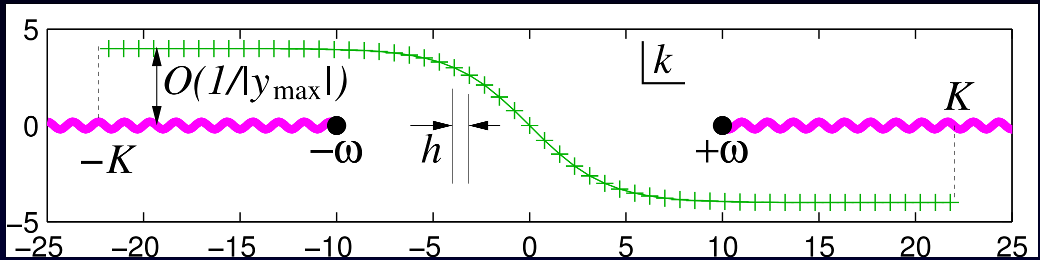

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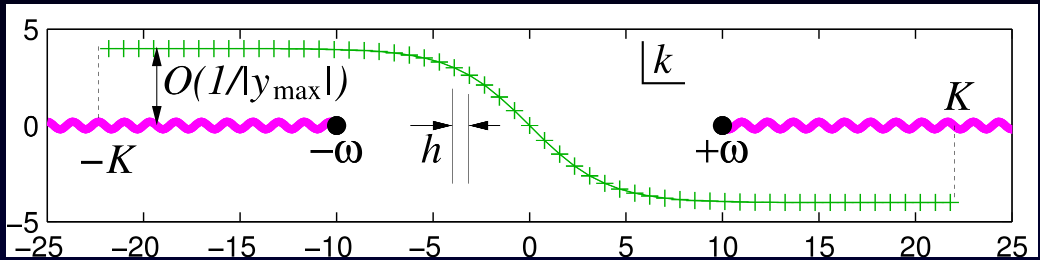

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Solve full $(N+2M)$-by-$(N+2M)$ linear system:

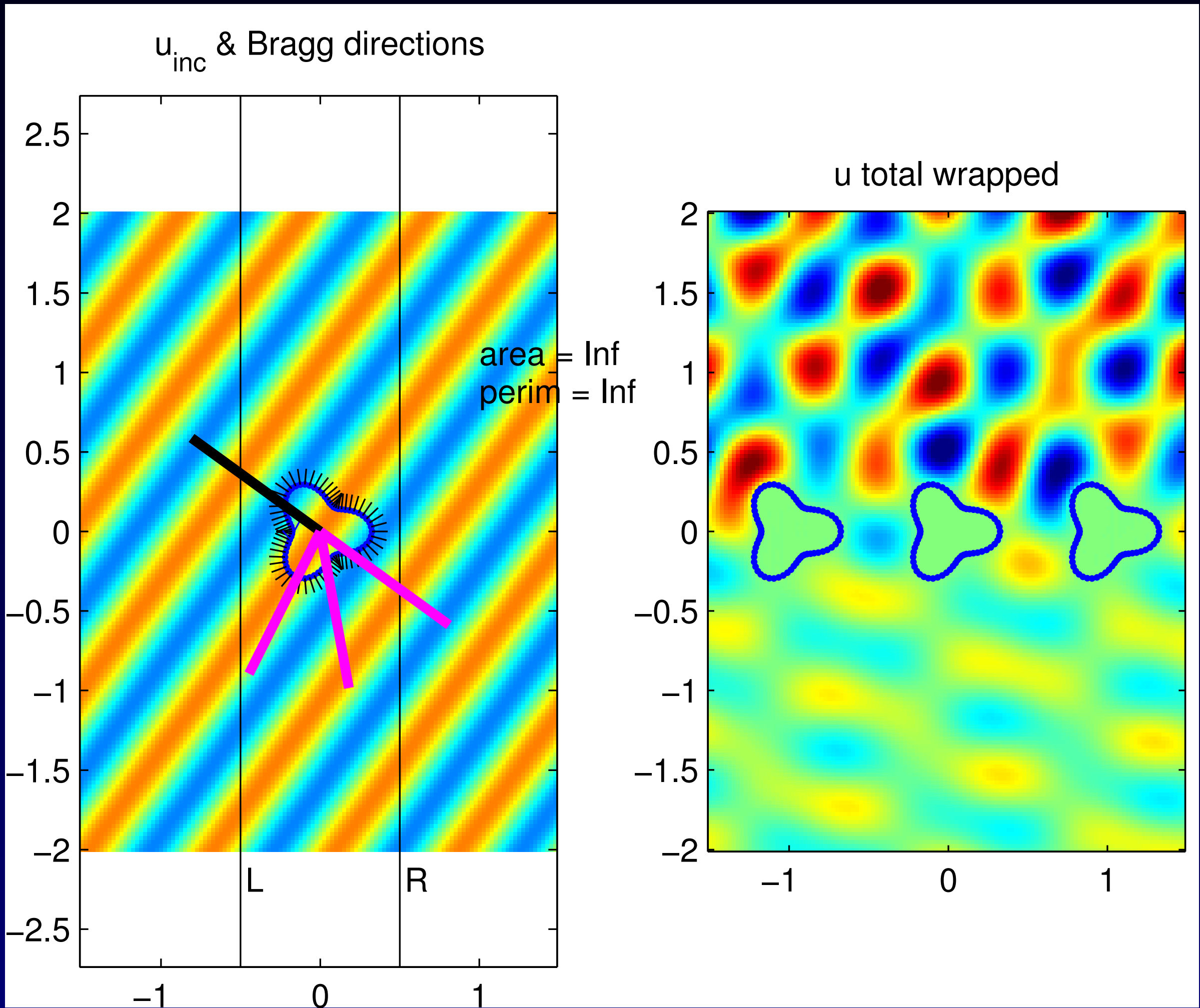
$$\begin{bmatrix} \boldsymbol{A} & \hat{\boldsymbol{B}} \\ \hat{\boldsymbol{C}} & \hat{\boldsymbol{Q}} \end{bmatrix} \begin{bmatrix} \boldsymbol{\tau} \\ \hat{\boldsymbol{\xi}} \end{bmatrix} = \begin{bmatrix} \boldsymbol{b} \\ \boldsymbol{0} \end{bmatrix}$$

$\leftarrow$ BC on $\partial\Omega$
$\leftarrow$ FT-y of discrep.

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

Results

(10-line code in 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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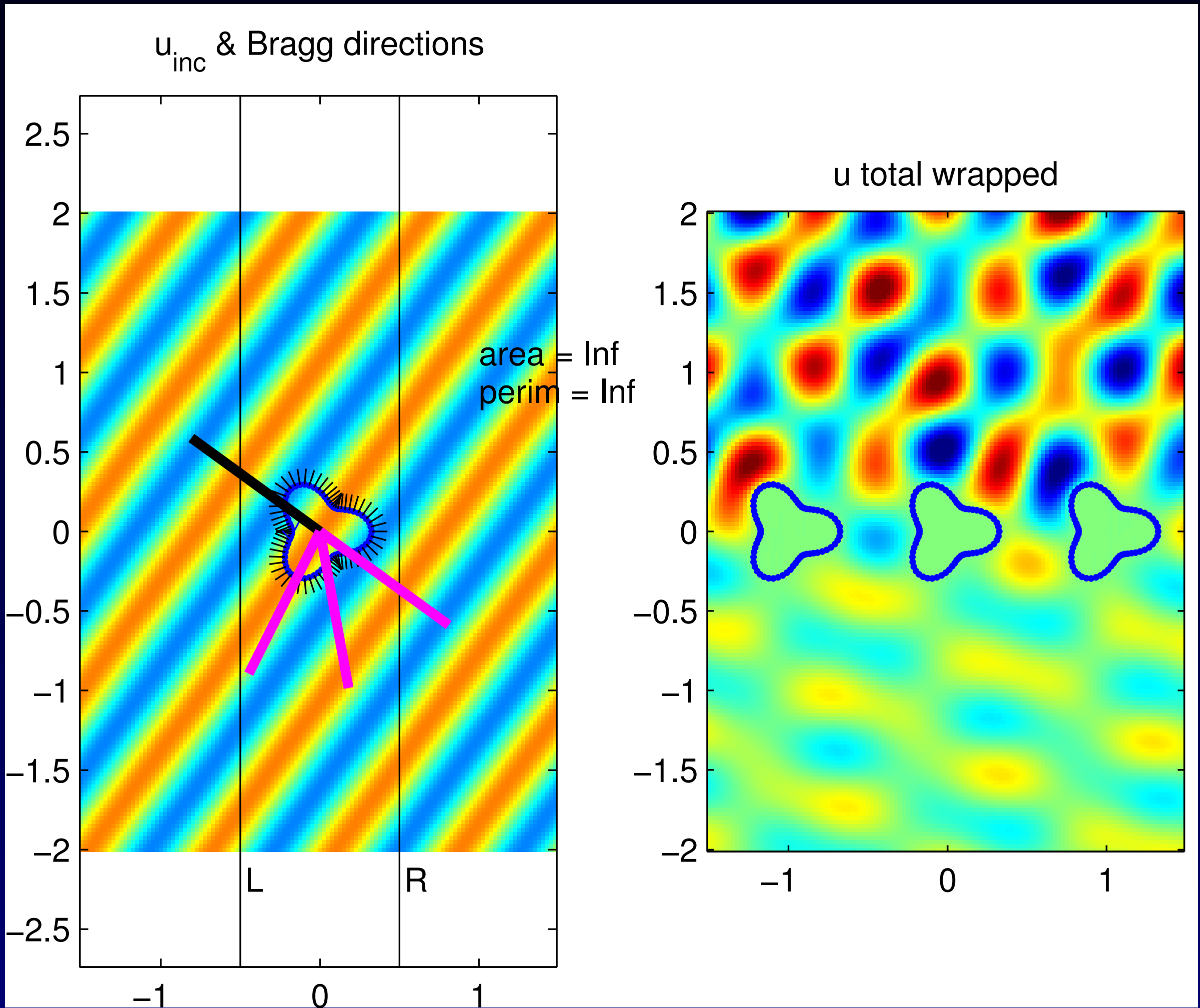
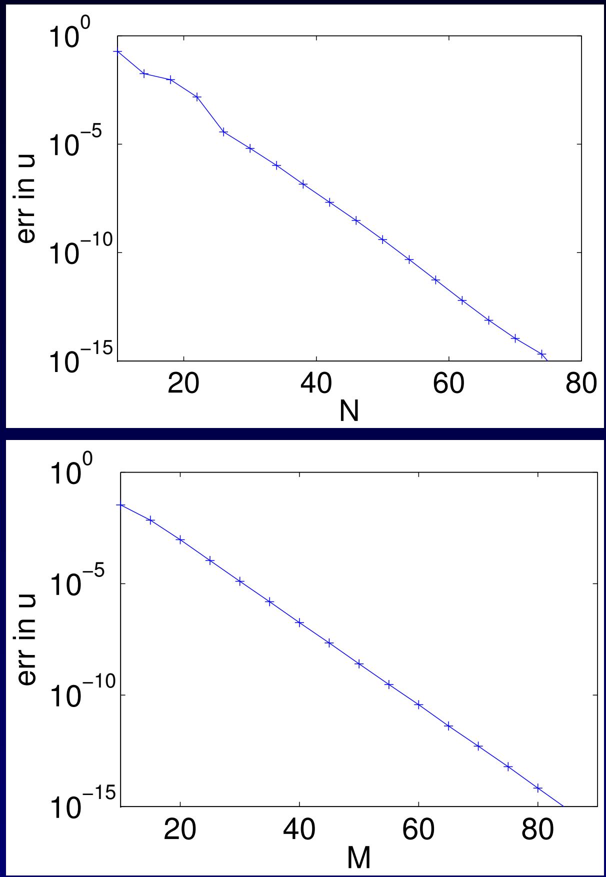


Exponential convergence:



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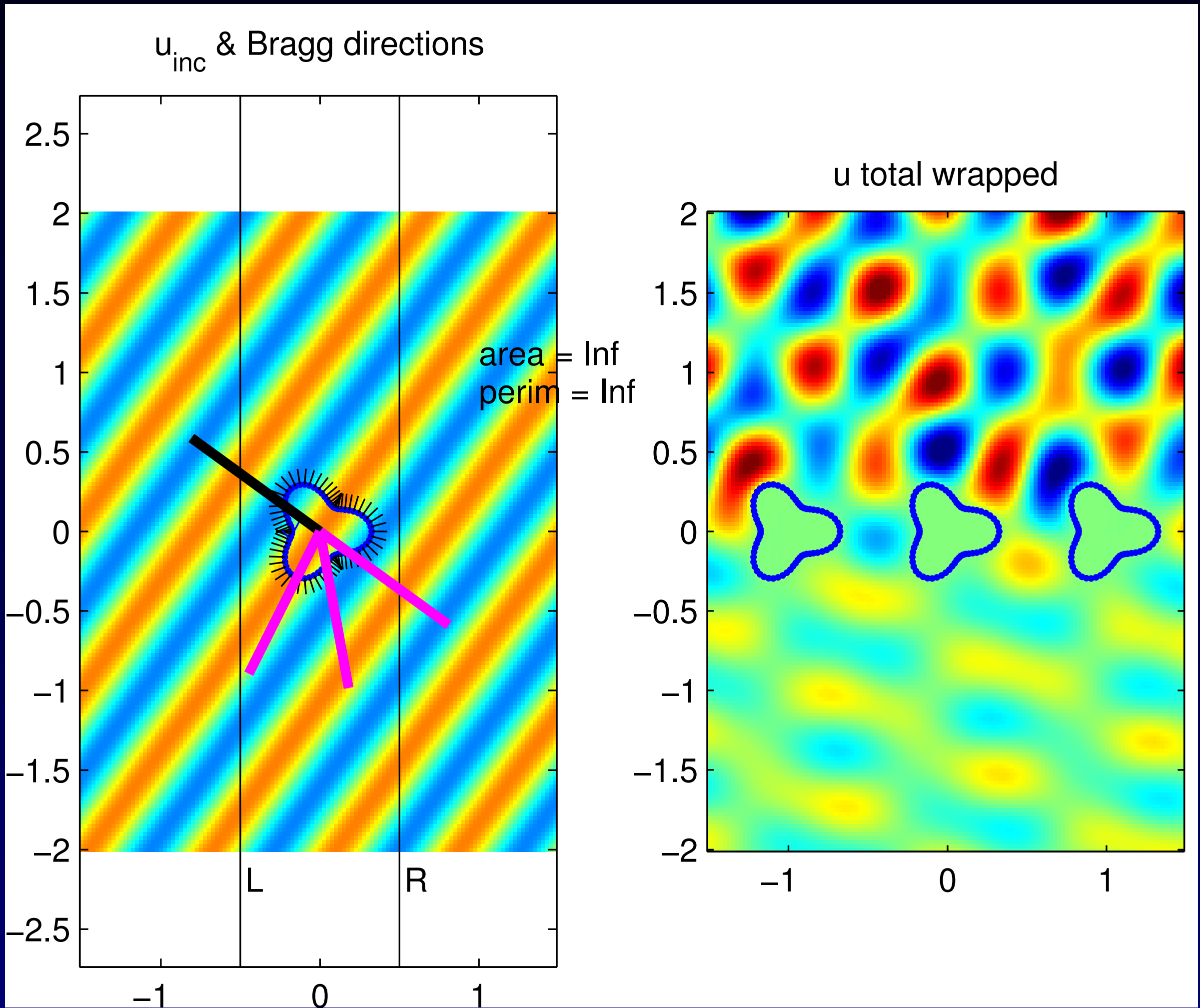

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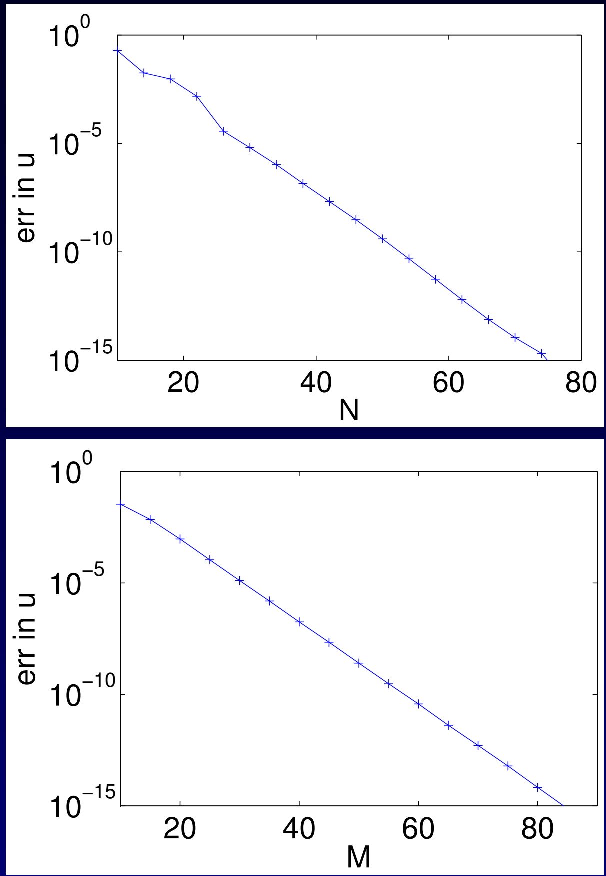

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- improved convergence rate by summing 1 or 2 $\partial\Omega$ neighbors directly
- low condition # $\sim 10^2$: solved to 14 digits in 55 GMRES iters.

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

recall k_n are Rayleigh–Bloch y-wavenumbers: $+k_n$ travels upwards, $-k_n$ downwards

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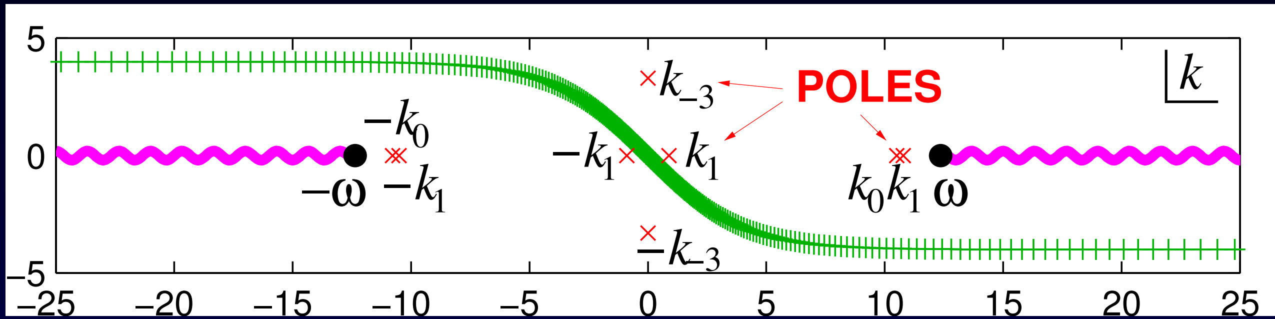

Why?

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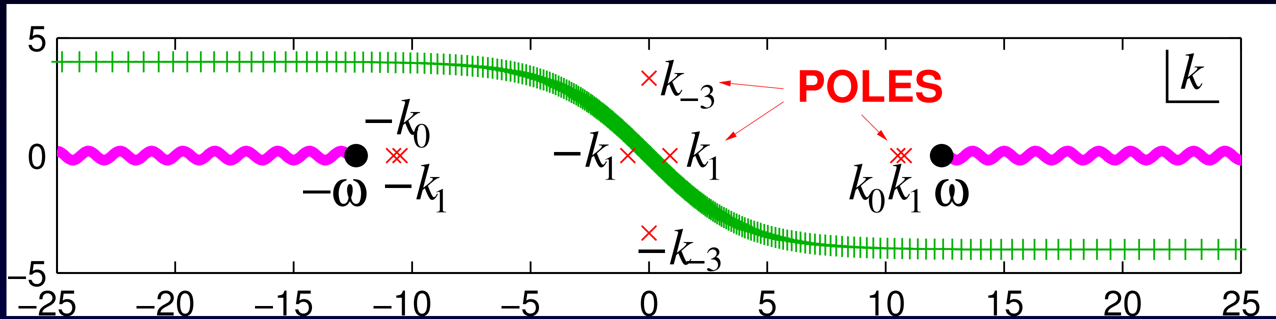
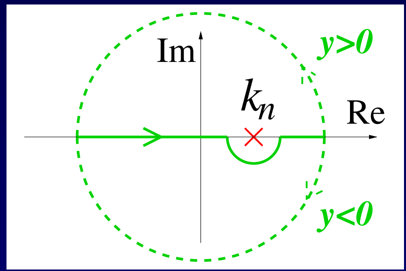
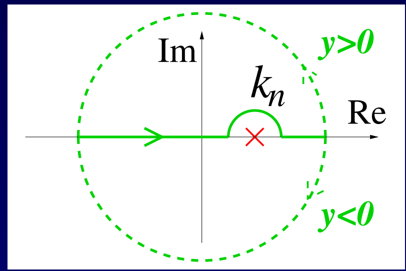


Why? $$\frac{i}{2\pi(k_n - k)} \overset{\text{FT}}{\longleftrightarrow} \begin{cases} e^{ik_n y}, & y > 0 \\ 0, & y < 0 \end{cases} \quad \text{or} \quad \begin{cases} 0, & y > 0 \\ -e^{ik_n y}, & y < 0 \end{cases}$$





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

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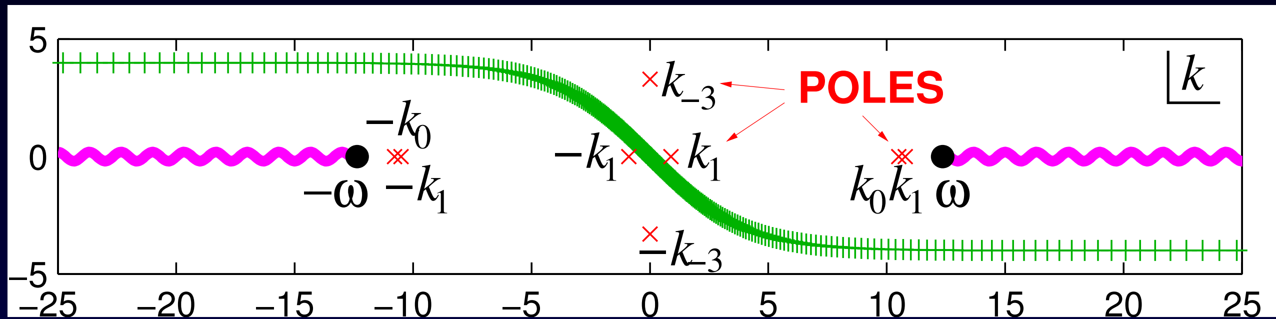

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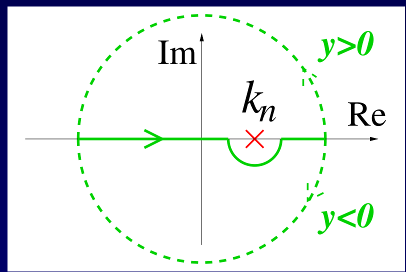
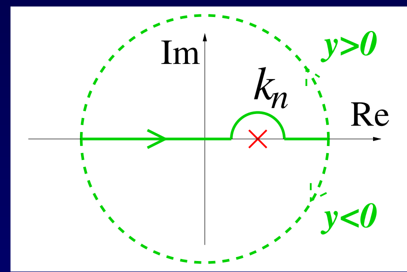




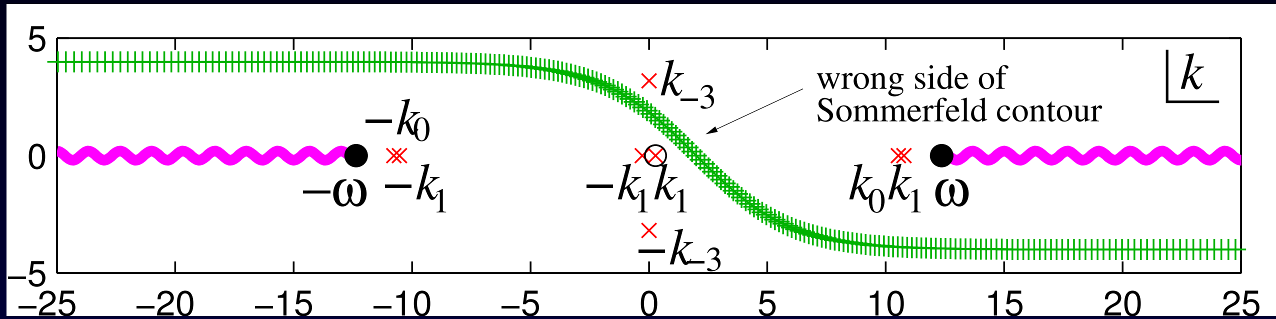
interpretation for $k_n > 0$: R–B outgoing above incoming below

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

- not robust: log blow-up of M, cond. # and $\|\hat{\xi}\|$ diverge!

Well-conditioned robust scheme near Wood's

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



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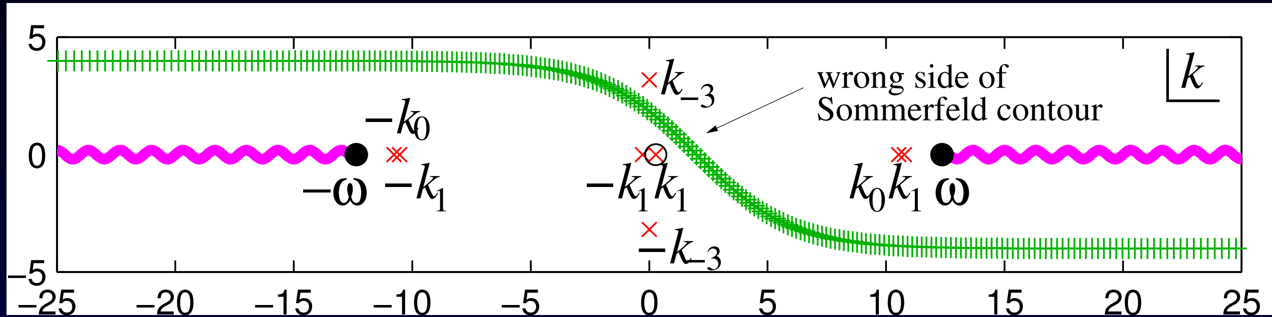

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The fix: (inspiration: Mikhlin '57)

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

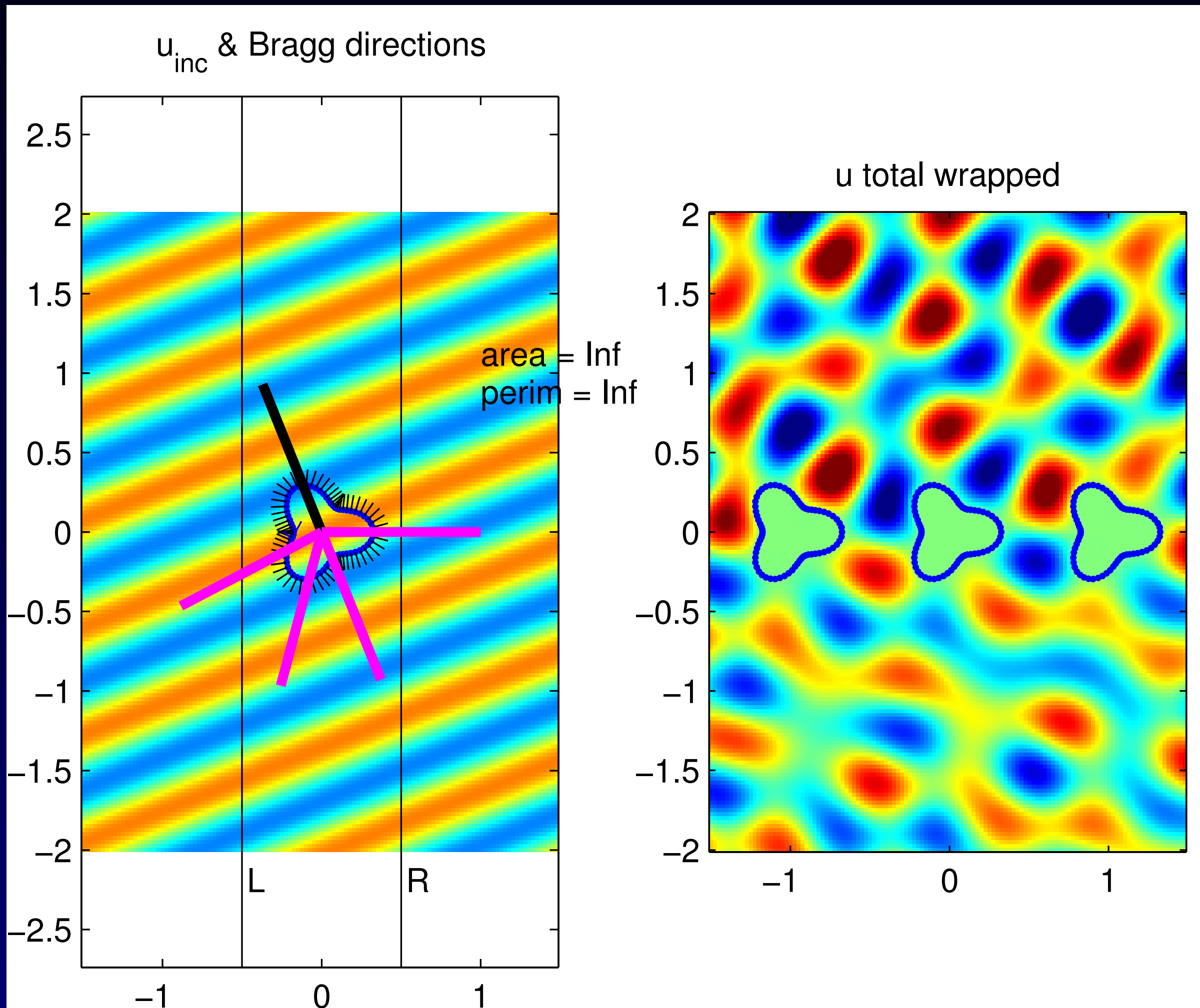
implement by projection of $u(\cdot, -y_0)$ onto n^{th} Fourier mode

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

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

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

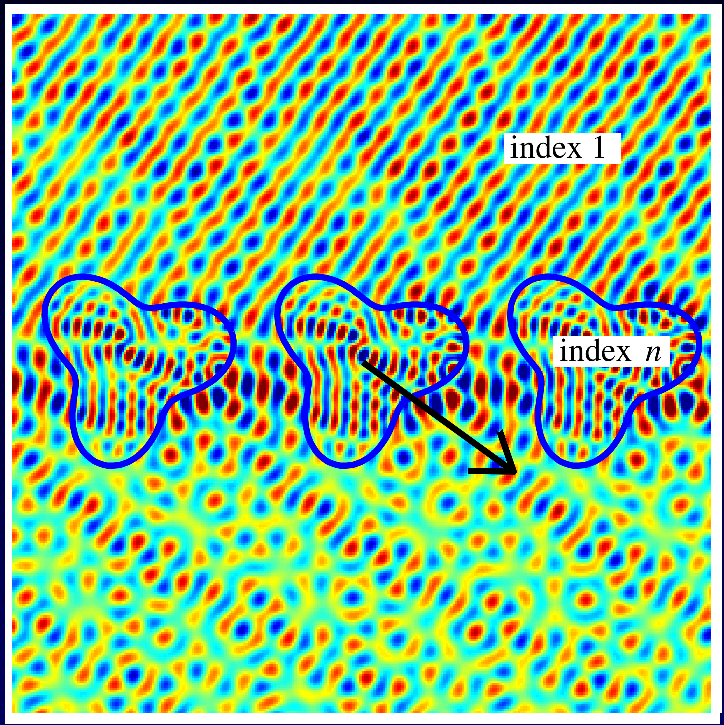
Results precisely at Wood's anomaly



$d = 1.6\lambda$ $N = 70$ $M = 90$ error 10^{-13} $t_{\text{fill+solve}} = 0.26$ s cond. # 10^3

- previously impossible to solve this via integral equations! MOVIES

Dielectric (transmission) obstacles



$$(\Delta + \omega^2)u = 0 \quad \text{in } \mathbb{R}^2 \setminus \overline{\Omega_{\mathbb{Z}}}$$

$$(\Delta + n^2\omega^2)u = 0 \quad \text{in } \Omega_{\mathbb{Z}}$$

$$\left.\begin{aligned} u^+ - u^- &= -u^i \\ u_n^+ - u_n^- &= -u_n^i \end{aligned}\right\} \text{on } \partial\Omega_{\mathbb{Z}}$$

matching (TM Maxwell)

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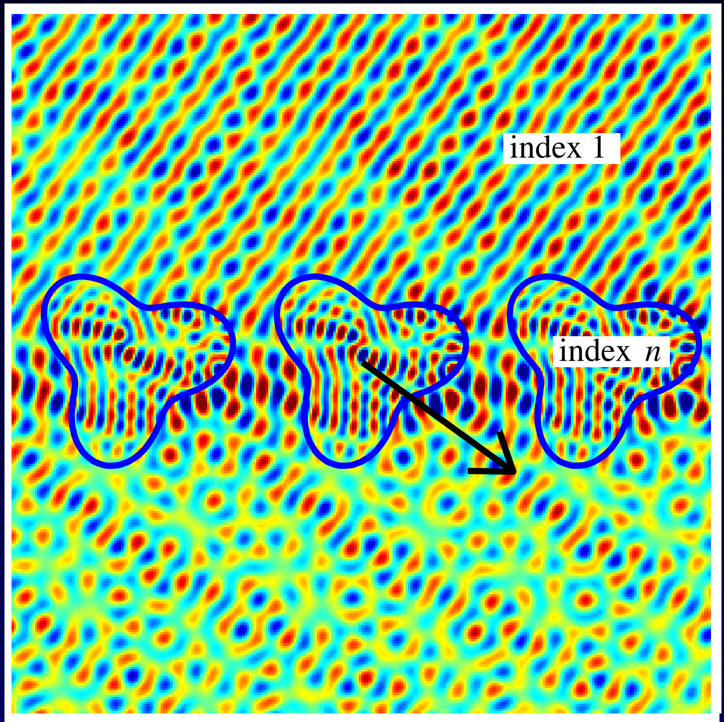

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non-periodic rep: (Müller '69, Rokhlin '83)

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2nd kind Fredholm $A\eta = b, \quad \eta = \begin{bmatrix} -\tau \\ \sigma \end{bmatrix}, \quad A = I + \begin{bmatrix} D - D_i & S_i - S \\ T - T_i & D_i^* - D^* \end{bmatrix}$

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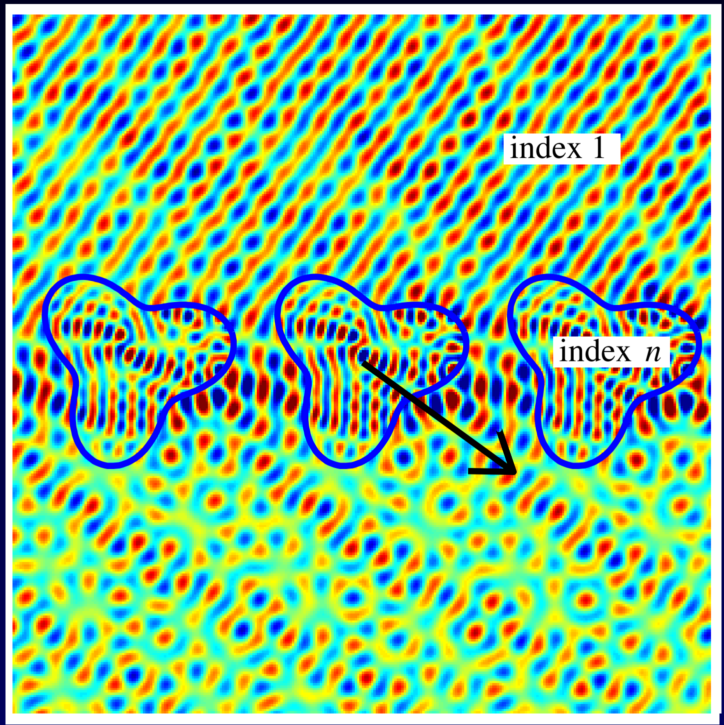

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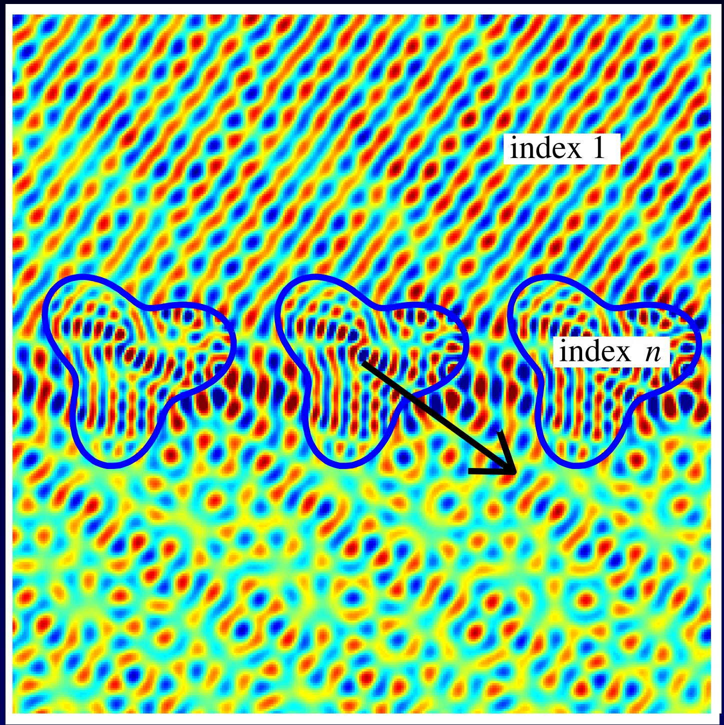
- periodize just as before (add $u_{\text{QP}}[\xi]$ in exterior only)

Dielectric (transmission) obstacles



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

$$\left.\begin{aligned}u^+-u^- &= -u^i\\ u^+_n-u^-_n &= -u^i_n\end{aligned}\right\}\text{ on } \partial\Omega_{\mathbb{Z}}$$

matching (TM Maxwell)

non-periodic rep: (Müller ’69, Rokhlin ’83)

$$u = \begin{cases}\mathcal{D}\tau+\mathcal{S}\sigma & \text{in } \mathbb{R}^2\setminus\overline{\Omega_{\mathbb{Z}}}\\ \mathcal{D}_i\tau+\mathcal{S}_i\sigma & \text{in } \Omega_{\mathbb{Z}}\end{cases}$$

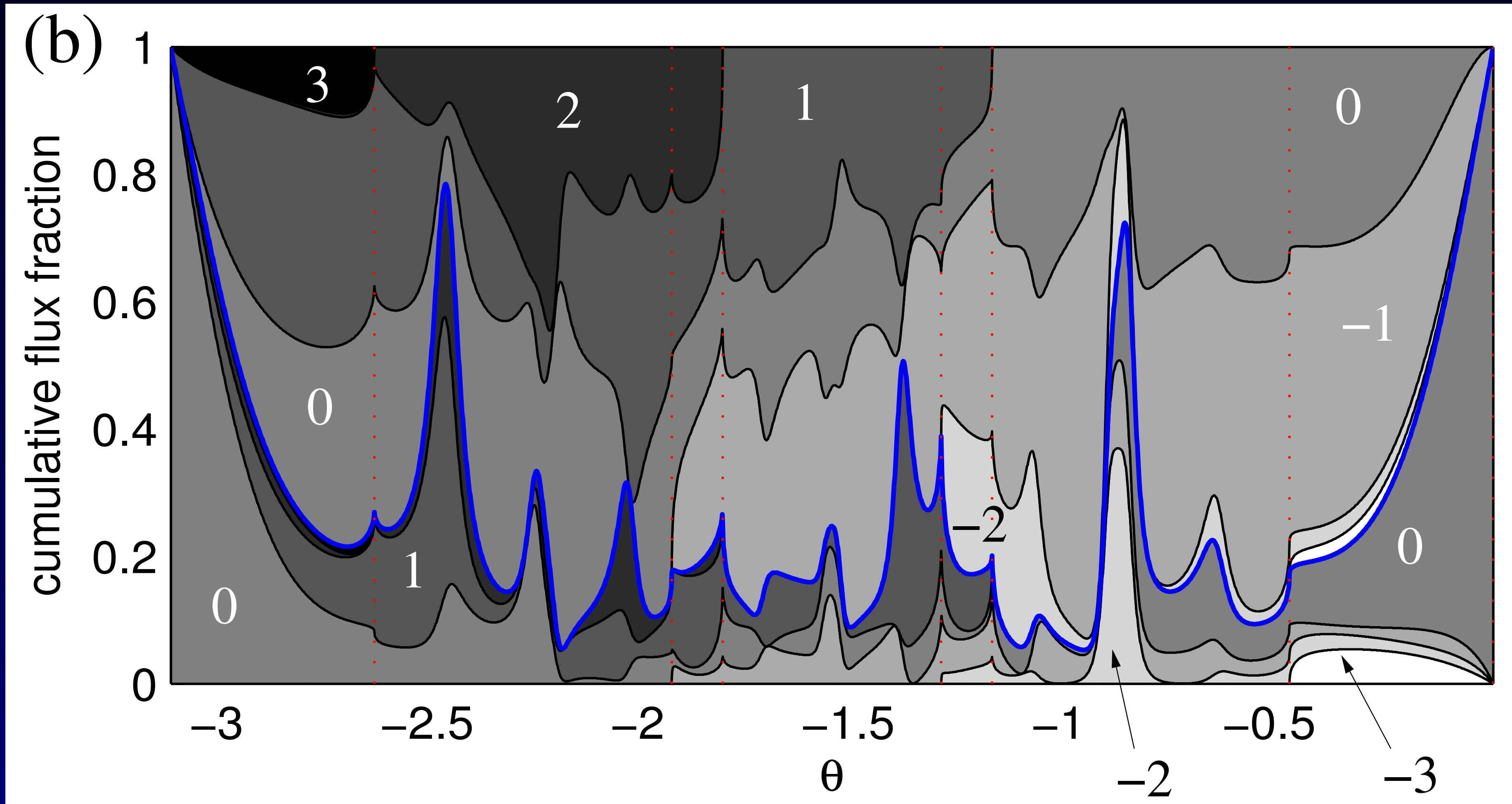
2nd kind Fredholm $A\eta=b,\quad \eta=\begin{bmatrix}-\tau\\ \sigma\end{bmatrix},\quad A=I+\begin{bmatrix}D-D_i & S_i-S\\ T-T_i & D_i^*-D^*\end{bmatrix}$

- periodize just as before (add $u_{\text{QP}}[\xi]$ in exterior only)

shown: $d=8\lambda$ $N=230$ $M=160$ err 10^{-14} $t_{\text{fill+solve}}=2.4$ s cond. # 10^3

Diffraction efficiencies vs inc. angle

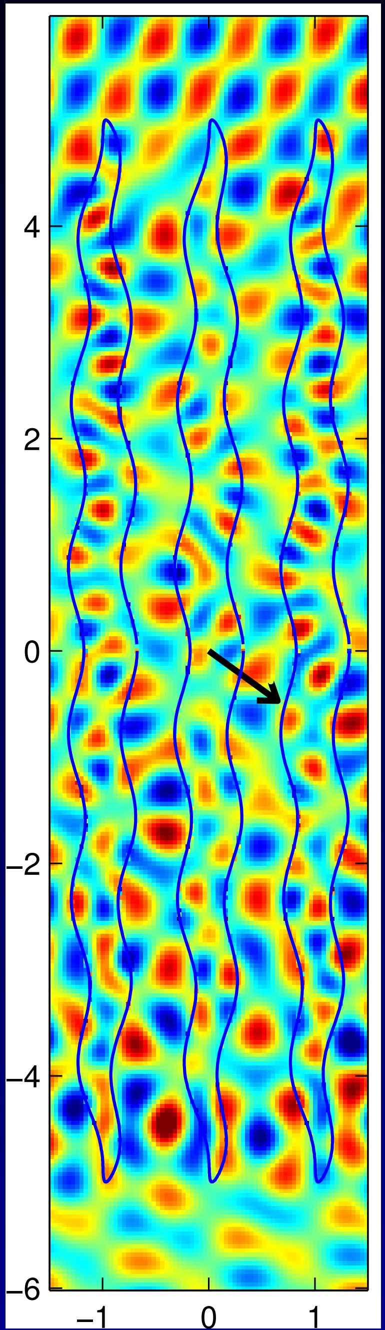
Power fractions scattered into each transmitted/reflected Bragg order:



$d = 1.6\lambda$ error 10^{-12} 3000 angles in 30 mins

- square-root type cusps at each Wood anomaly (dotted red)

Results: high aspect ratio dielectric



height $H = 10\,d$ (24λ in interior)

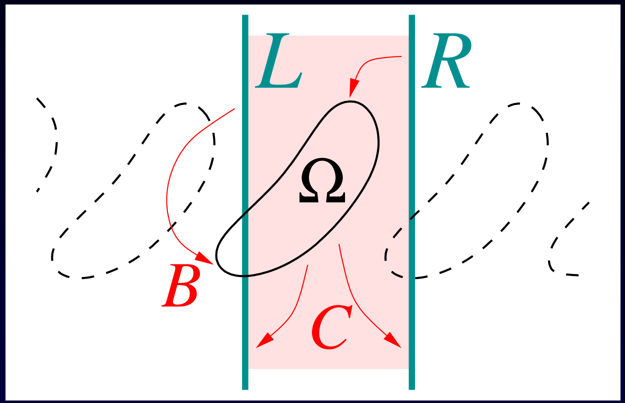
if lattice sums were used:
would need > 10 neighbor copies of $\partial\Omega$
to be summed directly ($> 10^2$ in 3D)

$d = 1.6\lambda \quad N = 500 \quad M = 330$

error $10^{-13} \quad t_{\text{fill}} = 9$ s $\quad t_{\text{solve}} = 4$ s

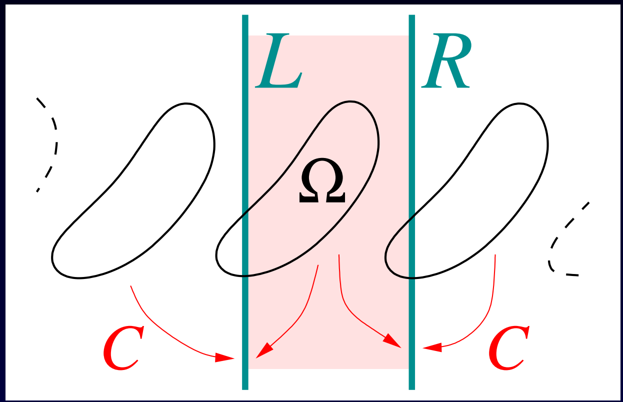
$M = O(\omega H)$ but prefactor small

Obstacle intersecting artificial unit cell walls



B and C blocks break

Obstacle intersecting artificial unit cell walls

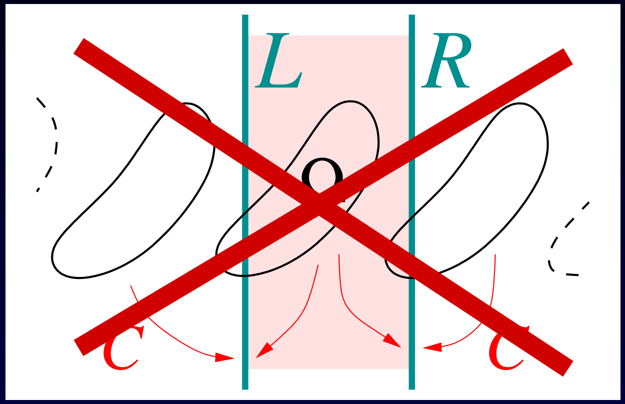


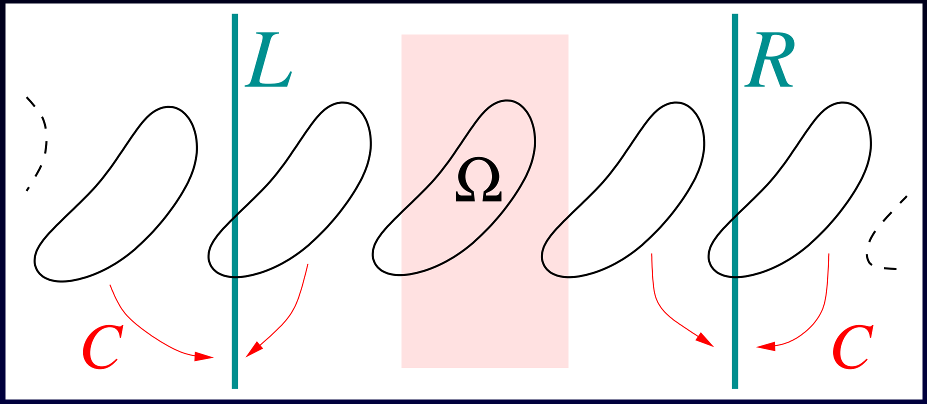
B and C blocks break

directly sum $\partial\Omega$ neighbors in u rep.:

cancels intersecting C terms!

Obstacle intersecting artificial unit cell walls





- L–R separation $3d$, Bloch phase α^3
- makes walls 'invisible' in scheme

Why works? **Lemma** (non-Wood case):
For L–R separation a whole # periods, solution density η equals that when periodizing in standard way via $\Phi_{\omega,\mathrm{QP}}$

Pf: *Schur complement* of upper-left block,

$$A_{\mathrm{QP}}\eta = (A - BQ^{-1}C)\eta = b$$

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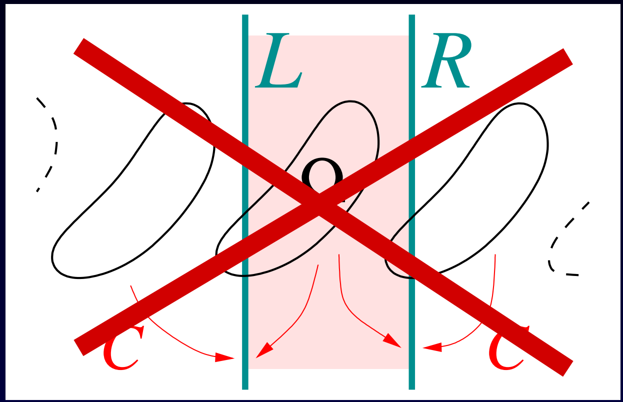

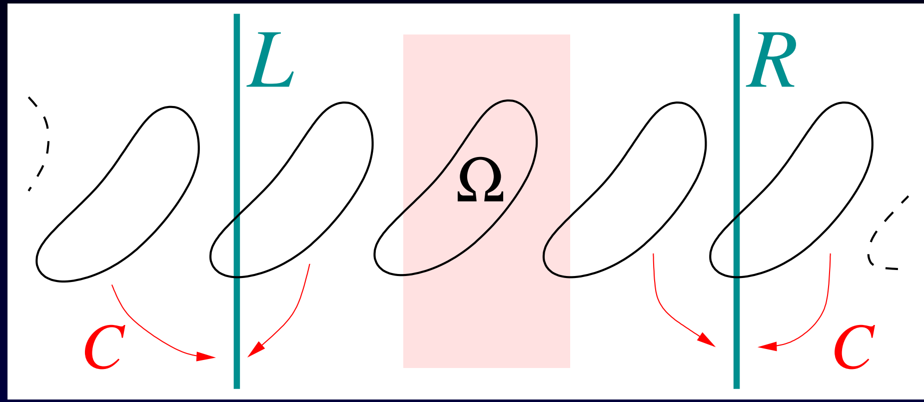

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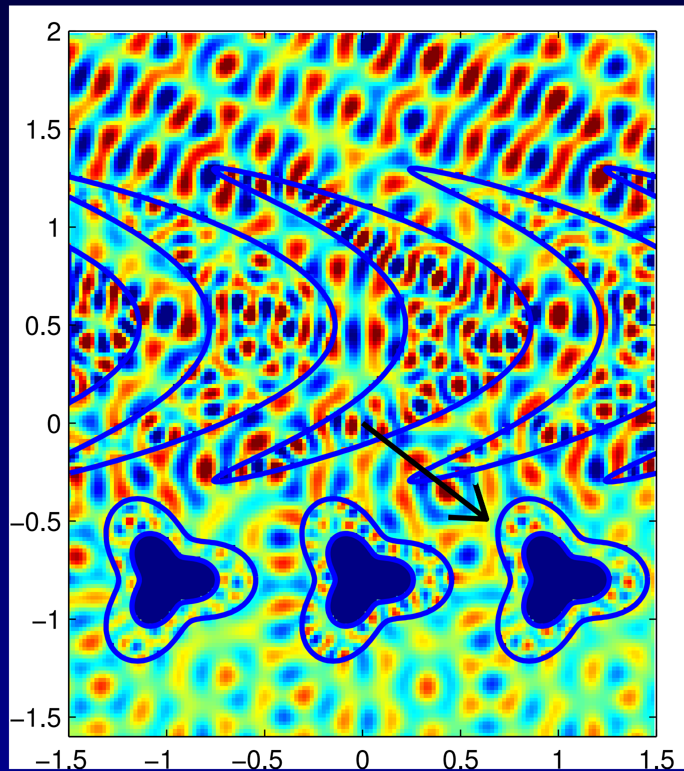

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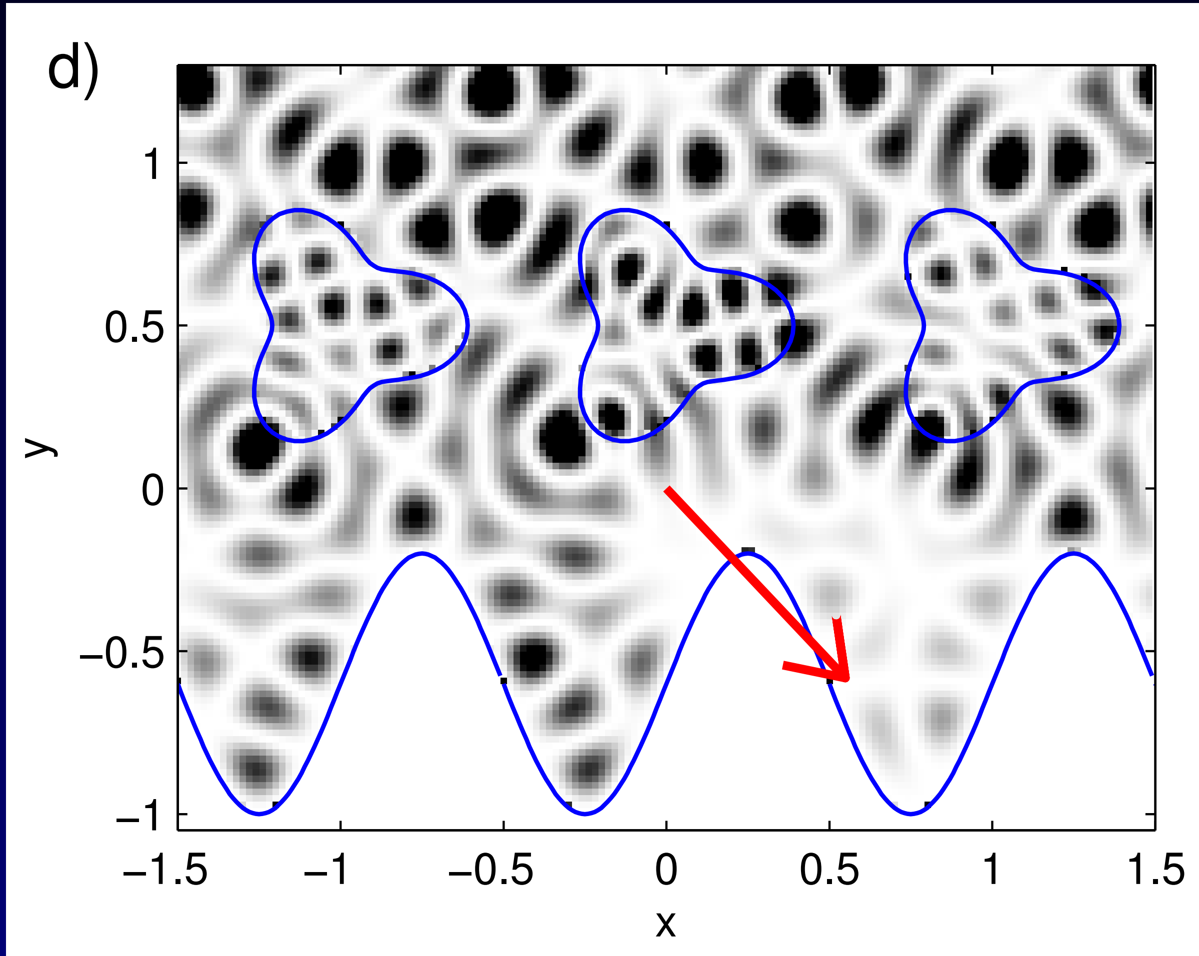
Preliminary results: multi-layer media

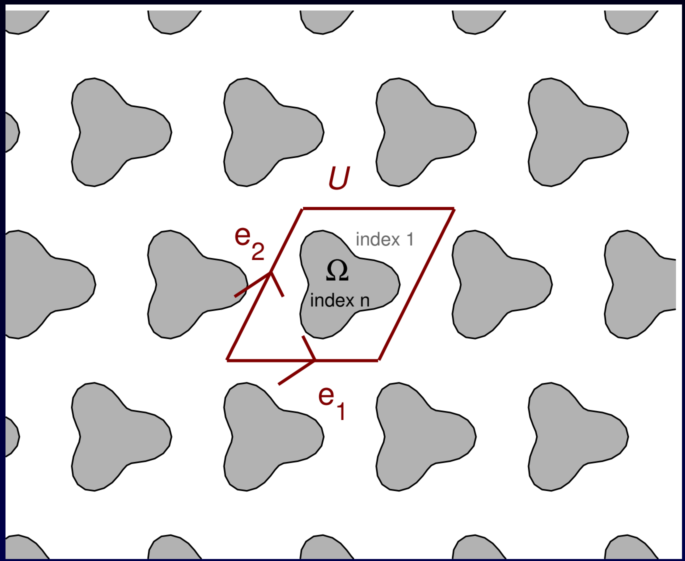
Periodic Dirichlet interface below dielectric inclusions:



$d = 3.2\lambda$ at Wood's anomaly error 10^{-4} ... low-order open-segment quadrature

- try high-order quadrature w/ endpoints (Alpert, Kapur–Rokhlin,...)

Idea also good for band structure (taste)



Doubly-periodic QP phases (α, β)

EVP: seek Bloch eigen-triples (ω, α, β)

- App: photonic crystal bandgap design

May periodize by replacing A by A_{QP}...

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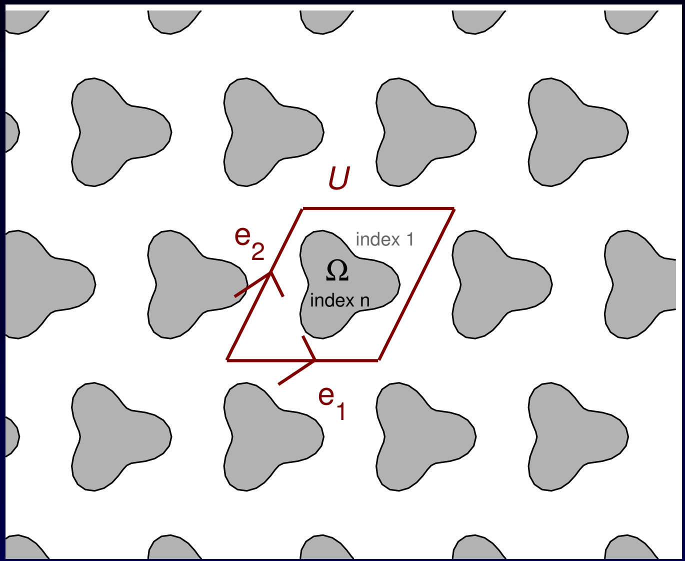

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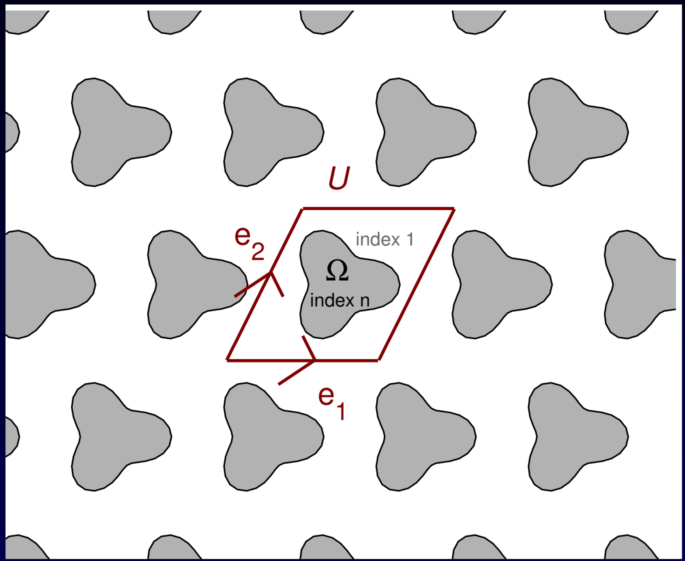

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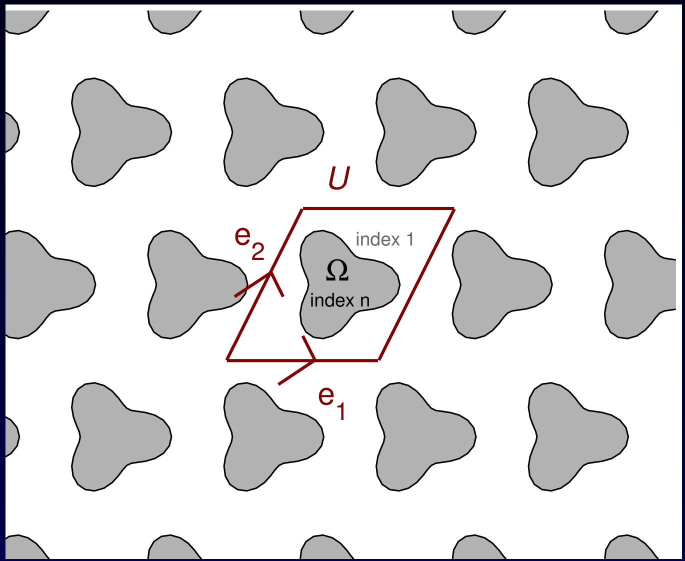

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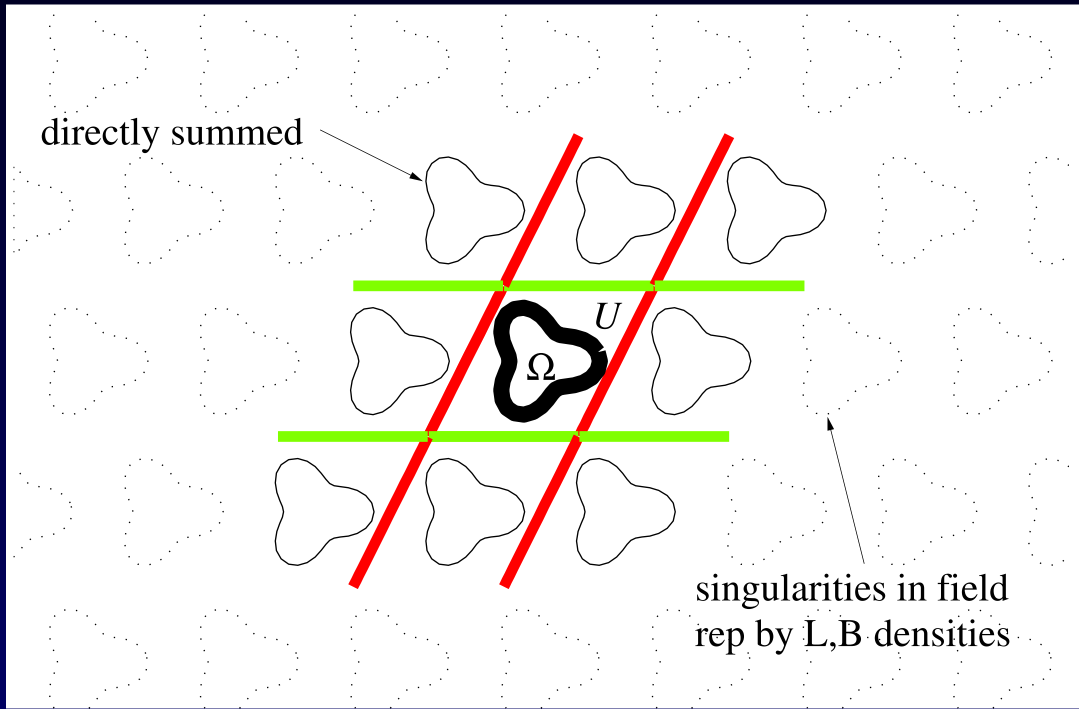
$\ldots$ but $\Phi_{\omega,\text{QP}}$ has poles at resonances of *empty* unit cell: scheme fails

Fix: as before, discard A_{QP} in favor of larger system $\begin{bmatrix} A & B \\ C & Q \end{bmatrix}$

- robust for all params, 2nd kind, couples to existing $\partial\Omega$ scatt. code

2nd kind ‘tic-tac-toe’ scheme (B–Greengard, JCP, 2010)

sticking-out phased copies of walls & 3x3 phased copies of $\partial\Omega$:



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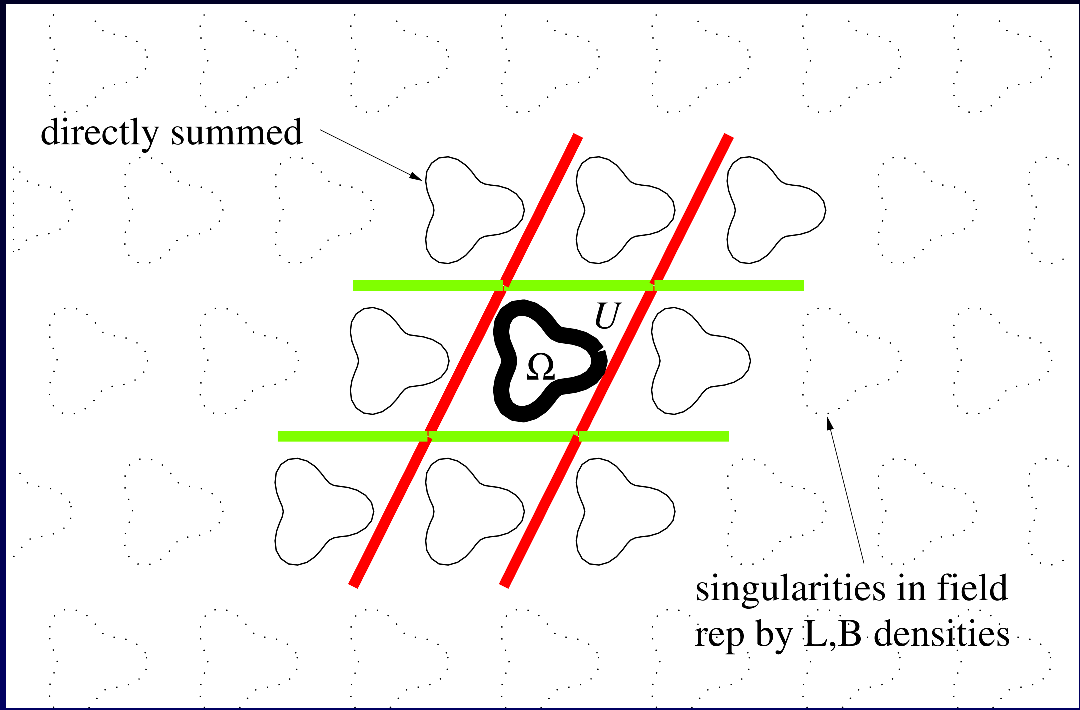


- Careful cancellations: B, C, Q have only interactions of distance ≥ 1
- Large dist increases convergence rate, i.e. large c in error = $O(e^{-cN})$

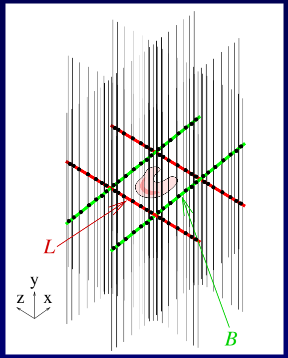
Philosophy: sum neighboring image sources directly, so fields due to remainder of lattice have distant singularities

Conclusions

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

Future:

- multi-layer; insert FMM for inclusion; 3D . . .



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

B–Greengard, J. Comput. Phys. '10
B–Greengard, BIT, *submitted*

funding: NSF DMS-0811005

http://math.dartmouth.edu/∼ahb

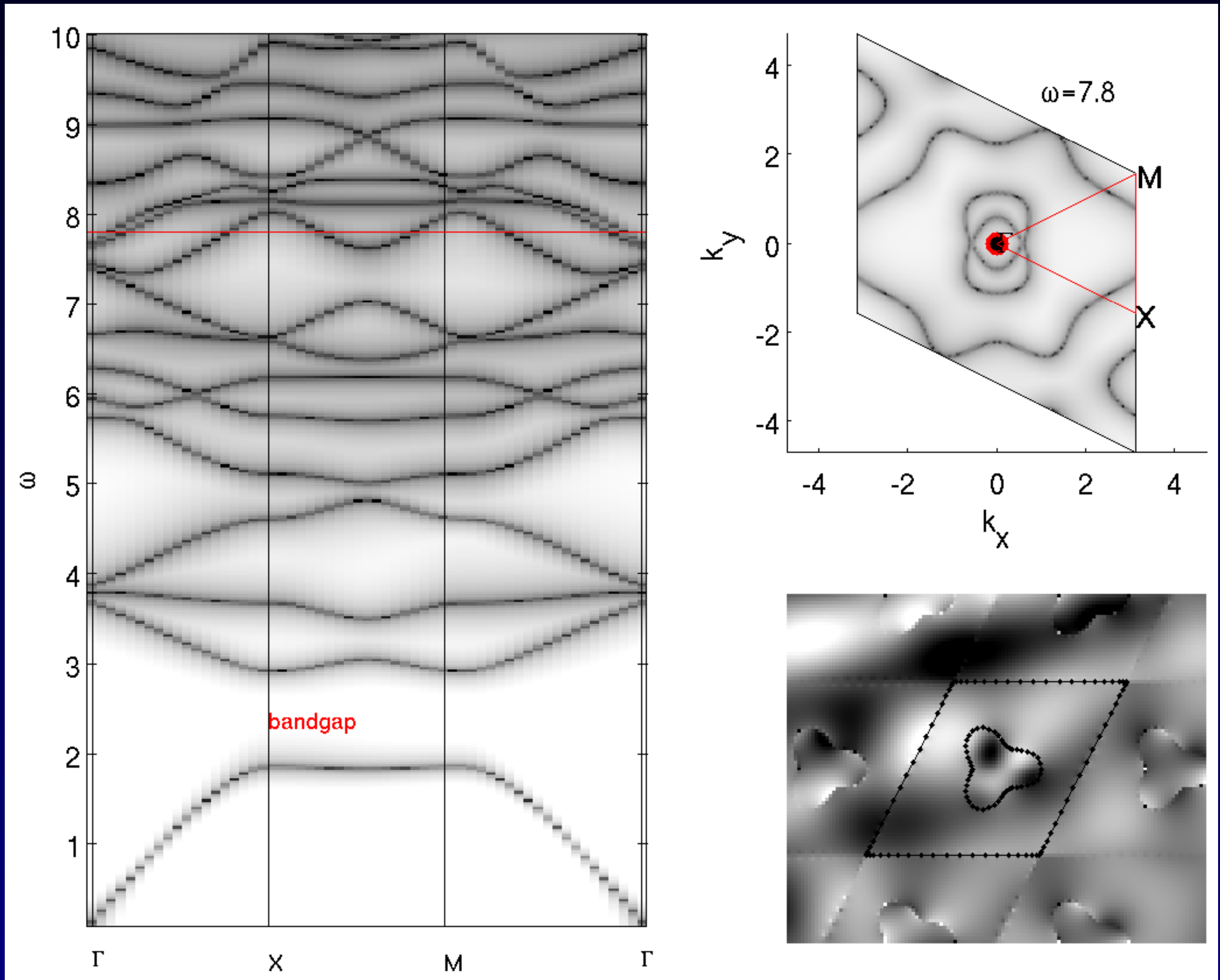
EXTRA SLIDES

Results: small inclusion

band structure: simply plot log min sing. val. of M vs $(\omega, k_x, k_y) \ldots$

Results: small inclusion

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



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