The Abdus Salam
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Spring College on Computational Nanoscience

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Computational Photonics: Band Structures and Dispersion Relations

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Computational Nanophotonics: Band Structures & Dispersion Relations

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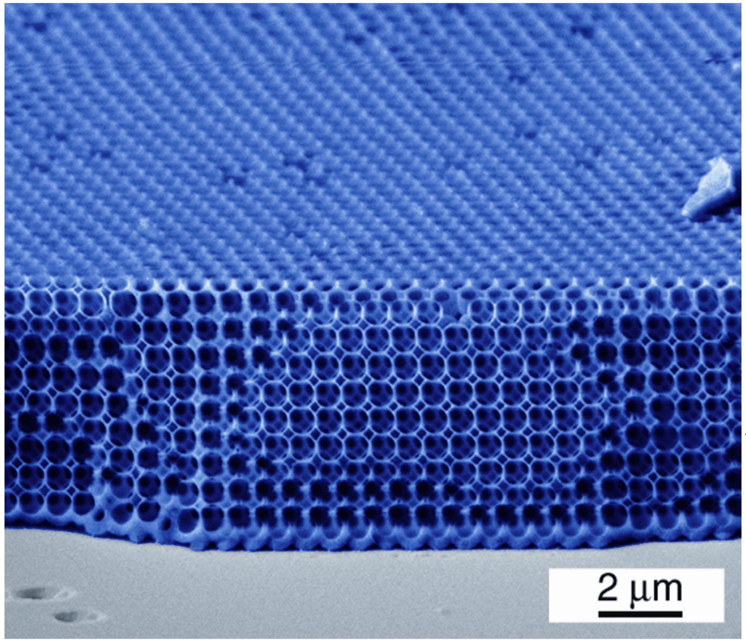
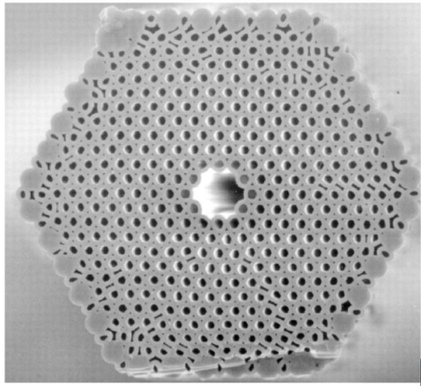
Nanophotonics:

classical electromagnetic effects can be
greatly altered by λ-scale structures
especially with *many* interacting scatterers

optical “insulators”

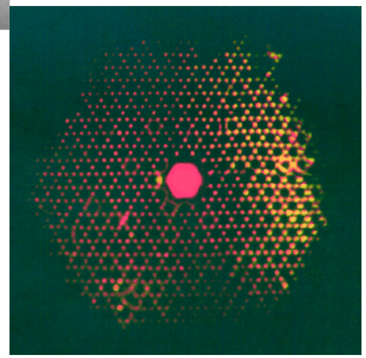


[D. Norris, UMN (2001)]

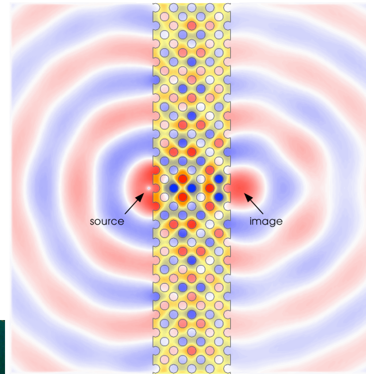


trapping/guiding
light in vacuum

[R. F. Cregan
(1999)]



flat “superlenses”



[Luo (2003)]

easy to study numerically, theory practically exact,
well-developed scalable 3d methods for arbitrary materials

Just solve this: Maxwell's equations

Faraday: $\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$

Ampere: $\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$

(nonzero frequency)

Gauss: $\nabla \cdot \mathbf{D} = \rho$

$\nabla \cdot \mathbf{B} = 0$

constitutive equations (here, linear media):

$$\mathbf{D} = \varepsilon \mathbf{E} \qquad \mathbf{B} = \mu \mathbf{H}$$

magnetic permeability
…usually $\approx \mu_0$ at infrared/visible ($\lambda \sim \mu$m)

electric permittivity
$\varepsilon_r = \varepsilon / \varepsilon_0$ = relative permittivity or dielectric constant
= n^2 (square of refractive index)

$c^2 = 1 / \varepsilon_0 \mu_0$

ε, μ depend on frequency (dispersion)
…negligible for transparent media in narrow bandwidth

theorists: often $\varepsilon_0 = \mu_0 = 1$
and/or $\varepsilon_r = \varepsilon$

Limits of validity at the nanoscale?

- Continuum material models (ε etc.) have generally proved very successful down to ~ few nm feature sizes
  [For metal features at < 20nm scale, some predictions of small nonlocal effects (ballistic transport), but this is mostly neglected]

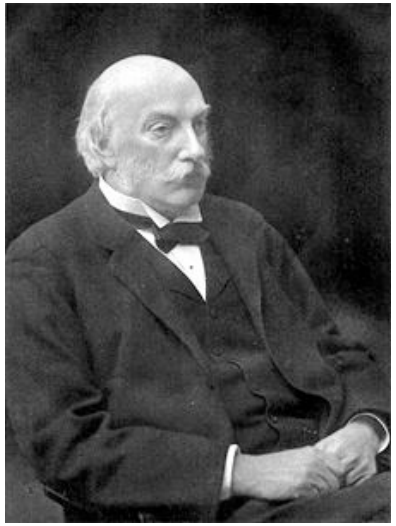
- Phenomena from resonant ~ nm features << λ (e.g. spontaneous emission) usually can be incorporated perturbatively / semiclassically
  (e.g. spontaneous emission ~ stochastic dipole source,
  spontaneous emission rate ~ local density of states
  ~ power radiated by dipole)

first, some perspective…

Development of Classical EM Computations

1 Analytical solutions

vacuum, single/double interfaces
various electrostatic problems, …



Lord Rayleigh

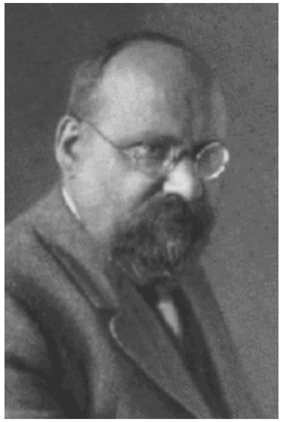
scattering from small particles,
periodic multilayers (Bragg mirrors), …

… & other problems with
very high symmetry
and/or separability
and/or small parameters

Development of Classical EM Computations

1. Analytical solutions

2. Semi-analytical solutions: series expansions



Gustav Mie
(1908)

e.g. Mie scattering of light by a sphere

Also called *spectral methods:*

Expand solution in *rapidly converging Fourier-like basis*

- *spectral integral-equation methods:*

  exactly solve homogeneous regions (Green's func.),
  & match boundary conditions via spectral basis
  (e.g. Fourier series, spherical harmonics)

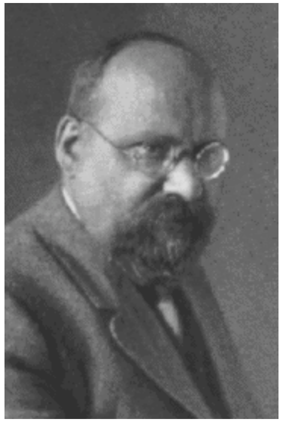
- *spectral PDE methods:*

  spectral basis for unknowns in inhomogeous space
  (e.g. Fourier series, Chebyshev polynomials, …)
  & plug into PDE and solve for coefficients

Development of Classical EM Computations

1. Analytical solutions

2. Semi-analytical solutions & spectral methods



Gustav Mie
(1908)

Expand solution in *rapidly converging Fourier-like basis*
e.g. Mie scattering of light by a sphere

Strength: can converge *exponentially fast*
— fast enough for hand calculation
— analytical insights, asymptotics, …

Limitation: fast ("spectral") convergence requires
basis to be redesigned for each geometry
(to account for any discontinuities/singularities
… complicated for complex geometries!)

(*Or:* brute-force Fourier series, polynomial convergence)

Development of Classical EM Computations

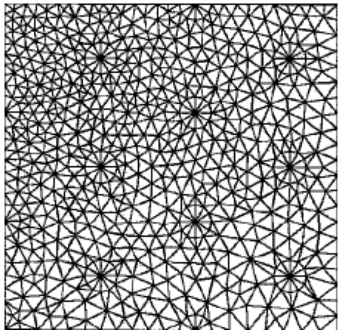
1. Analytical solutions
2. Semi-analytical solutions & spectral methods
3. Brute force: generic grid/mesh

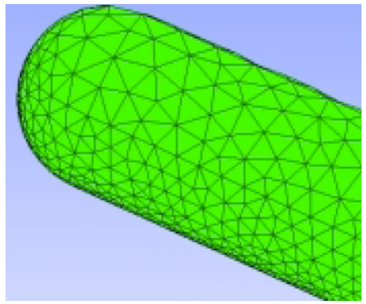
PDEs: discretize space into grid/mesh
— simple (low-degree polynomial) approximations in each pixel/element

integral equations:
— boundary elements mesh
surface unknowns coupled by Green's functions

←finite differences
(*or Fourier series*)

& finite elements→





lose orders of magnitude in performance … *but* re-usable code
\$ computer time << \$\$\$\$ programmer time

Computational EM: Three Axes of Comparison

- What *problem* is solved?
  - — eigenproblems: harmonic modes $\sim e^{-i\omega t}$ $(\mathbf{J} = 0)$
  - — frequency-domain response: $\mathbf{E}, \mathbf{H}$ from $\mathbf{J}(\mathbf{x})e^{-i\omega t}$
  - — time-domain response: $\mathbf{E}, \mathbf{H}$ from $\mathbf{J}(\mathbf{x}, t)$
  - — PDE or integral equation?

- What *discretization*?

  infinitely many unknowns
  $\rightarrow$ finitely many unknowns

  - — finite differences (FD)
  - — finite elements (FEM) / boundary elements (BEM)
  - — spectral / Fourier
  - — …

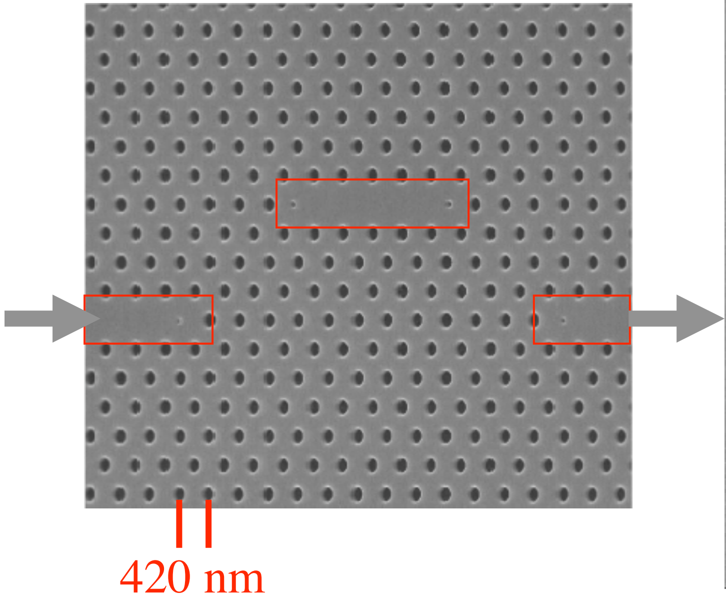
- What *solution method*?
  - — dense linear solvers (LAPACK)
  - — sparse-direct methods
  - — iterative methods

A few lessons of history

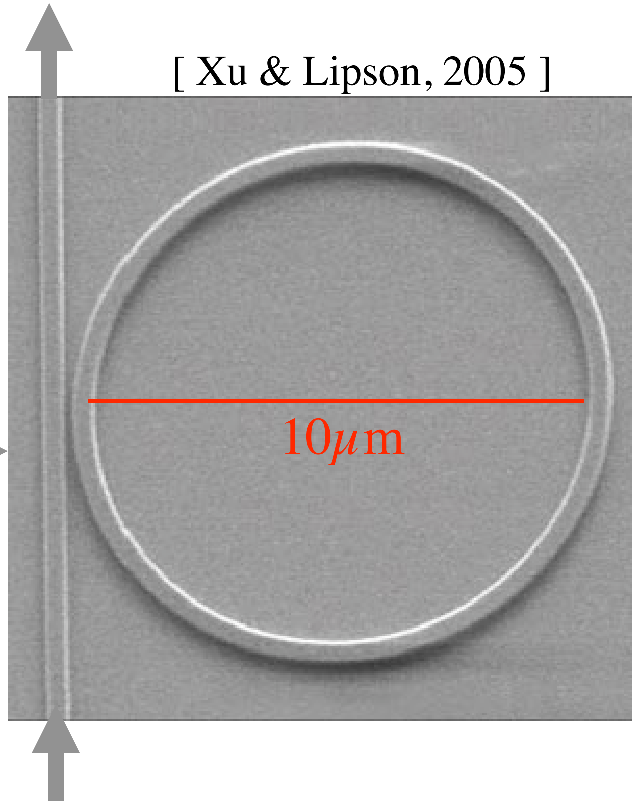
- All approaches still in widespread use
  - brute force methods in 90%+ of papers, typically the first resort to see what happens in a new geometry
  - geometry-specific spectral methods still popular, especially when particular geometry of special interest
  - analytical techniques used less to solve new geometries than to prove theorems, treat small perturbations, etc.
- No single numerical method has "won" in general
  - each has strengths and weaknesses, e.g. tradeoff between simplicity/generalizability and performance/scalability
  - very mature/standardized problems (e.g. capacitance extraction) use increasingly sophisticated methods (e.g. BEM), research fields (e.g. nanophotonics) tend to use simpler methods that are easier to modify (e.g. FDTD)

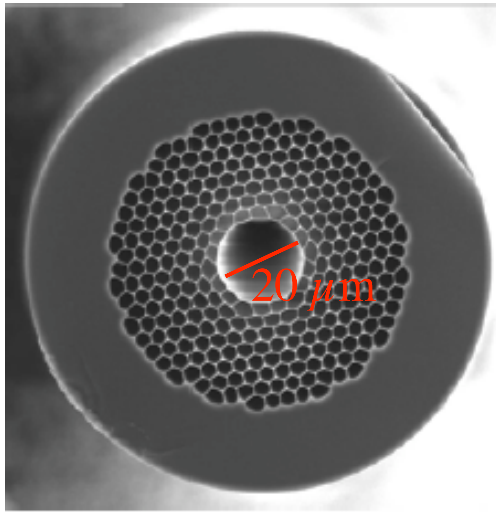
Understanding Photonic Devices

[Notomi *et al*. (2005).]



[Xu & Lipson, 2005]





[Mangan, *et al*., OFC 2004 PDP24]

Model the whole thing at once? Too hard to understand & **design**.

Break it up into pieces first: periodic regions, waveguides, cavities

Building Blocks: Eigenmodes

- Want to know what solutions exist in different regions and how they can interact: look for time-harmonic modes $\sim e^{-i\omega t}$

$$\vec{\nabla} \times \vec{E} = -\cancelto{1}{\mu} \frac{\partial}{\partial t} \vec{H} \rightarrow i\omega \vec{H}$$

$$\vec{\nabla} \times \vec{H} = \varepsilon \frac{\partial}{\partial t} \vec{E} + \cancelto{0}{\vec{J}} \rightarrow -i\omega\varepsilon \vec{E}$$

First task:

get rid of this mess

$$\underbrace{\nabla \times \frac{1}{\varepsilon} \nabla \times}_{\text{eigen-operator}} \vec{H} = \underbrace{\omega^2}_{\text{eigen-value}} \vec{H}$$

eigen-field

(Hermitian for lossless/real ε!)

+ constraint

$$\nabla \cdot \vec{H} = 0$$

Electronic & Photonic Eigenproblems

Electronic

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi = E\psi$$

nonlinear eigenproblem

(V depends on e density $|\psi|^2$)

(+ nasty quantum entanglement)

Photonic

$$\nabla \times \frac{1}{\varepsilon} \nabla \times \vec{H} = \left(\frac{\omega}{c}\right)^2 \vec{H}$$

simple linear eigenproblem

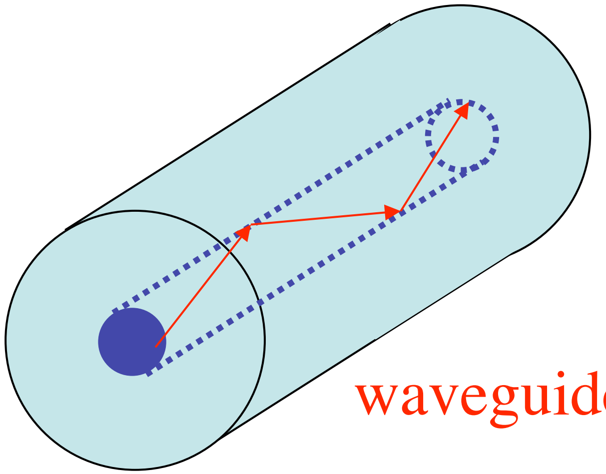
(for linear materials
with negligible dispersion)

— many well-known
computational techniques

Hermitian = real E & ω, … *Periodicity* = *Bloch's theorem*…

Building Blocks: Periodic Media

homogeneous
media

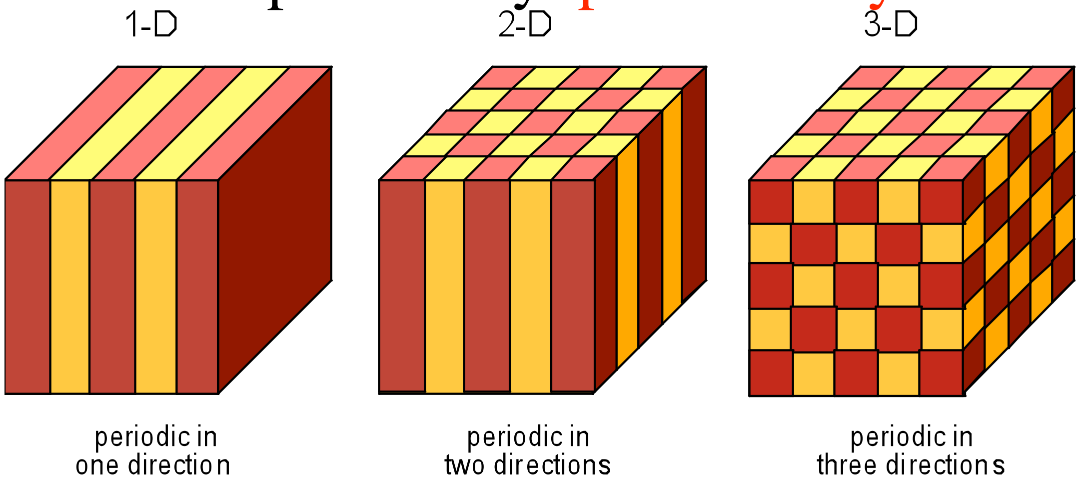


waveguides

common thread:

translational
symmetry

discrete periodicity: photonic crystals



Periodic Hermitian Eigenproblems

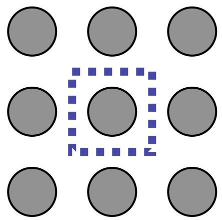
[G. Floquet, "Sur les équations différentielles linéaries à coefficients périodiques," *Ann. École Norm. Sup.* **12**, 47–88 (1883).]
[F. Bloch, "Über die quantenmechanik der electronen in kristallgittern," *Z. Physik* **52**, 555–600 (1928).]

if eigen-operator is periodic, then Bloch-Floquet theorem applies:

can choose: $$\vec{H}(\vec{x},t) = \underbrace{e^{i(\vec{k}\cdot\vec{x}-\omega t)}}_{\text{planewave}}\underbrace{\vec{H}_{\vec{k}}(\vec{x})}_{\text{periodic “envelope”}}$$

Corollary 1: **k** is conserved, *i.e.* no scattering of Bloch wave

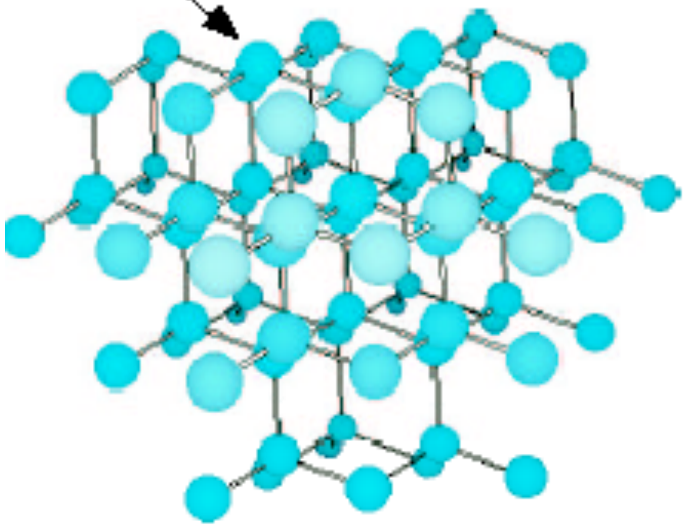
Corollary 2: $\vec{H}_{\vec{k}}$ given by finite unit cell,
so ω are discrete $\omega_n(\mathbf{k})$



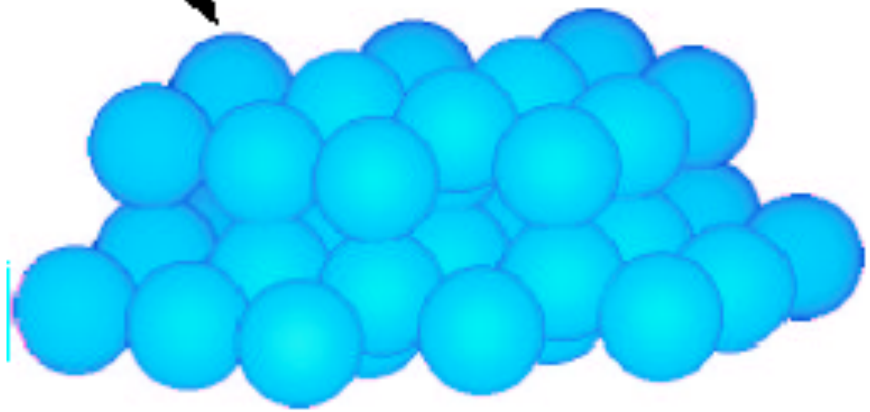
Electronic and Photonic Crystals

Periodic Medium

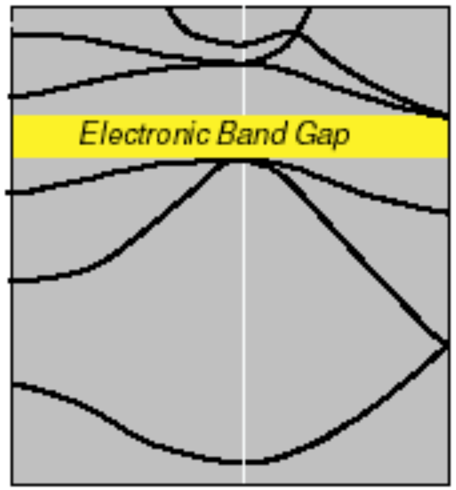
atoms in diamond structure



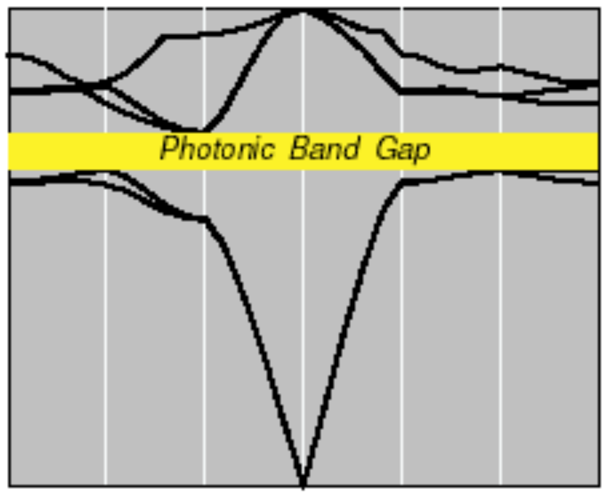
dielectric spheres, diamond lattice



Bloch waves: **Band Diagram**



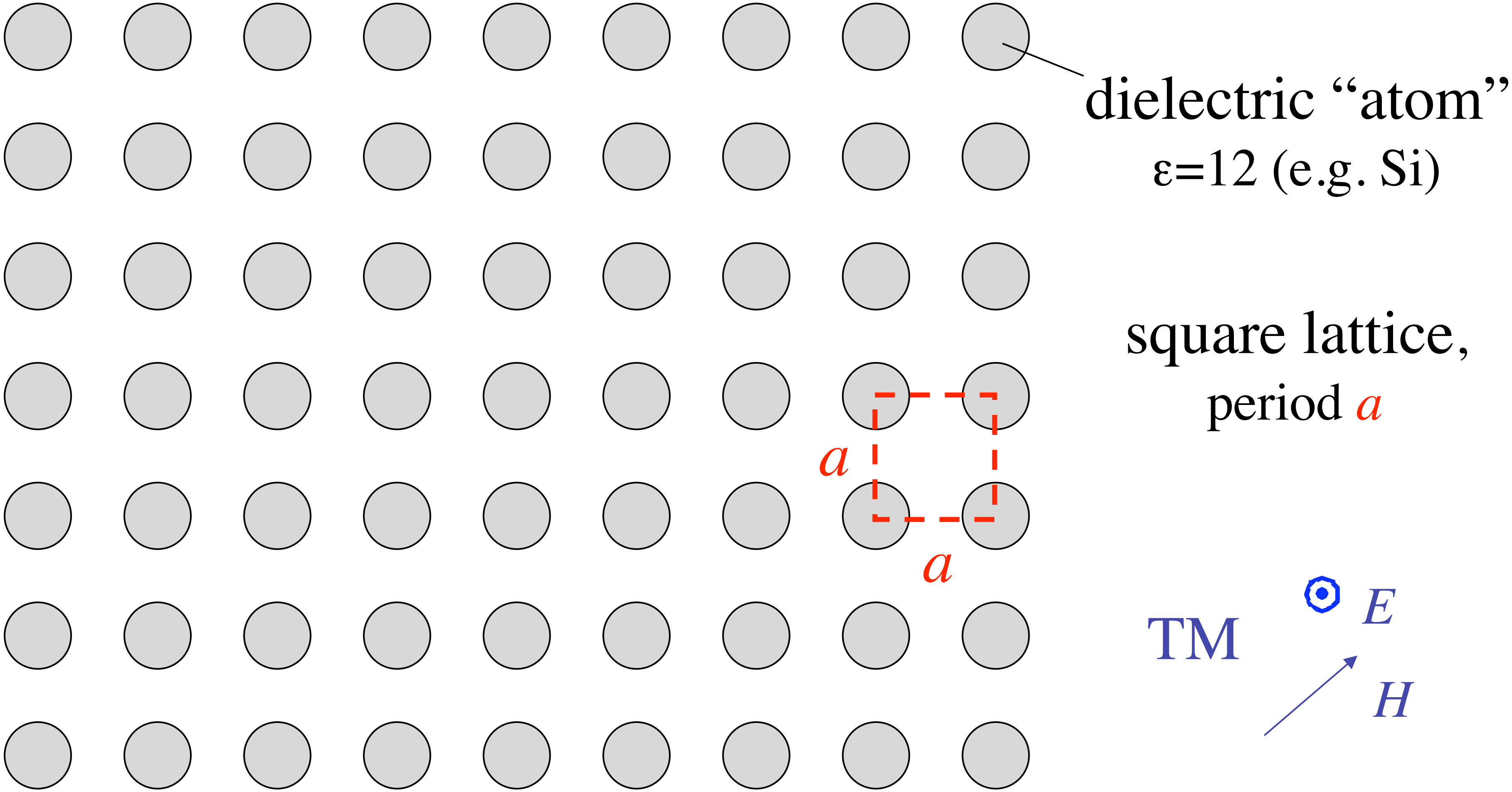
strongly interacting fermions



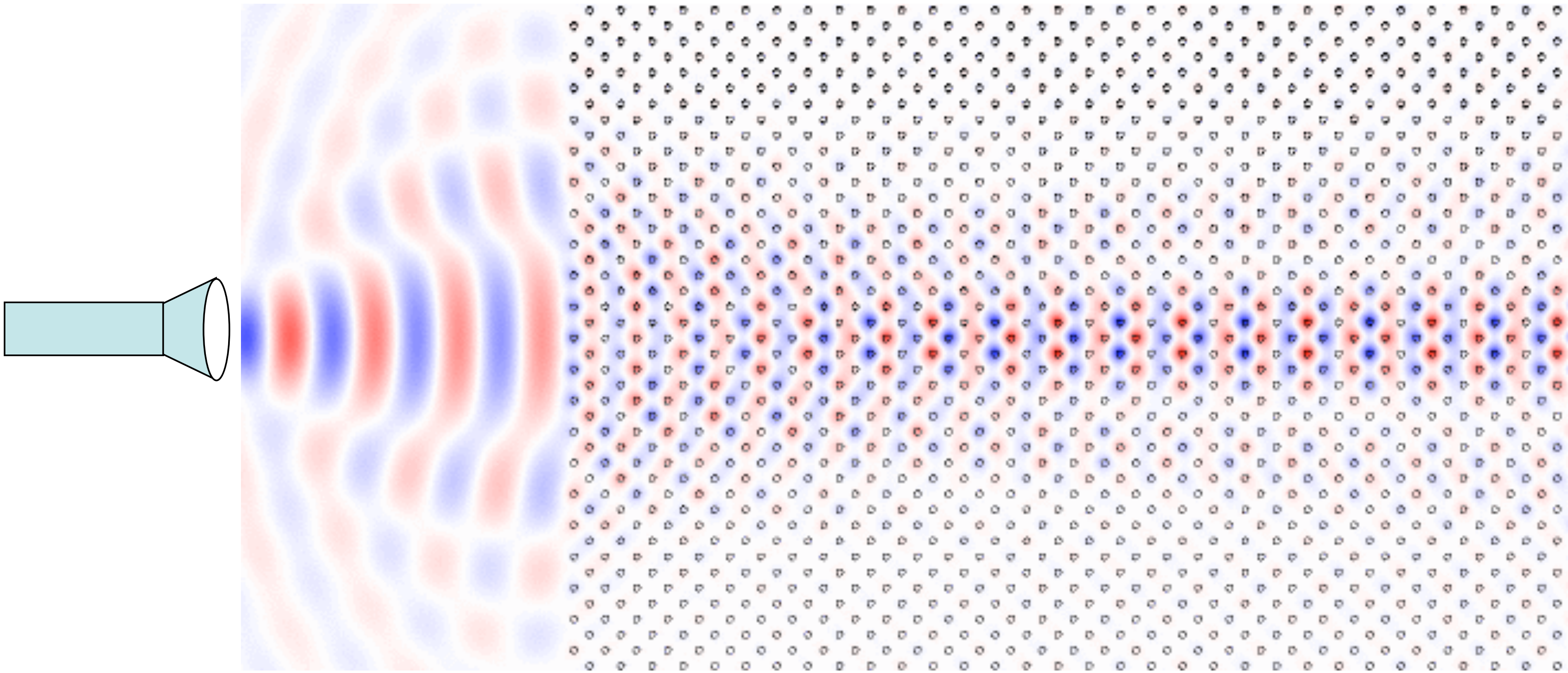
weakly-interacting bosons

… many design degrees of freedom

A 2d Model System



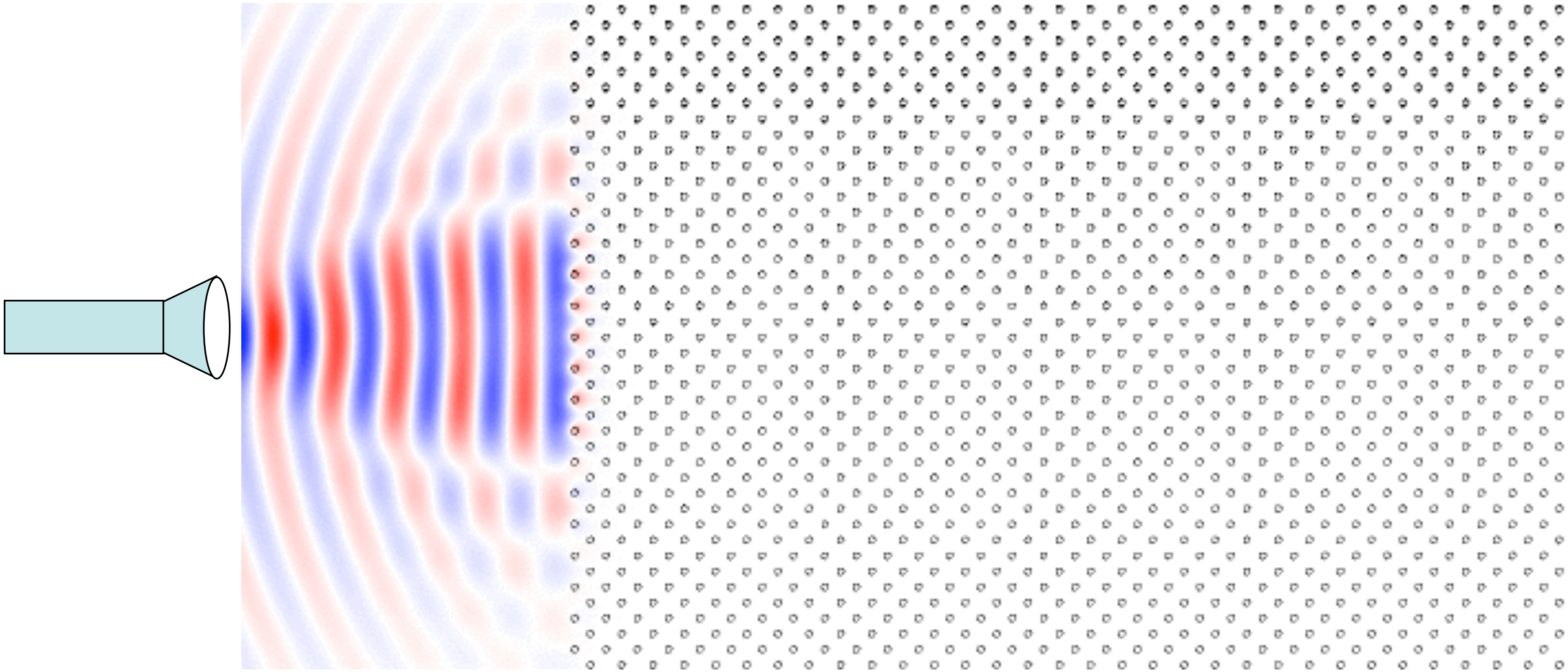
The magic of periodicity: Bloch waves



the light seems to form several *coherent beams*
that propagate *without scattering*
… and almost *without diffraction* (*supercollimation*)

A slight change? Shrink λ by 20%

an "optical insulator" (photonic bandgap)



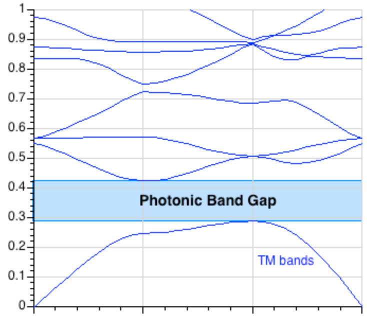
light cannot penetrate the structure at this wavelength!

all of the scattering destructively interferes

Solving the Maxwell Eigenproblem

Finite cell ➔ *discrete* eigenvalues ω_n

Want to solve for $\omega_n(\mathbf{k})$,
& plot vs. "all" $\mathbf{k}$ for "all" n,



$$(\nabla + i\mathbf{k}) \times \frac{1}{\varepsilon}(\nabla + i\mathbf{k}) \times \mathbf{H}_n = \frac{\omega_n^2}{c^2}\mathbf{H}_n$$

constraint: $(\nabla + i\mathbf{k}) \cdot \mathbf{H}_n = 0$

where field = $\mathbf{H}_n(\mathbf{x})\, e^{i(\mathbf{k}\cdot\mathbf{x} - \omega t)}$

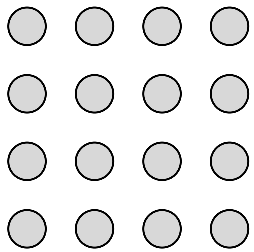
1. Limit range of $\mathbf{k}$: irreducible Brillouin zone

2. Limit degrees of freedom: expand $\mathbf{H}$ in finite basis

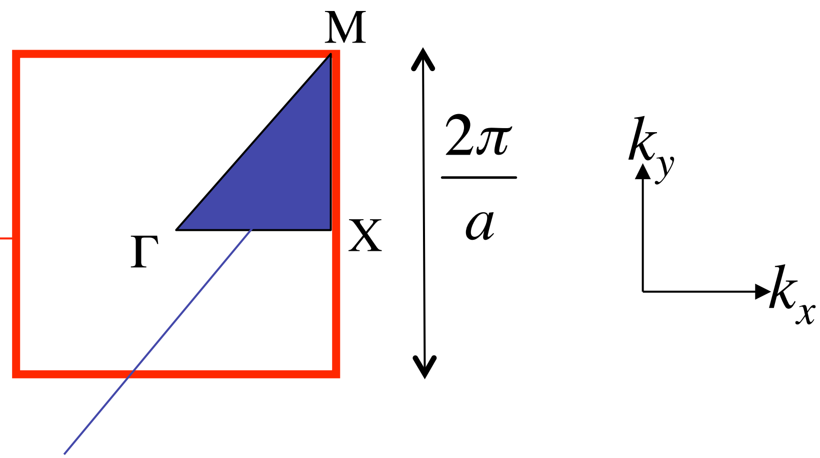
3. Efficiently solve eigenproblem: iterative methods

Solving the Maxwell Eigenproblem: 1

1. Limit range of **k**: irreducible Brillouin zone



—Bloch's theorem: solutions are periodic in **k**



first Brillouin zone
= minimum |**k**| "primitive cell"

irreducible Brillouin zone: reduced by symmetry

2. Limit degrees of freedom: expand **H** in finite basis

3. Efficiently solve eigenproblem: iterative methods

Solving the Maxwell Eigenproblem: 2a

1. Limit range of $\mathbf{k}$: irreducible Brillouin zone

2. Limit degrees of freedom: expand $\mathbf{H}$ in finite basis (N)

$$|\mathbf{H}\rangle = \mathbf{H}(\mathbf{x}_t) = \sum_{m=1}^{N} h_m \mathbf{b}_m(\mathbf{x}_t) \qquad \text{solve: } \hat{A}|\mathbf{H}\rangle = \omega^2 |\mathbf{H}\rangle$$

finite matrix problem: $$Ah = \omega^2 Bh$$

$$\langle \mathbf{f} | \mathbf{g} \rangle = \int \mathbf{f}^* \cdot \mathbf{g} \qquad A_{m\ell} = \langle \mathbf{b}_m | \hat{A} | \mathbf{b}_\ell \rangle \qquad B_{m\ell} = \langle \mathbf{b}_m | \mathbf{b}_\ell \rangle$$

3. Efficiently solve eigenproblem: iterative methods

Solving the Maxwell Eigenproblem: 2b

1. Limit range of $\mathbf{k}$: irreducible Brillouin zone

2. Limit degrees of freedom: expand $\mathbf{H}$ in finite basis

— must satisfy constraint: $(\nabla + i\mathbf{k}) \cdot \mathbf{H} = 0$

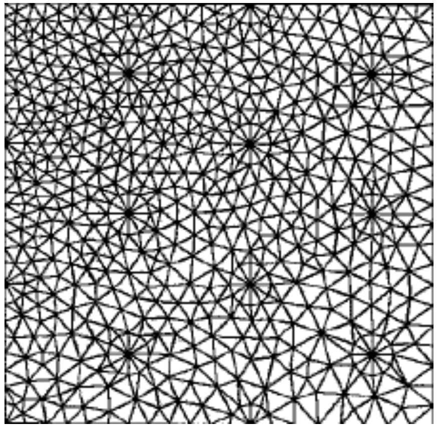
Planewave (FFT) basis

$$\mathbf{H}(\mathbf{x}_t) = \sum_{\mathbf{G}} \mathbf{H}_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{x}_t}$$

constraint: $\mathbf{H}_{\mathbf{G}} \cdot (\mathbf{G} + \mathbf{k}) = 0$

uniform "grid," periodic boundaries,
simple code, O(N log N)

Finite-element basis



[figure: Peyrilloux *et al.*, *J. Lightwave Tech.* **21**, 536 (2003)]

constraint, boundary conditions:

Nédélec elements

[Nédélec, *Numerische Math.* **35**, 315 (1980)]

nonuniform mesh,
more arbitrary boundaries,
complex code & mesh, O(N)

3. Efficiently solve eigenproblem: iterative methods

Solving the Maxwell Eigenproblem: 3a

1. Limit range of **k**: irreducible Brillouin zone

2. Limit degrees of freedom: expand **H** in finite basis

3. Efficiently solve eigenproblem: iterative methods

$$Ah = \omega^2 Bh$$

Slow way: compute A & B, ask LAPACK for eigenvalues

— requires $O(N^2)$ storage, $O(N^3)$ time

Faster way:

— start with *initial guess* eigenvector h_0

— *iteratively* improve

— $O(Np)$ storage, ~ $O(Np^2)$ time for p eigenvectors

(p smallest eigenvalues)

Solving the Maxwell Eigenproblem: 3b

1. Limit range of **k**: irreducible Brillouin zone
2. Limit degrees of freedom: expand **H** in finite basis
3. Efficiently solve eigenproblem: iterative methods

$$Ah = \omega^2 Bh$$

Many iterative methods:

— Arnoldi, Lanczos, Davidson, Jacobi-Davidson, …, Rayleigh-quotient minimization

Solving the Maxwell Eigenproblem: 3c

1. Limit range of **k**: irreducible Brillouin zone
2. Limit degrees of freedom: expand **H** in finite basis
3. Efficiently solve eigenproblem: iterative methods

$$Ah = \omega^2 Bh$$

Many iterative methods:

— Arnoldi, Lanczos, Davidson, Jacobi-Davidson, …, Rayleigh-quotient minimization

for Hermitian matrices, smallest eigenvalue ω_0 minimizes:

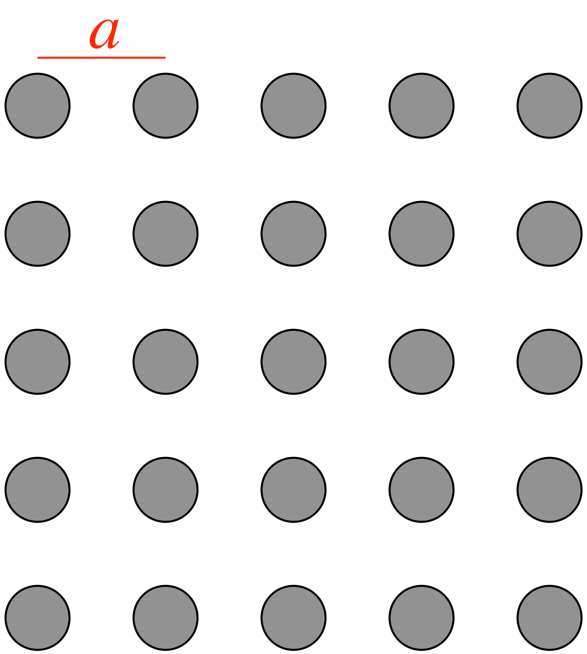
variational / min–max theorem

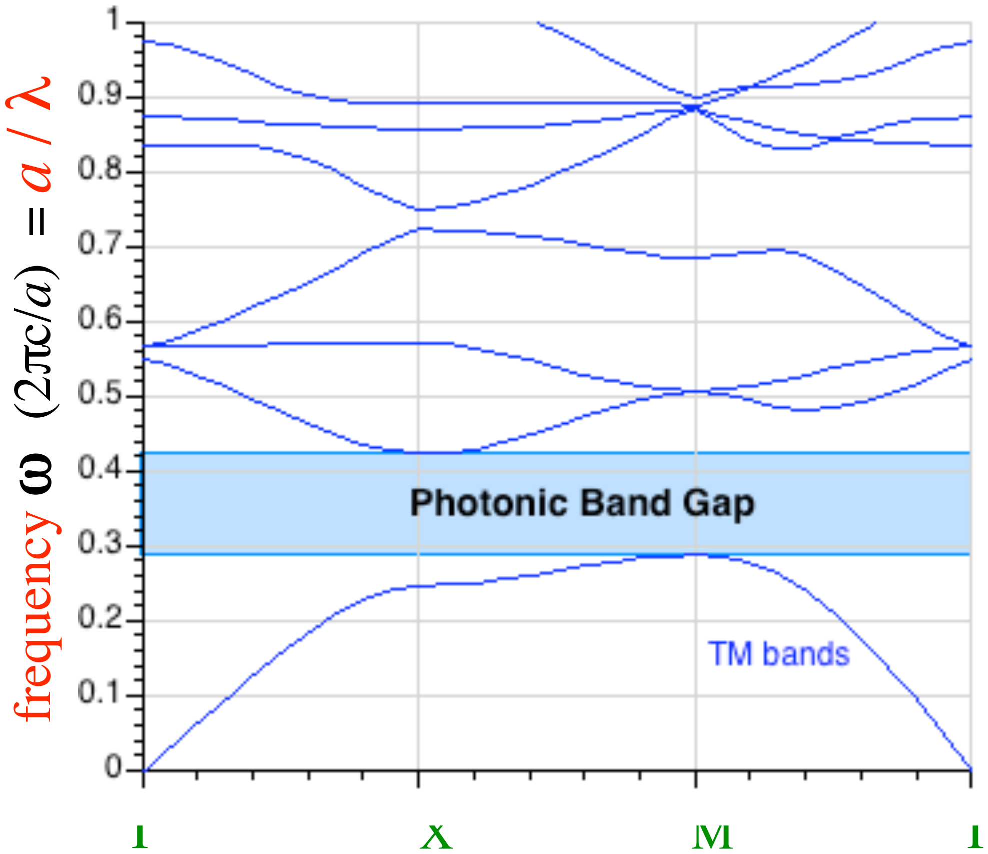
$$\omega_0^2 = \min_h \frac{h^* Ah}{h^* Bh}$$

minimize by preconditioned conjugate-gradient (or…)

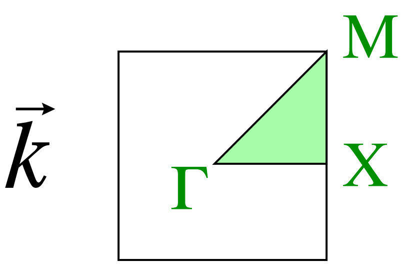
Band Diagram of 2d Model System

(radius 0.2a rods, ε=12)





irreducible Brillouin zone



gap for

n > ~1.75:1

Origin of the Band Gap

Hermitian eigenproblems:

solutions are orthogonal and satisfy a variational theorem

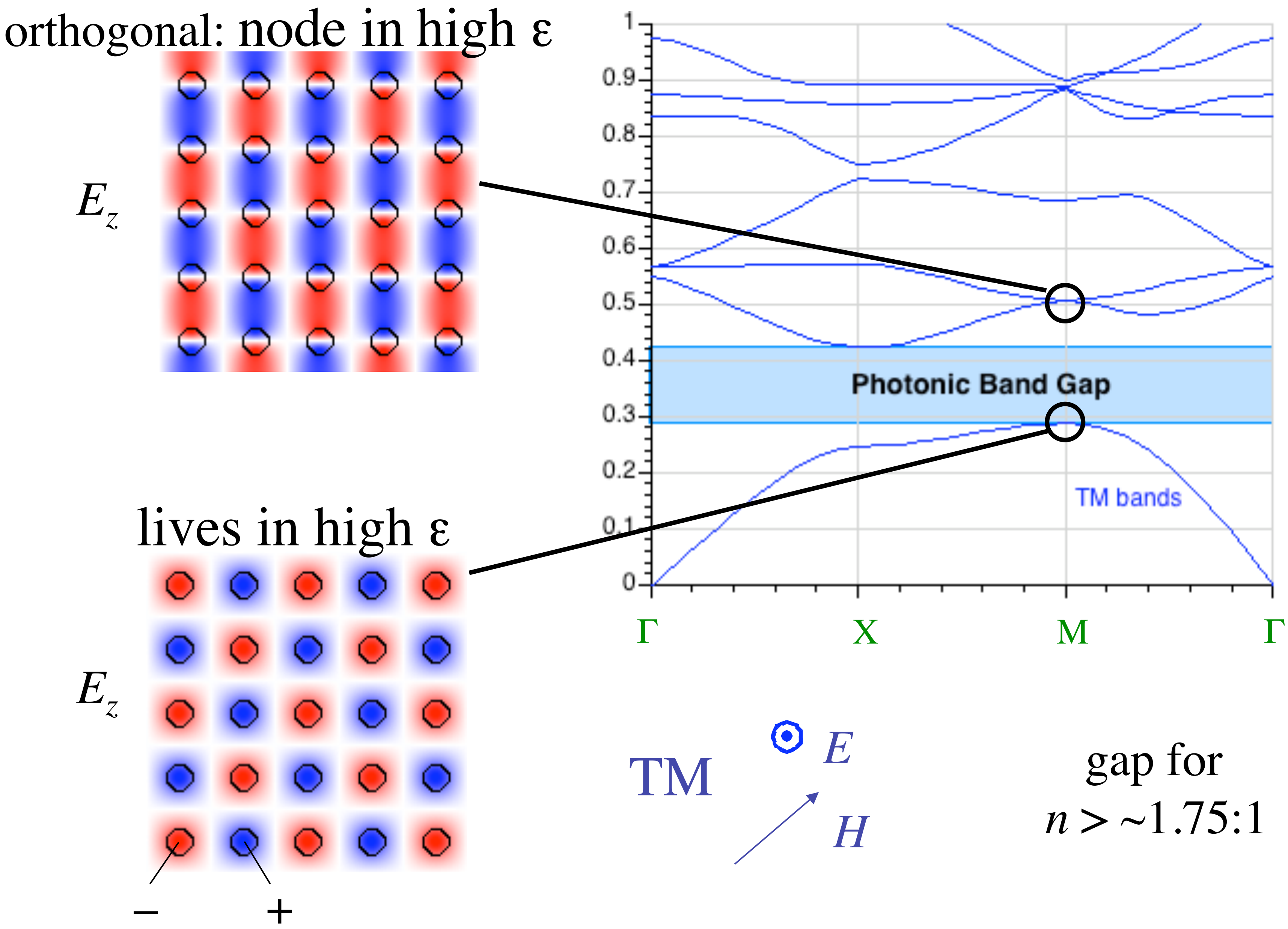
Electronic	Photonic
• minimize kinetic + potential energy (e.g. “bonding” state)	• minimize: $\dfrac{\text{field oscillations}}{\text{field in high } \varepsilon}$ $$\omega^2 = \min_{\vec{E}} \frac{\int \left\lvert \nabla \times \vec{E} \right\rvert^2}{\int \varepsilon \left\lvert \vec{E} \right\rvert^2} c^2$$

• higher bands orthogonal to lower —

must oscillate (high kinetic) or be in low ε (high potential)

(e.g. “anti-bonding” state)

Origin of Gap in 2d Model System



gap for
$n >$ ~1.75:1

The Iteration Scheme is *Important*

(minimizing function of 10^4–10^8+ variables!)

$$\omega_0^2 = \min_h \frac{h^* A h}{h^* B h} = f(h)$$

Steepest-descent: minimize ($h + \alpha\, \nabla f$) over α … repeat

Conjugate-gradient: minimize ($h + \alpha\, d$)

— d is ∇f + (stuff): *conjugate* to previous search dirs

Preconditioned steepest descent: minimize ($h + \alpha\, d$)

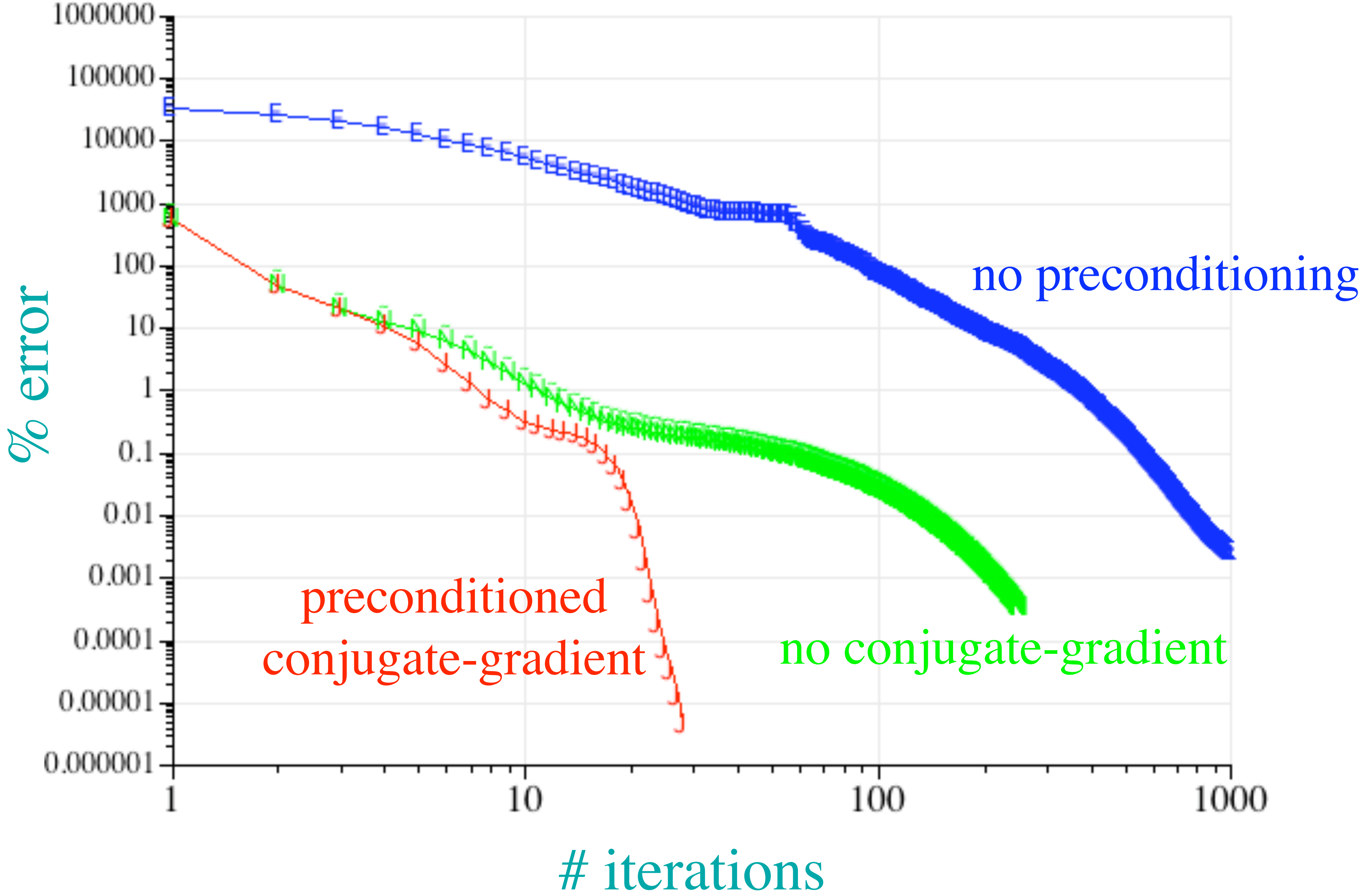
— d = (approximate A^{-1}) ∇f ~ Newton's method

Preconditioned conjugate-gradient: minimize ($h + \alpha\, d$)

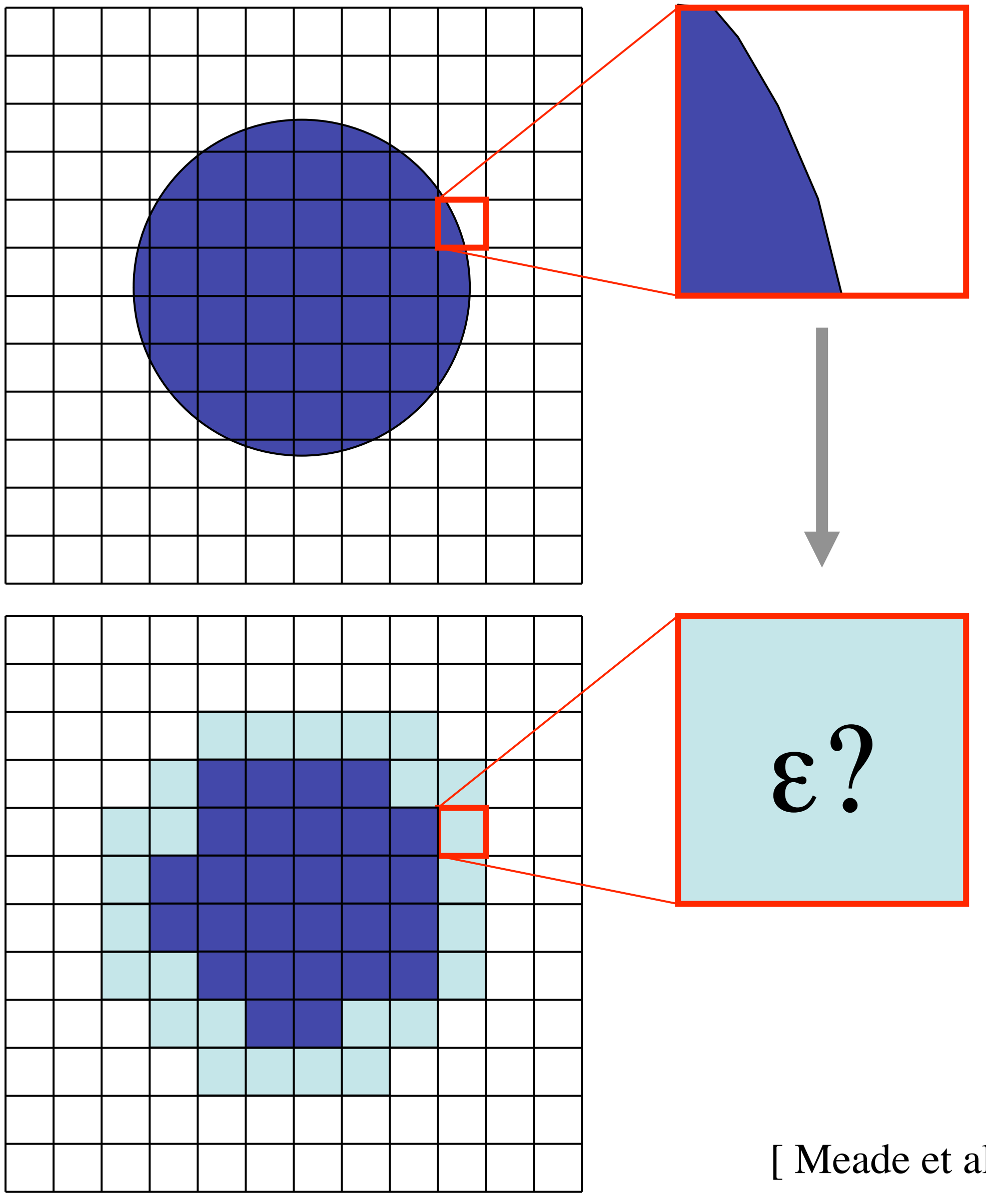
— d is (approximate A^{-1}) [∇f + (stuff)]

The Iteration Scheme is *Important*

(minimizing function of ~40,000 variables)



The Boundary Conditions are Tricky



$\mathbf{E}_{||}$ is continuous

$\mathbf{E}_{\perp}$ is discontinuous

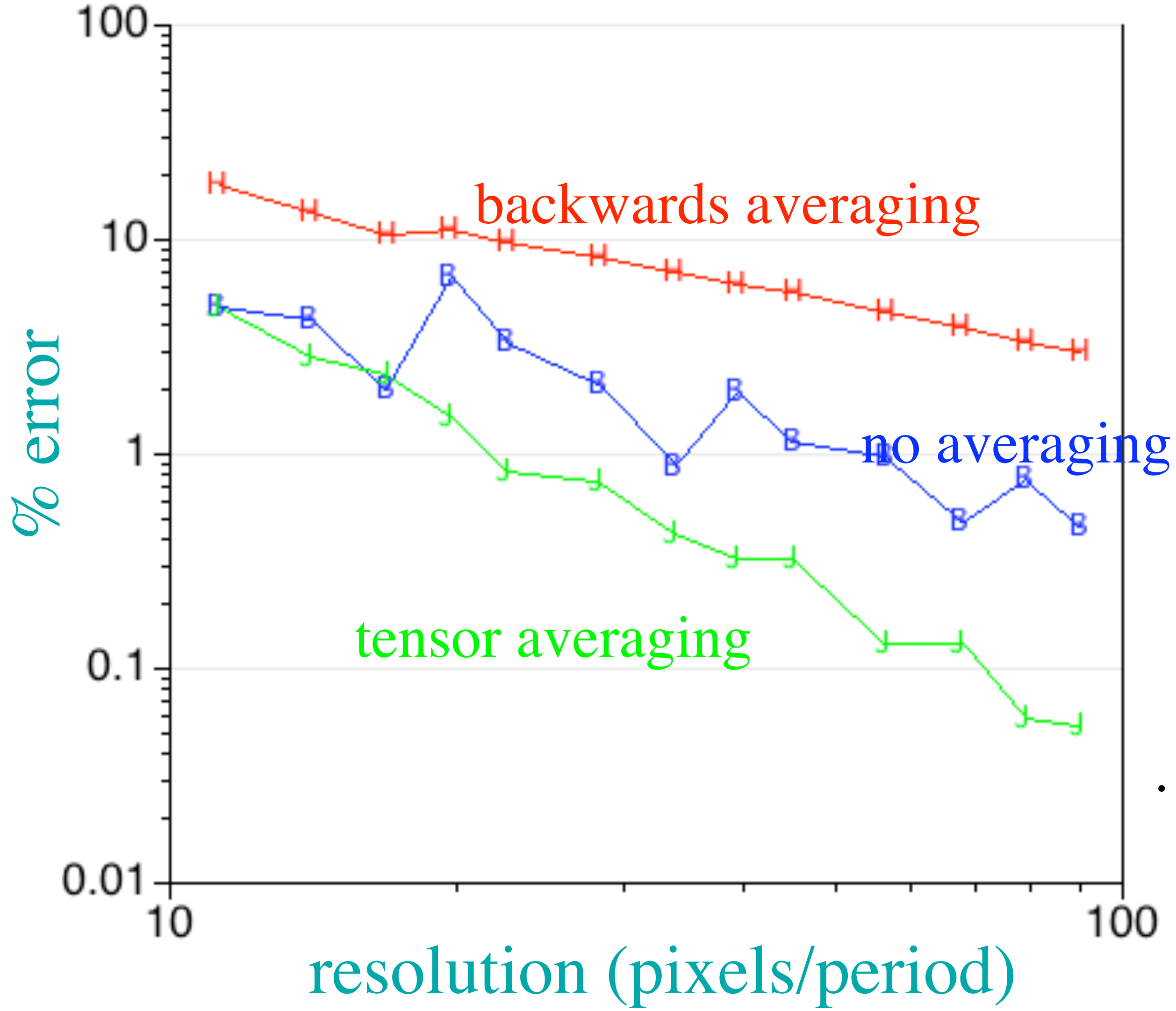
($\mathbf{D}_{\perp} = \varepsilon\mathbf{E}_{\perp}$ is continuous)

Use a tensor ε:

$$\begin{array}{cc} \begin{pmatrix} \langle\varepsilon\rangle & & \\ & \langle\varepsilon\rangle & \\ & & \langle\varepsilon^{-1}\rangle^{-1} \end{pmatrix} & \begin{array}{l} \Big| \; \mathbf{E}_{||} \\ \\ \mathbf{E}_{\perp} \end{array} \end{array}$$

[Meade et al. (1993)]

The ε-averaging is *Important*



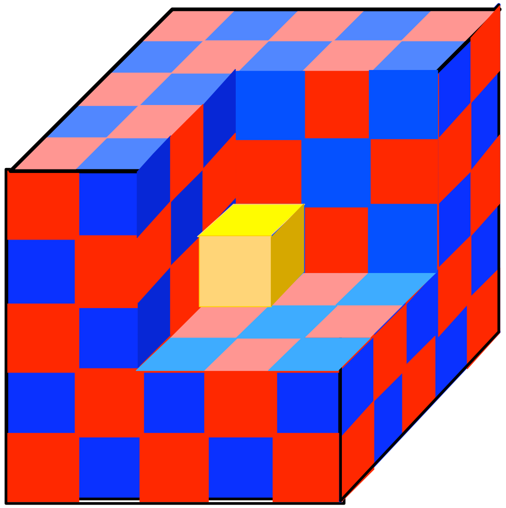
correct averaging changes *order* of convergence from Δx to Δx^2

reason in a nutshell:
averaging
= smoothing ε
= changing structure
… must pick smoothing with zero 1st-order perturbation

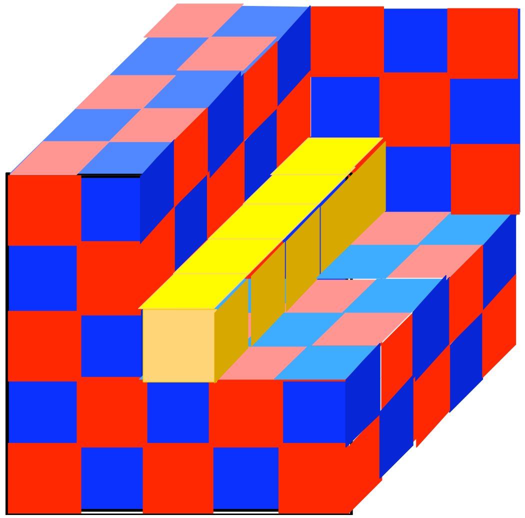
[Farjadpour et al. (2006)]

Intentional "defects" are good

microcavities



waveguides ("wires")

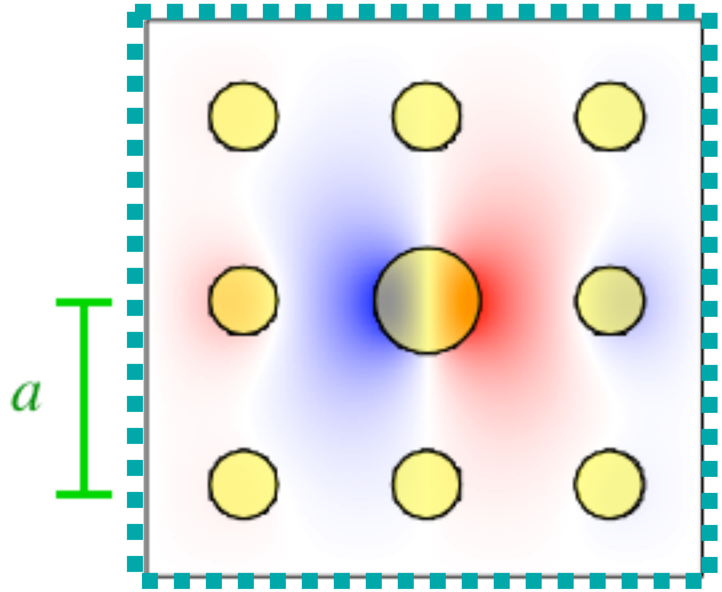


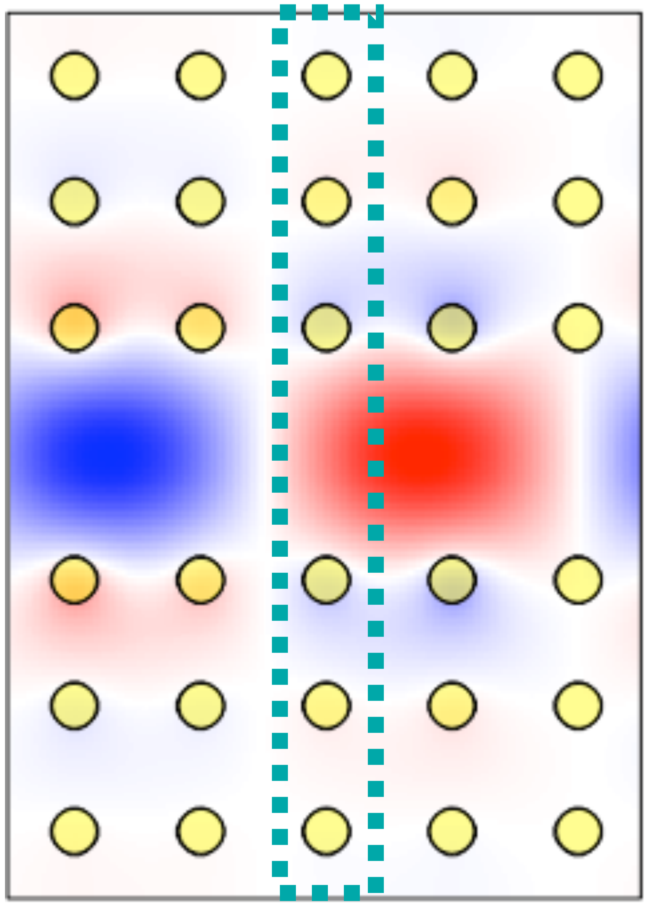
Intentional “defects” in 2d

(Same computation, with supercell = many primitive cells)

waveguides

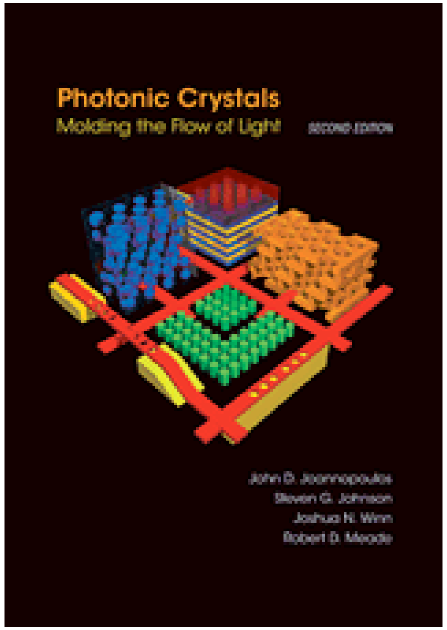
microcavities





(boundary conditions ~ irrelevant
for exponentially localized modes)

to be continued…



Further reading:

Photonic Crystals book: http://jdj.mit.edu/book

Bloch-mode eigensolver: http://jdj.mit.edu/mpb