Solving the Maxwell Eigenproblem

Want to solve for \( \omega_0(k) \), find \( \omega \) vs. \( k \) for "all" \( k \).

- Limit range of \( k \): irreducible Brillouin zone
- Limit degrees of freedom: expand \( H \) in finite basis
- Efficiently solve eigenproblem: iterative methods

\( (V + \mathbf{k}) \mathbf{H} = \omega \mathbf{H} \)

where:

\[ H_{jk} = \frac{1}{\epsilon_{jk}} \]

Limit degrees of freedom: expand \( H \) in finite basis

\[ \mathbf{H} = \sum_{x} \mathbf{b}_x(x) \]

solve: \( \mathbf{A}[\mathbf{H}] = \omega^2 \mathbf{H} \)

finite matrix problem:

\[ \mathbf{A} = \mathbf{H} \]

Many iterative methods:
- Arnoldi, Lanczos, Davidson, Jacobs-Davidson, ..., Rayleigh-quotient minimization

for Hermitian matrices, smallest eigenvalue \( \omega_0 \) minimizes:

\[ \omega_0^2 = \min \left( \frac{\mathbf{H} \mathbf{h}}{\mathbf{h}^T \mathbf{H} \mathbf{h}} \right) \]

where \( \mathbf{h} \) is arbitrary function

\( \epsilon \)-averaging is Important

correct averaging changes order of convergence from \( \Delta x \) to \( \Delta x^2 \)

The Boundary Conditions are Tricky

- \( E_z \) is continuous
- \( E_x \) is discontinuous
- \( \mathbf{E}_f \) is continuous

Any single scalar fail

(\( \mathbf{D} \) or \( \mathbf{E} \))

Use a tensor \( \mathbf{E} \):

\[ \left( \begin{array}{c} \psi_1 \end{array} \right) = \mathbf{E}_f \left( \begin{array}{c} \psi_1 \end{array} \right) \]

The Iteration Scheme is Important

(minimizing function of \( 10^3 - 10^5 \) variables!)

\[ \omega_0^2 = \min_{\mathbf{h}} \frac{\mathbf{h}^T \mathbf{A} \mathbf{h}}{\mathbf{h}^T \mathbf{B} \mathbf{h}} = f(h) \]

Steeped descent: minimize \((h + \alpha \nabla f)\) over \( \alpha \) ... repeat

Conjugate gradient: minimize \((h + \alpha d)\)

- \( d \) is \( \nabla f + \text{(stuff)} \): conjugate to previous search dir

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

- \( d \) is approximate \( \nabla f - \text{(approximate)} \text{(stuff)} \)

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

- \( d \) is approximate \( A^{-1} \text{(stuff)} \)

The Iteration Scheme is Important

(minimizing function of \( \approx 40,000 \) variables)

\[ \mathbf{H} = \sum_{x} \mathbf{b}_x(x) \]

solve:

\[ \mathbf{A} = \mathbf{H} \]

finite matrix problem:

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