ECE 595, Section 10
Numerical Simulations
Lecture 20: Bandstructure Concepts

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Outline

• Recap from Friday
• Bandstructure Problem Formulation
• Bloch’s Theorem
• Reciprocal Lattice Space
• Numerical Solutions
  – 1D crystal
  – 2D triangular lattice
  – 3D diamond lattice
Recap from Friday: FEM for Electronic Transport

- Physics-based device modeling
- Electronic transport theory
- FEM electronic transport model
- Numerical results
- Error Analysis
Bandstructure Problem

• Amounts to solving an eigenvalue equation for a system with discrete translational symmetry

• Examples include:
  – Electronic bandstructure:
    \[ -\frac{\hbar^2}{2m} \nabla^2 + V(x) \Psi(x) = \hbar \omega \Psi(x) \]
  – Photonic bandstructure:
    \[ \nabla \times [\epsilon^{-1}(\nabla \times H)] = \left(\frac{\omega}{c}\right)^2 H \]
  – Phononic bandstructure:
    \[ \nabla \times [C(\nabla \times \mathbf{u})] = -\rho \omega^2 \mathbf{u} \]
Bloch Theorem

- Asserts that solution in periodic potential is always a product of two terms:
  - a periodic function (with the same period)
  - a plane wave

- Mathematically, we can write:

\[ \Psi(r) = A e^{ik \cdot r} u(r) \]

where \( u(r + R) = u(r) \)
Bloch Theorem

• Use Bloch’s theorem to solve this eigenproblem:
\[
\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r})\right] [e^{i\mathbf{k} \cdot \mathbf{r}} u(\mathbf{r})] = E(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x}} u(\mathbf{r})
\]

• What basis to use for periodic function?
Reciprocal Lattice Vectors

- If working in Fourier space, define a set of reciprocal lattice vectors $G$ such that $e^{iG \cdot R} = 1$
- Then we can construct a complex Fourier series approximating any $R$-periodic function with: $f(r) = \sum_G f_G e^{iG \cdot r}$
- Each coefficient calculated using orthogonality relations: $f_G = \int_V d\mathbf{r} f(\mathbf{r}) e^{-iG \cdot \mathbf{r}}$
- In 1D lattice of period $a$, $G = (2\pi m/a)\hat{x}$
Reciprocal Lattice Vectors

• For 2D lattice, will have two directions for our reciprocal lattice vectors, depending on lattice

• For square lattice: $G_1 = (2\pi/a)\hat{x}$; $G_2 = (2\pi/a)\hat{y}$; $G = mG_1 + pG_2$

• For triangular lattice: $G_1 = (2\pi/a)\hat{x}$; $G_2 = (\pi/a)(\hat{x} + \sqrt{3}\hat{y})$; $G = mG_1 + pG_2$

• Other types include rectangular, rhombic, and oblique
Reciprocal Lattice Vectors

• In 3D, there are 14 total Bravais lattices:
Reciprocal Lattice Vectors

• In 3D, can’t just construct reciprocal lattice vectors by inspection.
• If we define lattice directions \{a_i\}, and lattice volume \( V = a_1 \cdot (a_2 \times a_3) \), then:

\[
\begin{align*}
  b_1 &= \frac{2\pi}{V} (a_2 \times a_3) \\
  b_2 &= \frac{2\pi}{V} (a_3 \times a_1) \\
  b_3 &= \frac{2\pi}{V} (a_1 \times a_2) \\
  \mathbf{G} &= m b_1 + p b_2 + q b_3
\end{align*}
\]
Reciprocal Lattice Vectors

• Brillouin Zone is constructed by drawing perpendicular bisectors between adjacent G’s in reciprocal space.

• BZ is where $\mathbf{k}$ can vary.

• Can also introduce further symmetries to make irreducible BZ.
Reciprocal Lattice Vectors

- Certain wavevectors have special designations:
  - \( \Gamma \): \( k = 0 \) Center
  - \( \Xi \): \( k = (\pi/a)\hat{x} \) Face center
  - \( L \): \( k = (\pi/a)(\hat{x} + \hat{y} + \hat{z}) \) BZ hex face center
  - \( W \): \( k = (\pi/a)(2\hat{x} + \hat{y}) \) Corner (fcc)
  - \( K \): \( k = (3\pi/2a)(\hat{x} + \hat{y}) \) Edge joins hex faces
  - \( U \): \( k = (\pi/2a)(4\hat{x} + \hat{y} + \hat{z}) \) Joins hex/square face
  - \( M \): \( k = (\pi/a)(\hat{x} + \hat{z}) \) Center of edge
Reciprocal Lattice Vectors

• In the case of electronic bandstructures:

\[
\left[- \frac{\hbar^2}{2m} \nabla^2 + V(x) \right] \Psi(x) = \hbar \omega \Psi(x)
\]

• We obtain the nice recursion relation:

\[
V_{G'} c_{G-G'} = \left[ E(k) - \frac{\hbar^2}{2m} (k + G)^2 \right] c_G
\]
Reciprocal Lattice Vectors

• In the case of photonic bandstructures:

\[ \nabla \times [\varepsilon^{-1} (\nabla \times H)] = \left(\frac{\omega}{c}\right)^2 H \]

• We can obtain:

\[ - (k + G) \times \left[ \varepsilon_{GG'}^{-1} (k + G') \times h_{G-G'} \right] = \left(\frac{\omega}{c}\right)^2 h_G \]

• Implemented numerically in MIT Photonic Bands (MPB): [http://jdj.mit.edu/mpb/](http://jdj.mit.edu/mpb/)
Photonic Bandstructures: 1D

(Above) photonic bandstructures obtained for increasing dielectric contrast

(Right) Electric fields associated with bandgap seen in middle bandstructure
Photonic Bandstructures: 2D

Frequency $\omega a/2\pi c$

TE modes

TM modes

$\Gamma$ X M $\Gamma$
Photonic Bandstructures: 2D
Next Class

- Is on Wednesday, Feb. 25
- Will discuss more about bandstructures
- Recommended reading: Joannopoulos, Chapter 3 and Appendix D