Nanophotonic Modeling
Lecture 1.14: Formulating the Photonic Bandstructure Calculation

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Maxwell Eigenproblem

- Maxwell's equations in QM notation:

$$\vec{\nabla} \times \frac{1}{\varepsilon} \vec{\nabla} \times |H\rangle = -\frac{1}{c^2} \frac{\partial^2}{\partial t^2} |H\rangle$$

$$\vec{\nabla} \cdot |H\rangle = 0.$$

- Choose: $$|H\rangle = e^{i(\vec{k}\cdot\vec{x}-\omega t)} \left|H_{\vec{k}}\right\rangle$$

- Such that: $$\hat{A}_{\vec{k}} \left|H_{\vec{k}}\right\rangle = (\omega/c)^2 \left|H_{\vec{k}}\right\rangle$$

$$\hat{A}_{\vec{k}} = \left(\vec{\nabla} + i\vec{k}\right) \times \frac{1}{\varepsilon} \left(\vec{\nabla} + i\vec{k}\right) \times$$

Maxwell Eigenproblem

- Choose basis such that: $\left\langle H_{\vec{k}}^{(n)} \middle| H_{\vec{k}}^{(m)} \right\rangle = \delta_{n,m}$

- Generally can expand H-field in the basis:

$$\left|H_{\vec{k}}\right\rangle \cong \sum_{m=1}^{N} h_m \left|b_m\right\rangle .$$

- Which yields:

$$Ah = \left(\frac{\omega}{c}\right)^2 Bh$$

h is a column vector

$$A_{\ell m} = \langle b_\ell | \hat{A}_{\vec{k}} | b_m \rangle \text{ and } B_{\ell m} = \langle b_\ell | b_m \rangle$$

Maxwell Eigenproblem

- Best algorithm to use?
  - Power method: $\lambda_1 = \frac{{v_k}^T A v_k}{{v_k}^T v_k}$
  - Inverse iteration: $\lambda = b_{k-1}(\boldsymbol{A} - \tau\mathbf{1})^{-1^T} \cdot \boldsymbol{A} \cdot (\boldsymbol{A} - \tau\mathbf{1})^{-1} b_{k-1}$
  - Transformation method: $A' = PAP$
  - Decomposition: $A_{k+1} = L_k Q_k = {Q_k}^T A_k Q_k$

Decomposition Timing

- Execution time:
  - total number of elements computed/stored: N^2
  - Total number of operations per element (average): N/3
  - Scaling: $\mathcal{O}(N^3)$

Alternative approaches

- May want to focus on first p bands, where $p \ll N$
- Now storage scales like $\mathcal{O}(pN)$
- Work scales like $\mathcal{O}(p^2N)$

Reformulating the Eigenproblem

- Choose planewave basis such that:

$$|b_{m_1,m_2,m_3}\rangle = e^{i\sum_j m_j \vec{G}_j \cdot \vec{x}}$$

- Now we can rewrite

$$|H_{\vec{k}}\rangle \cong \sum_{\{m_j\}} \vec{h}_{\{m_j\}} e^{i\sum_{j,k} m_j \vec{G}_j \cdot n_k \vec{R}_k / N_k} = \sum_{\{m_j\}} \vec{h}_{\{m_j\}} e^{2\pi i \sum_j m_j n_j / N_j}$$

- This is in fact a discrete Fourier transform!

Reformulating the Eigenproblem

- While a normal DFT scales like $\mathcal{O}(N^2)$, but
- A fast Fourier transform (FFT) scales like $\mathcal{O}(N \log N)$
- A succession of FFT and inverse FFT's, i.e.:

$$A_{\ell m} = -\left(\vec{k} + \vec{G}_\ell\right) \times \cdots \mathrm{IFFT} \cdots \widetilde{\varepsilon^{-1}} \cdots \mathrm{FFT} \cdots \left(\vec{k} + \vec{G}_m\right) \times$$

…would have the same scaling