# 6, Eigenvalues and Eigenvectors

The eigenvalue/eigenvector of an $N \times N$ matrix **A** are defined as a scalar $\lambda$ and a nonzero vector **v** satisfying

$$\begin{aligned} \mathbf{A} \cdot \mathbf{x} &= \lambda \mathbf{x}, \\ (\mathbf{A} - \lambda \mathbf{I})\mathbf{v} &= \mathbf{0}, \qquad (\mathbf{v} \neq \mathbf{0}). \end{aligned}$$

- the matrix $[\mathbf{A} - \lambda \mathbf{I}]$ should be *sigular*, its determinant should be zero det$(\mathbf{A} - \lambda \mathbf{I}) = 0$,
- the determinant of the matrix $[\mathbf{A} - \lambda \mathbf{I}]$ is a polynomial of degree $N$ in terms of $\lambda$.

# Eigenvalues and Eigenvectors

1. find the eigenvalue $\lambda$'s by solving the characteristic equation,

$$|\mathbf{A} - \lambda \mathbf{I}| = \lambda^N + a_{N-1}\lambda^{N-1} + \cdots + a_1\lambda + a_0 = 0,$$

2. then substitute the $\lambda_i$'s, one by one, into

$$(\mathbf{A} - \lambda \mathbf{I})\mathbf{v} = \mathbf{0},$$

to solve it for the eigenvector $\mathbf{v}_i$'s.

# Scaled power method: Largest magnitude

Suppose all of the eigenvalues of an $N \times N$ matrix $\mathbf{A}$ are distinct with the magnitudes,

$$|\lambda_1| > |\lambda_2| \geq |\lambda_3| \geq \cdots \geq |\lambda_N|.$$

- For any initial vector $\mathbf{x}_0$, such as

$$\mathbf{x}_0 = \left[\begin{array}{cccc} 1 & 1 & \cdots & 1 \end{array}\right],$$

- consequently, any initial vector $\mathbf{x}_0$ can be expressed as a linear combination of the eigenvecotrs,

$$\mathbf{x}_0 = \alpha_1 \mathbf{v}_1 + \alpha_2 \mathbf{v}_2 + \cdots + \alpha_N \mathbf{v}_N.$$

- For $\mathbf{A}\mathbf{v}_n = \lambda_n \mathbf{v}_n$,we have

$$\begin{aligned} \mathbf{A}\mathbf{x}_0 &= \alpha_1 \lambda_1 \mathbf{v}_1 + \alpha_2 \lambda_2 \mathbf{v}_2 + \cdots + \alpha_N \lambda_N \mathbf{v}_N \\ &= \lambda_1 (\alpha_1 \mathbf{v}_1 + \alpha_2 \frac{\lambda_2}{\lambda_1} \mathbf{v}_2 + \cdots + \alpha_N \frac{\lambda_N}{\lambda_1} \mathbf{v}_N), \end{aligned}$$

# Scaled power method: Largest magnitude

- repeat this multiplication over and over again to obtain,

$$
\begin{aligned}
\mathbf{x}_k &= \mathbf{A}^k \mathbf{x}_0 \\
&= \lambda_1^k (\alpha_1 \mathbf{v}_1 + \alpha_2 (\frac{\lambda_2}{\lambda_1})^k \mathbf{v}_2 + \cdots + \alpha_N (\frac{\lambda_N}{\lambda_1})^k \mathbf{v}_N) \\
&\rightarrow \lambda_1^k \alpha_1 \mathbf{v}_1,
\end{aligned}
$$

- we must keep scaling before multiplying at every iteration to prevent the overflow or underflow,

$$
\begin{aligned}
\mathbf{x}_{k+1} &= \mathbf{A} \frac{\mathbf{x}_k}{||\mathbf{x}_k||_\infty} \\
&\rightarrow \lambda_1 \frac{\mathbf{v}_1}{||\mathbf{v}_1||_\infty},
\end{aligned}
$$

where $||\mathbf{x}||_\infty = \text{Max}\{|\mathbf{x}_n|\}$.

# Inverse power method: smallest magnitude

- If the matrix is nonsigular **A**, then

$$\begin{aligned} \mathbf{A} \cdot \mathbf{x} &= \lambda \mathbf{x}, \\ \rightarrow \mathbf{A}^{-1} \mathbf{x} &= \lambda^{-1} \mathbf{x}, \end{aligned}$$

- this implies that the inverse matrix $\mathbf{A}^{-1}$ has the eigenvalues that are the reciprocals of the eigenvalues of the original matrix $A$, but with the same eigenvectors.
- we can apply the scaled power method for the eigenvalues with largest magnitude,

$$\lambda_N = \frac{1}{\text{the largest eigenvalue of } \mathbf{A}^{-1}},$$

to find the smallest (magnitude) eigenvalue $\lambda_N$.

# Shifted inverse power method

- To find the eigenvalue that is not necessarily of the largest or smallest magnitude, we substract the eigenvalue equation by $s\mathbf{v}$ ($s$ is a number that does not happen to equal any eigenvalue,)

$$
\begin{aligned}
\mathbf{A} \cdot \mathbf{x} &= \lambda \mathbf{x}, \\
\rightarrow [\mathbf{A}^{-1} - s\mathbf{I}]\mathbf{x} &= (\lambda - s)\mathbf{x},
\end{aligned}
$$

- this implies that $(\lambda - s)$ is the eigenvalue of $[\mathbf{A} - s\mathbf{I}]$, we apply the inverse power method to get its smallest magnitude eigenvalue,
- then we add $s$ to obtain the eigenvalue of the original matrix **A** which is closest to the number $s$,

$$
\lambda_N = \frac{1}{\text{the largest eigenvalue of} \quad [\mathbf{A} - s\mathbf{I}]} + s,
$$

to find the smallest (magnitude) eigenvalue $\lambda_N$.

# Eigenpackages of Canned eigenroutines

- LAPACK: Linear Algebra Package
- EISPACK: Matrix Eigensystem Routines
- IMSL: Visual Numerics
- NAG: Numerical Algorithms Group
- . . .

# Eigenpackages of Canned eigenroutines

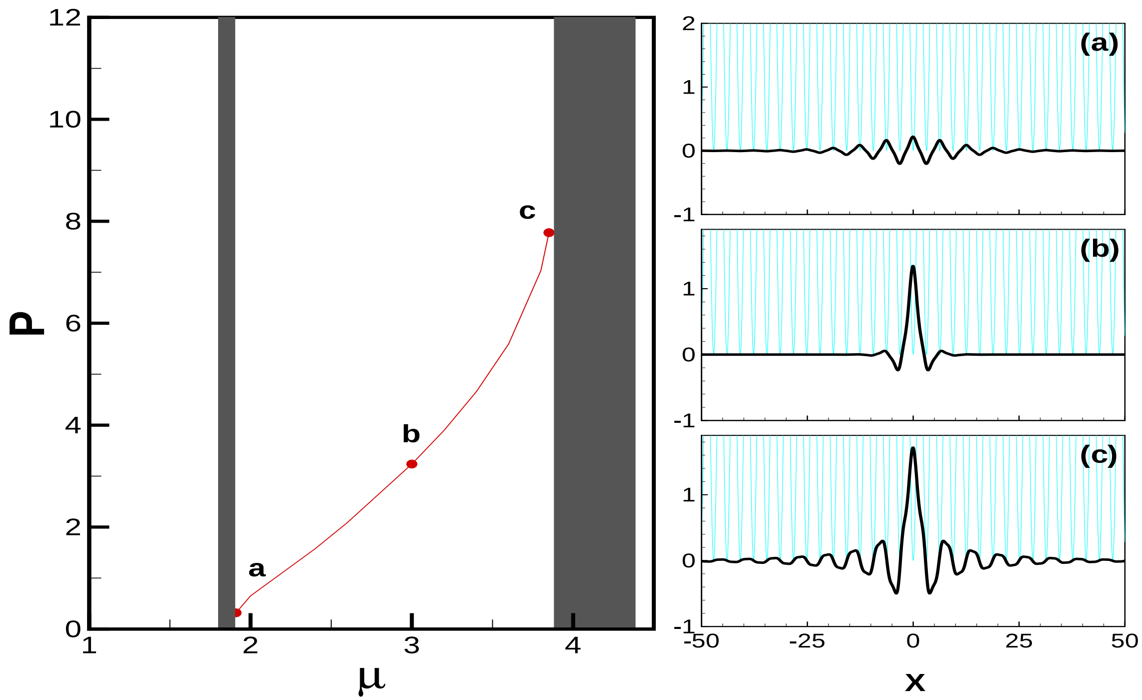
- all eigenvalues and no eigenvectors,
- all eigenvalues and some corresponding eigenvectors,
- all eigenvalues and all corresponding eigenvectors,
- real, symmetric, tridiagonal,
- real, symmetric, banded,
- real, symmetric, full,
- real nonsymmetric,
- complex, Hermitian,
- complex, non-Hermitian.

# Gap solitons in optical lattices

1-D Gross-Pitaevskii equation with periodic potentials, $V(x) = V_0 \sin^2(k_0 x)$,

$$i\hbar \frac{\partial}{\partial t}\Phi_0(t,x) = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\Phi_0(t,x) + V(x)\Phi_0(t,x) + g_{1D}|\Phi_0(t,x)|^2\Phi_0(t,x)$$

which has gap soliton solutions.




by FS + NK methods, $N_x$ = 512, no. of iterations $< 10$; gpeol.m.

R.-K. Lee, E. A. Ostrovskaya, Yu. S. Kivshar, and Y. Lai, *Phys. Rev. A* **72**, 033607 (2005).

# Band-Gap spectrum

1-D Gross-Pitaevskii equation with periodic potentials, $V(x) = V_0 \sin^2(k_0 x)$,

$$i\hbar \frac{\partial}{\partial t}\Phi_0(t,x) = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\Phi_0(t,x) + V(x)\Phi_0(t,x) + g_{1D}|\Phi_0(t,x)|^2\Phi_0(t,x).$$

For the stationary solution,

$$\Phi_0(t,x) = \phi(x)\mathrm{exp}(-i\mu t),$$

one have *time-independent* GP equation,

$$\frac{1}{2}\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2} - [V_0 \sin^2(Kx)\phi - \mu\phi] - g_{1D}|\phi|^2\phi = 0.$$

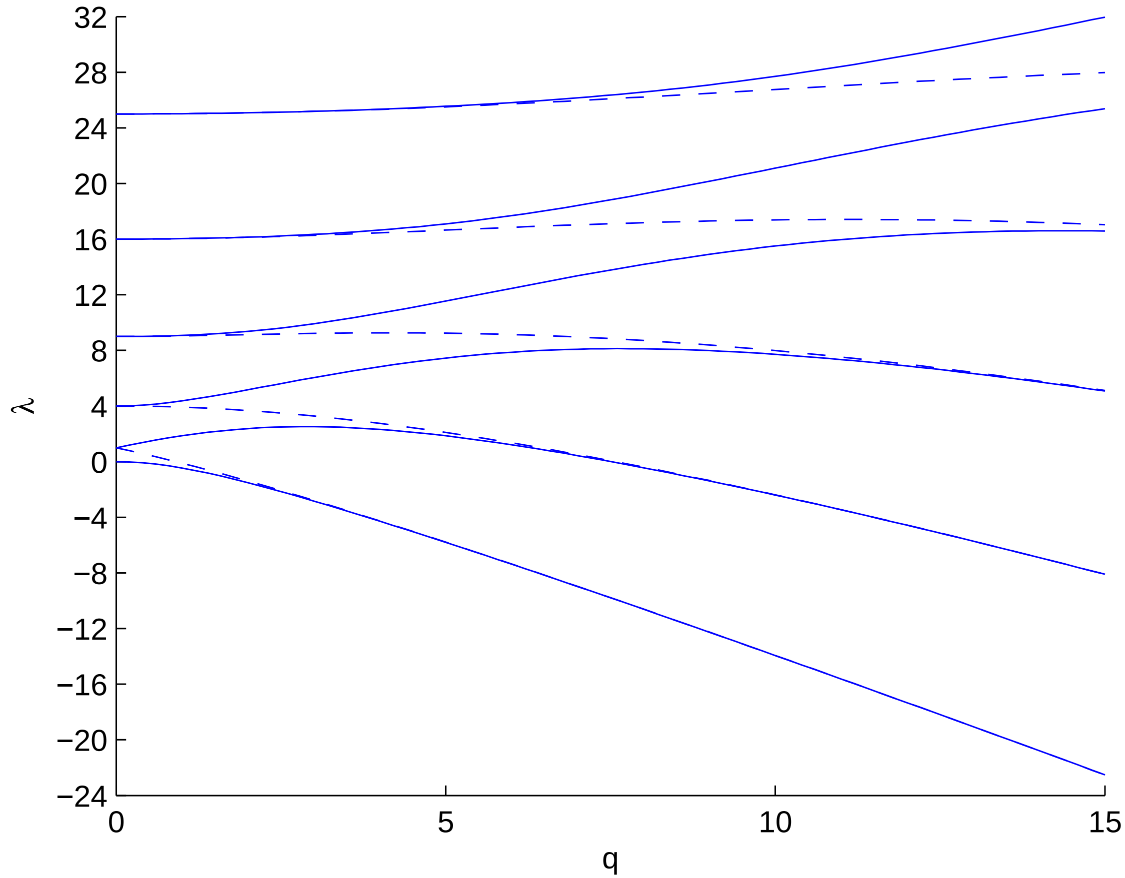
For the *linear case* (non-interacting condensate), $g_{1D} = 0$,

$$\frac{1}{2}\frac{\mathrm{d}^2\phi}{\mathrm{d}y^2} - [2q\cos(2y) - p]\phi = 0,$$

where $y = Kx$, $q = -V_0/(2K^2)$, and $p = 2(q + \mu/K^2)$, which is the Mathieu's equation.

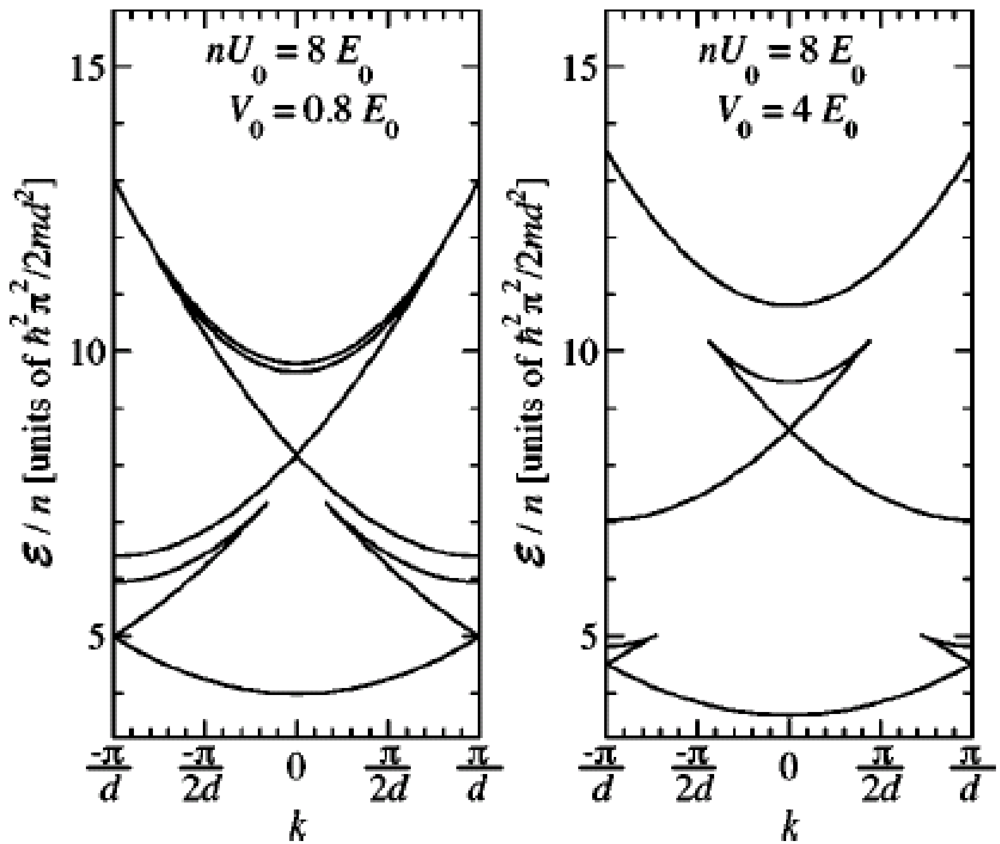
# Mathieu equation

Mathieu equation: $-u_{xx} + 2q\cos(2x)u = \lambda u,$



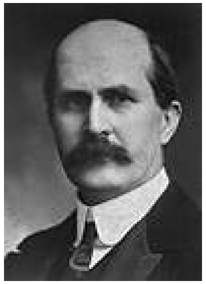
# Nonlinear band structure for BEC in OL

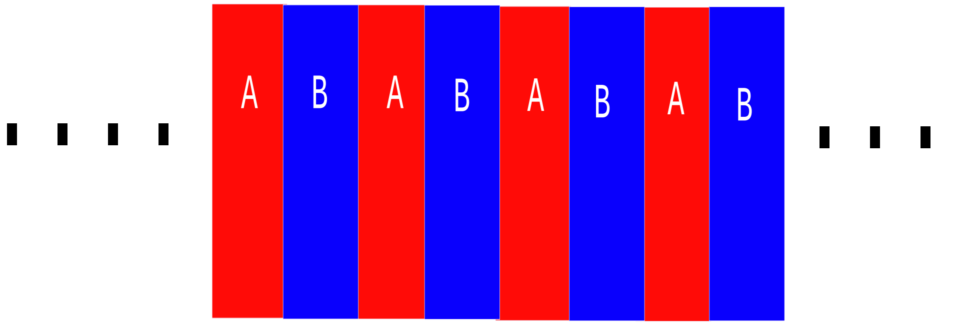
$$\frac{1}{2}\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2} - [V_0 \sin^2(Kx)\phi - \mu\phi] - \sigma|\phi|^2\phi = 0.$$

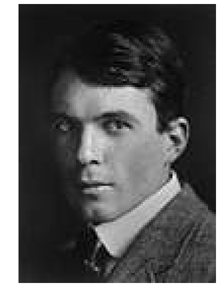


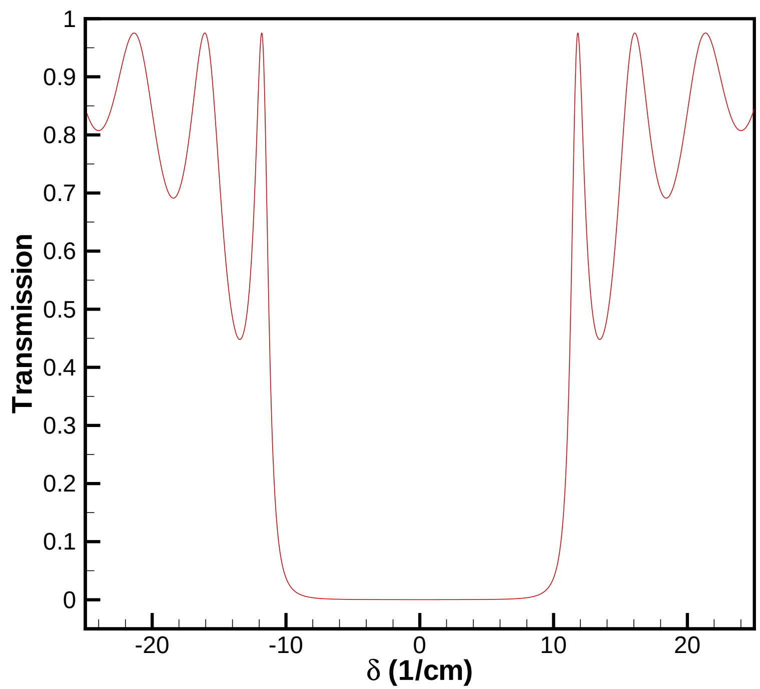

M. Machholm *et al.*, *Phys. Rev. A* **67**, 053613 (2003).

# Bragg reflectors





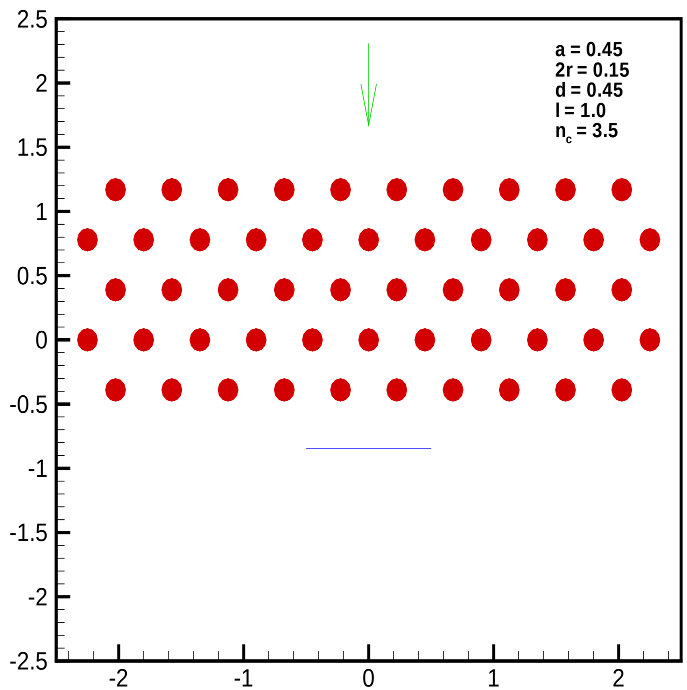



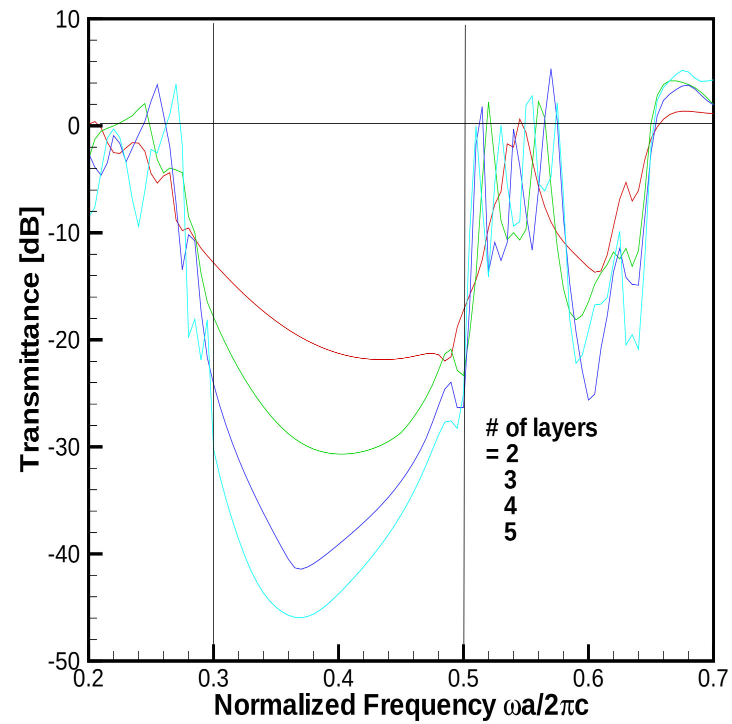



Nobel laureates William Henry Bragg and William Lawrence Bragg in 1915,

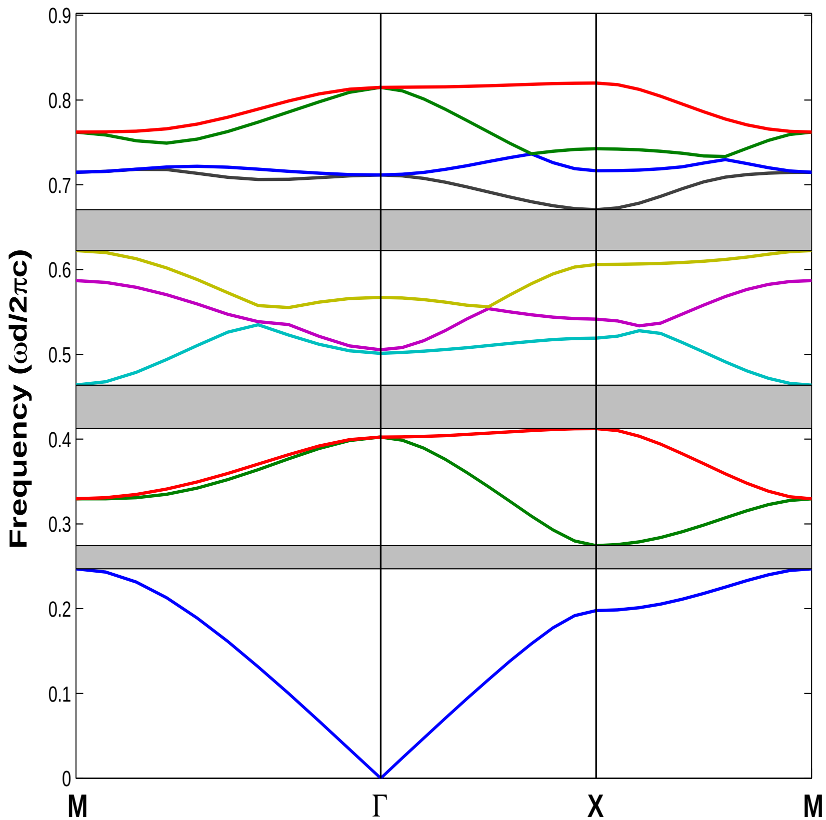
for their contribution to the X-ray diffraction analysis (Bragg diffraction).

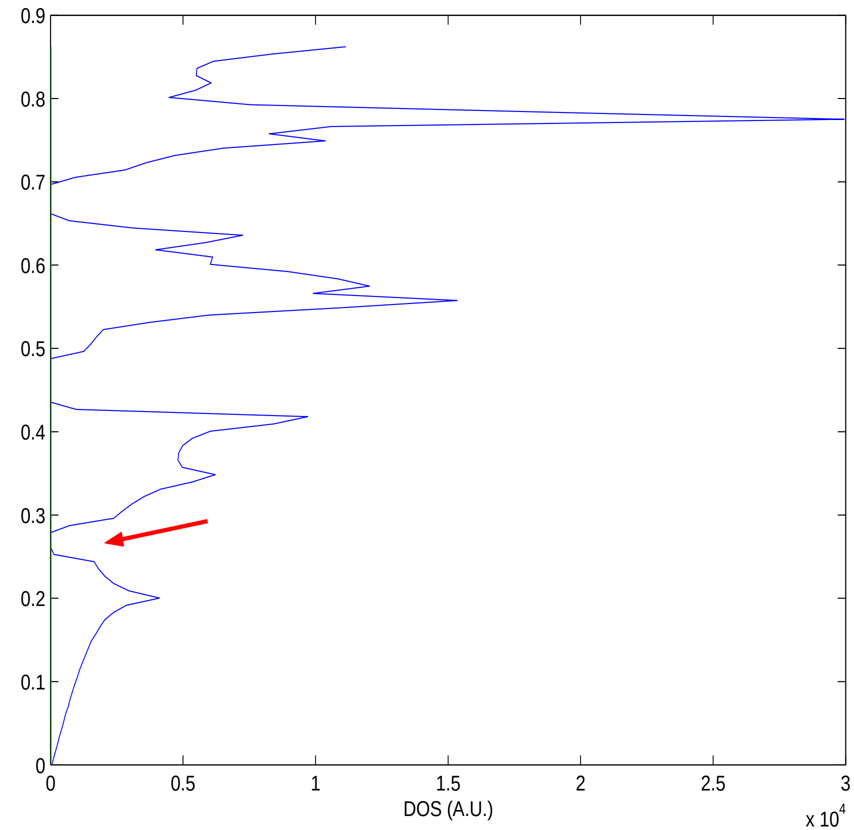
# Photonic Bandgap Crystals: two(high)-dimension



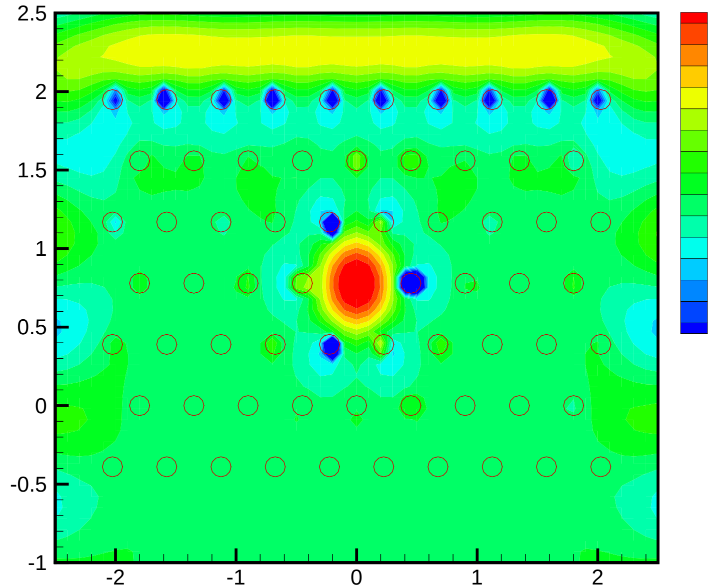



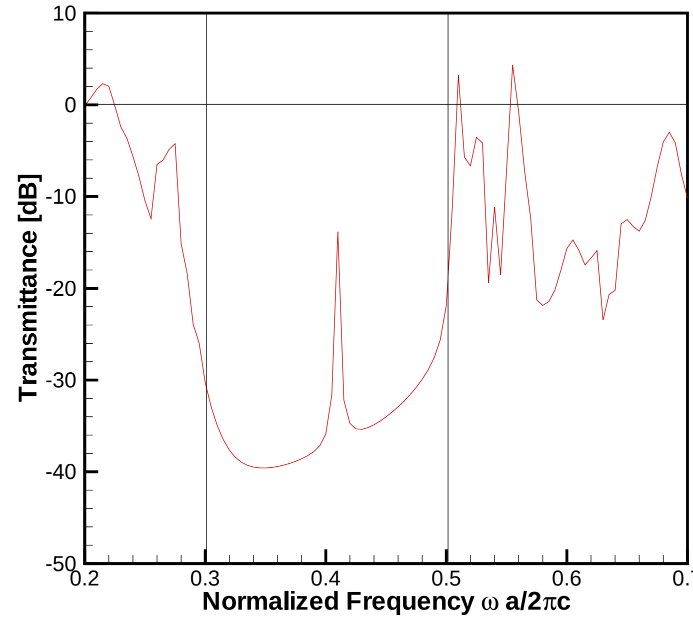
# Band diagram and Density of States

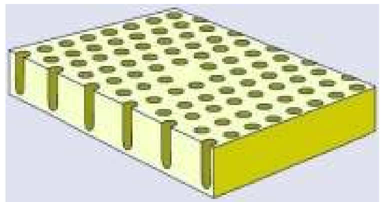


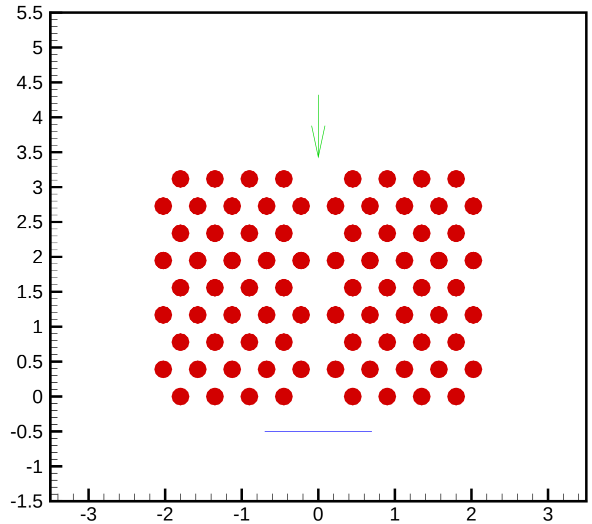
# Photonic Bandgap Crystals:point-defect (localized field)

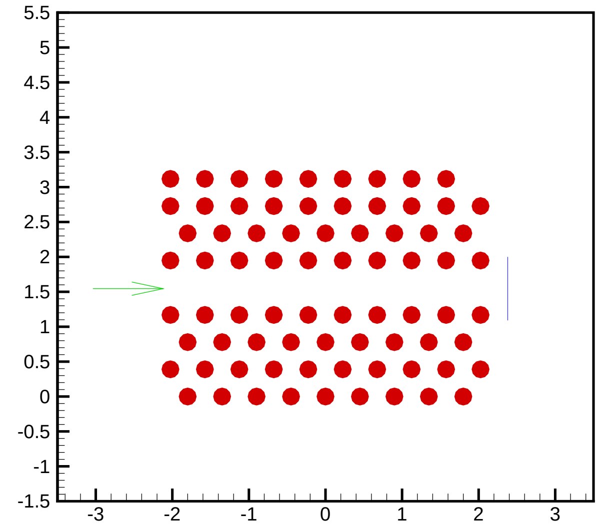


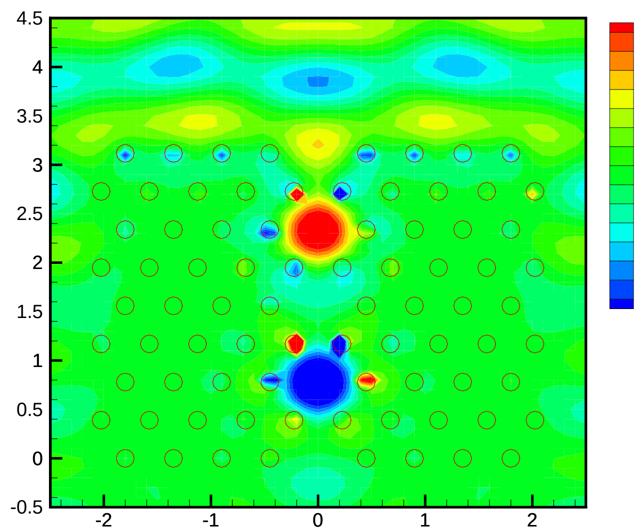



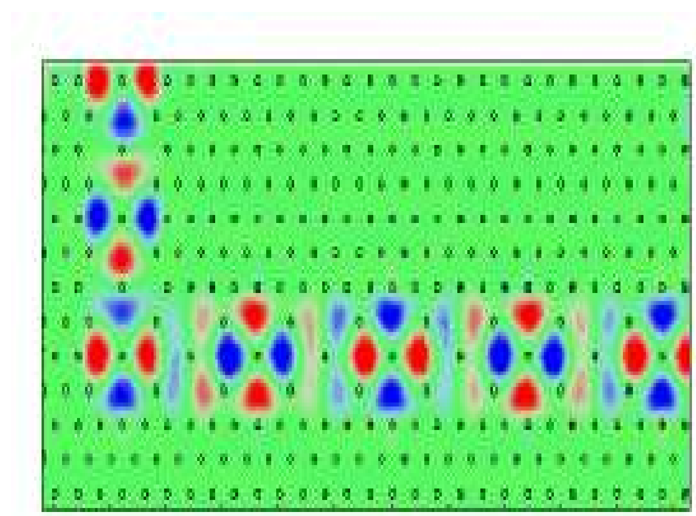



# Photonic Bandgap Crystals:line-defects









Courtesy: Bin-Shei Lin

# Maxwell equations

- For a linear, isotropic nondispersive material,

$$
\begin{aligned}
\mathbf{B} &= \mu \mathbf{H}, \\
\mathbf{D} &= \epsilon \mathbf{E}.
\end{aligned}
$$

- magnetic conduction current:

$$\mathbf{J}_m = \rho' \mathbf{H}.$$

- electric conduction current:

$$\mathbf{J}_e = \sigma \mathbf{E}.$$

Then the Maxwell's curl equations becom

$$
\begin{aligned}
\frac{\partial}{\partial t}\mathbf{H} &= -\frac{1}{\mu}\nabla \times \mathbf{E} - \frac{\rho'}{\mu}\mathbf{H} \\
\frac{\partial}{\partial t}\mathbf{E} &= \frac{1}{\epsilon}\nabla \times \mathbf{H} - \frac{\sigma}{\epsilon}\mathbf{E}.
\end{aligned}
$$

# Periodic structrures

- For a periodic structure,

$$\mathbf{D}(\mathbf{r},t) = \epsilon_0 \epsilon(\mathbf{r}) \mathbf{E}(\mathbf{r},t)$$

the periodicity of $\epsilon(\mathbf{r})$ implies

$$\epsilon(\mathbf{r}+\mathbf{a}_i) = \epsilon(\mathbf{r}), \qquad (i = 1,2,3).$$

- then the Maxwell equations become,

$$\begin{aligned}
\nabla \cdot \{\epsilon(\mathbf{r})\mathbf{E}(\mathbf{r},t)\} &= 0, \\
\nabla \cdot \mathbf{H}(\mathbf{r},t) &= 0, \\
\nabla \times \mathbf{E}(\mathbf{r},t) &= -\mu_0 \frac{\partial}{\partial t}\mathbf{H}(\mathbf{r},t), \\
\nabla \times \mathbf{H}(\mathbf{r},t) &= \epsilon_0 \epsilon(\mathbf{r}) \frac{\partial}{\partial t}\mathbf{E}(\mathbf{r},t).
\end{aligned}$$

# Wave equations and plane wave expansion

- then one can obtain the wave equations,

$$\begin{aligned}\frac{1}{\epsilon(\mathbf{r})}\nabla\times\{\nabla\times\mathbf{E}(\mathbf{r},t)\} &= -\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\mathbf{E}(\mathbf{r},t),\\ \nabla\times\{\frac{1}{\epsilon(\mathbf{r})}\nabla\times\mathbf{H}(\mathbf{r},t)\} &= -\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\mathbf{H}(\mathbf{r},t),\end{aligned}$$

- use plane wave solution as basis,

$$\begin{aligned}\mathbf{E}(\mathbf{r},t) &= \mathbf{E}(\mathbf{r})e^{-i\omega t},\\ \mathbf{H}(\mathbf{r},t) &= \mathbf{H}(\mathbf{r})e^{-i\omega t},\end{aligned}$$

- then the wave equations become the *eigenvalue equations*,

$$\begin{aligned}\mathcal{L}_{\mathcal{E}}\mathbf{E}(\mathbf{r}) &= \frac{1}{\epsilon(\mathbf{r})}\nabla\times\{\nabla\times\mathbf{E}(\mathbf{r},t)\} = \frac{\omega^2}{c^2}\mathbf{E}(\mathbf{r},t),\\ \mathcal{L}_{\mathcal{H}}\mathbf{H}(\mathbf{r}) &= \nabla\times\{\frac{1}{\epsilon(\mathbf{r})}\nabla\times\mathbf{H}(\mathbf{r},t)\} = \frac{\omega^2}{c^2}\mathbf{H}(\mathbf{r},t),\end{aligned}$$

# Brillouin zone

- For a wave vector $\mathbf{k}$ in the first Brillouin zone and a band index $n$, we can express the field as,

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_{\mathbf{k}n}(\mathbf{r}) = \mathbf{u}_{\mathbf{k}n}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}},$$

where $\mathbf{u}_{\mathbf{k}n}(\mathbf{r})$ is a periodic function satisfying,

$$\mathbf{u}_{\mathbf{k}n}(\mathbf{r}+\mathbf{a}_i) = \mathbf{u}_{\mathbf{k}n}(\mathbf{r}).$$

- only consider the $\mathbf{E}$-field in two-dimensional space,

$$\frac{1}{\epsilon(\mathbf{r})}\nabla \times \{\nabla \times \mathbf{E}(\mathbf{r})\} = \frac{\omega^2}{c^2}\mathbf{E}(\mathbf{r}),$$

- which can be reduced to

$$\mathcal{L}_E^{(2)}\mathbf{E}_z(\mathbf{r}) = -\frac{1}{\epsilon(\mathbf{r})}\{\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\}\mathbf{E}_z(\mathbf{r}) = \frac{\omega^2}{c^2}\mathbf{E}(\mathbf{r}),$$

# Brillouin zone

- apply Bloch's theorem,

$$\begin{aligned} \mathbf{E}_z(\mathbf{r}) &= \mathbf{E}_{z,\mathbf{k}n}(\mathbf{r}) \\ &= \sum_{\mathbf{G}} \mathbf{E}_{z,\mathbf{k}n}(\mathbf{G}) \exp\{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}\}, \end{aligned}$$

  wher **k** and **G** are the reciprocal lattice vector in two dimensions,

$$\mathbf{G} = l_1\mathbf{b}_1 + l_2\mathbf{b}_2,$$

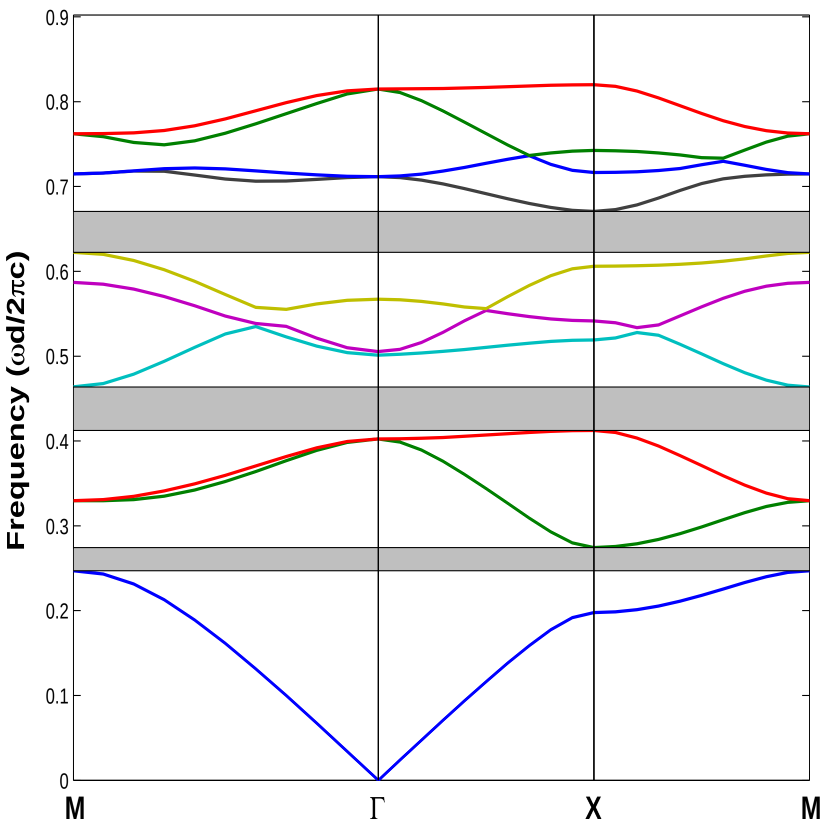
  where $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$ and $\{l_i\}$ are arbitrary integers.

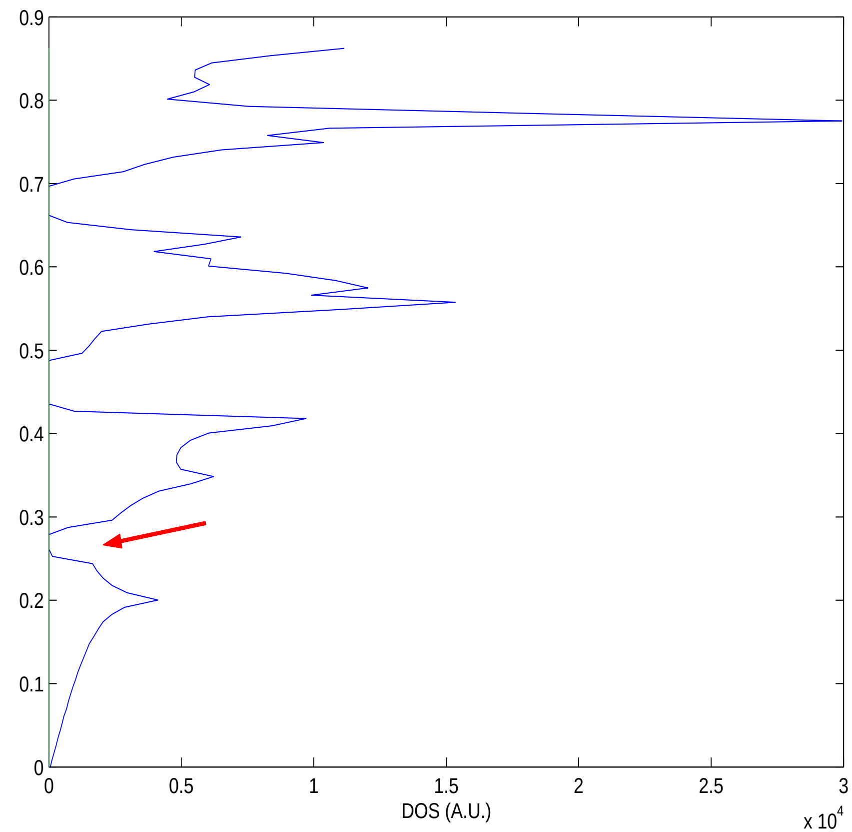
- the final eigenvalue equation to solve is,

$$\sum_{\mathbf{G}'} \frac{1}{\epsilon(\mathbf{G}-\mathbf{G}')} |\mathbf{k}+\mathbf{G}'|^2 \mathbf{E}_{z,\mathbf{k}n}(\mathbf{G}') = \frac{\omega_{\mathbf{k}n}^2}{c^2} \mathbf{E}_{z,\mathbf{k}n}(\mathbf{G}').$$

# Band diagram and Density of States

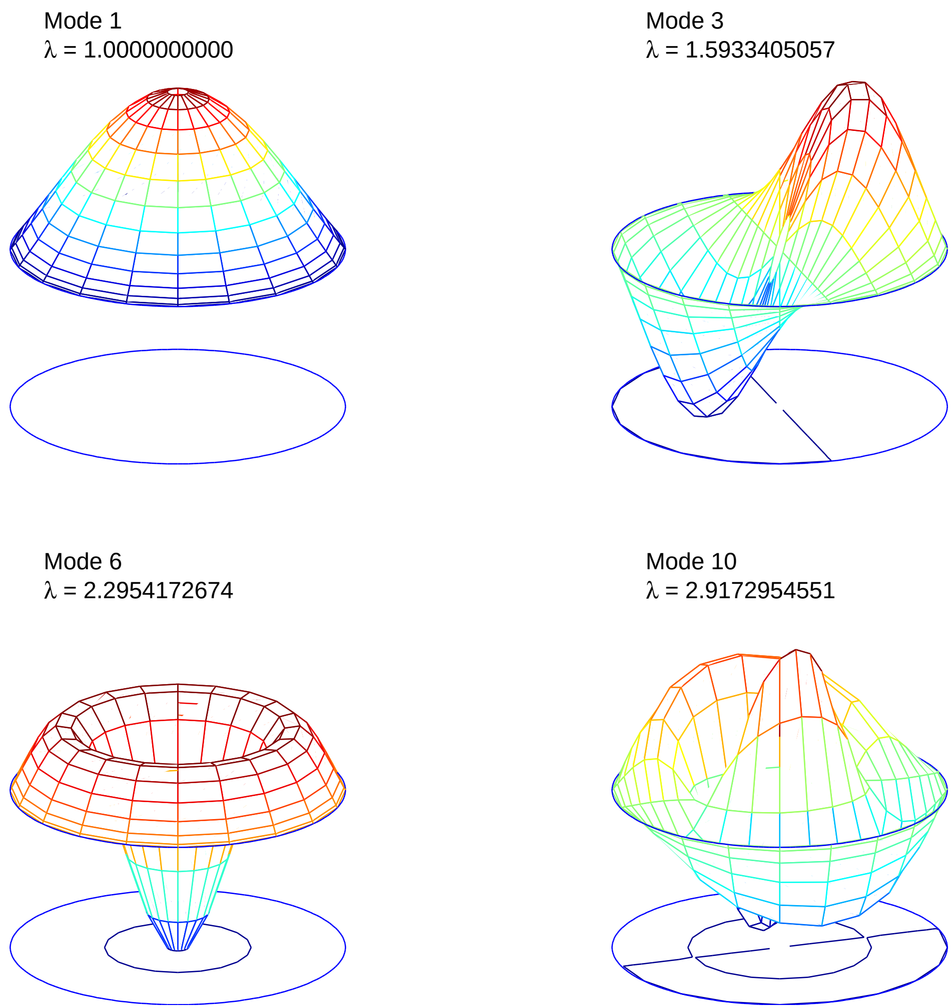
$$\frac{1}{\epsilon(\mathbf{r})}\nabla \times \{\nabla \times \mathbf{E}(\mathbf{r})\} = \frac{\omega^2}{c^2}\mathbf{E}(\mathbf{r}),$$



# Laplacian equation in a disk

Eigenmodes of Laplacian equations, $[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial x^2}]u(x,y) = -\lambda f(x,y)$.




L. N. Trefethen, *"Spectral methods in Matlab,"* SIAM (2000).

# Nonlinear eigenvalue problems

For example,

$$(\mathbf{A}\lambda^2 + \mathbf{B}\lambda + \mathbf{C}) \cdot \mathbf{x} = 0,$$

introduce an additional unkown eigenvector **y** and solve the $2N \times 2N$ eigensystem,

$$\begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{A}^{-1} \cdot \mathbf{C} & -\mathbf{A}^{-1} \cdot \mathbf{B} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}$$

This technique generalizes to higher-order polynomials in $\lambda$. Apolynomial of degree $M$ produces a linear $MN \times MN$ eigensystem.