Advanced Computation:

Computational Electromagnetics

Implementation of the Plane Wave Expansion Method

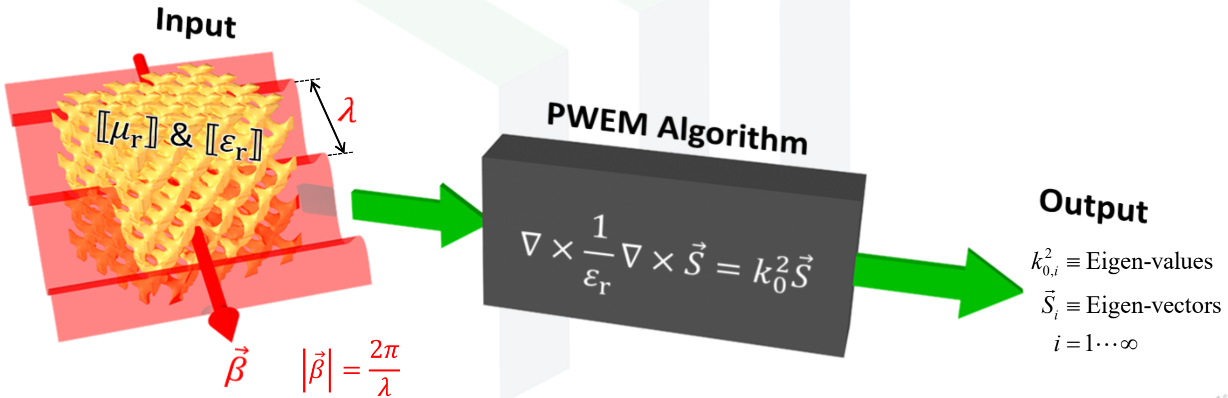
Outline

- Implementation
- Calculation of Band Diagrams
- Example – Computing the band diagram for a photonic crystal with square symmetry

Implementation

PWEM from a User's Perspective

Given the unit cell of an infinitely periodic lattice and the Bloch wave vector (i.e. wave direction and spatial period), the PWEM calculates all the modes with these conditions. The eigen-values contain the frequencies and the eigen-vectors contain the fields.



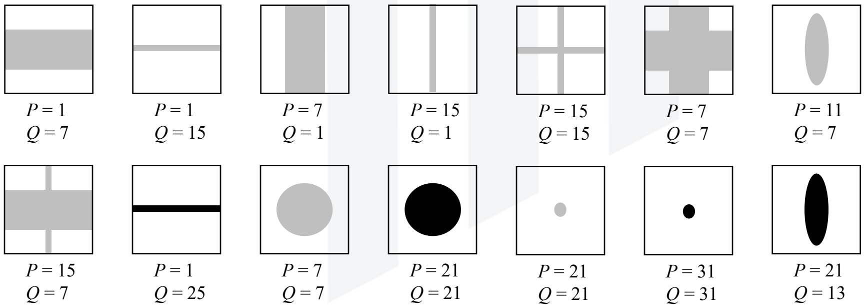
Choosing the Number of Spatial Harmonics

The only true way to determine the correct number of spatial harmonics is to test for convergence.

There are, however, some rules of thumb to follow in order to make a good initial guess.

$$\# \approx \frac{10a}{\lambda_{\min}}$$ For each direction.

Here are some examples…



Normalizing the Frequency

The eigen-value problem was derived so that k_0 (frequency) is the eigen-value.

$$\mathbf{K}_z [\![\mu_r]\!]^{-1} \mathbf{K}_z \mathbf{s} = \boxed{k_0^2} [\![\varepsilon_r]\!] \mathbf{s}$$

Think of k_0 as frequency because it is frequency ω divided by a constant c_0.

$$k_0 = \frac{\omega}{c_0}$$

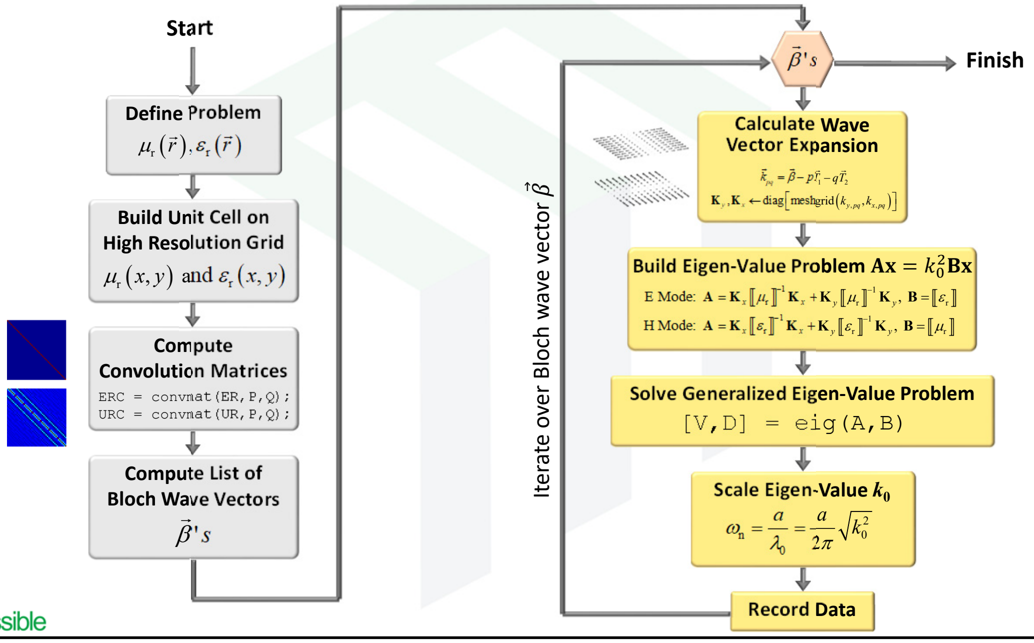
It is very useful when designing devices to scale the eigen-value to a/λ_0.

$$\omega_n = \frac{a}{\lambda_0} = \frac{a}{2\pi}\sqrt{k_0^2} = \frac{\omega a}{2\pi c_0}$$

Many papers like to label the normalized frequency this way. Crazy, huh?

The more meaningful a/λ_0 notation conveys that a design is easily scaled to operate at any wavelength λ_0 desired.

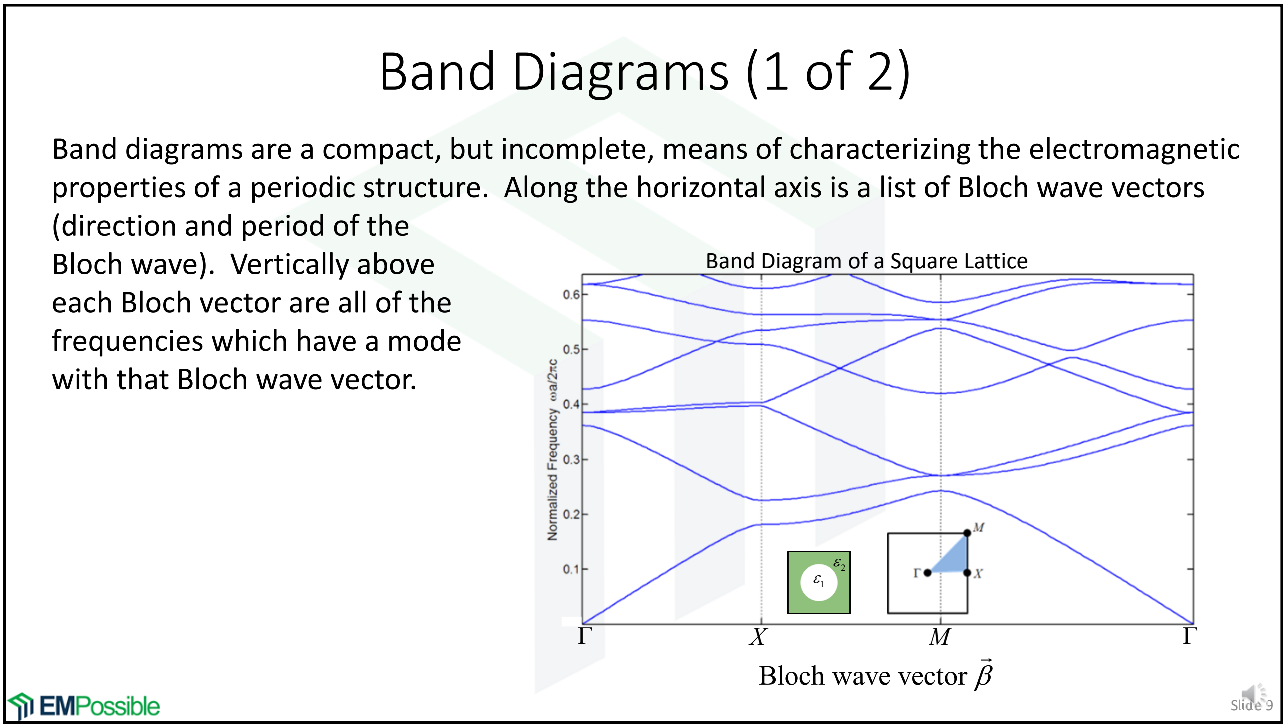
Block Diagram of 2D Analysis



```
ERC = convmat(ER,P,Q);
URC = convmat(UR,P,Q);
```

```
[V,D] = eig(A,B)
```

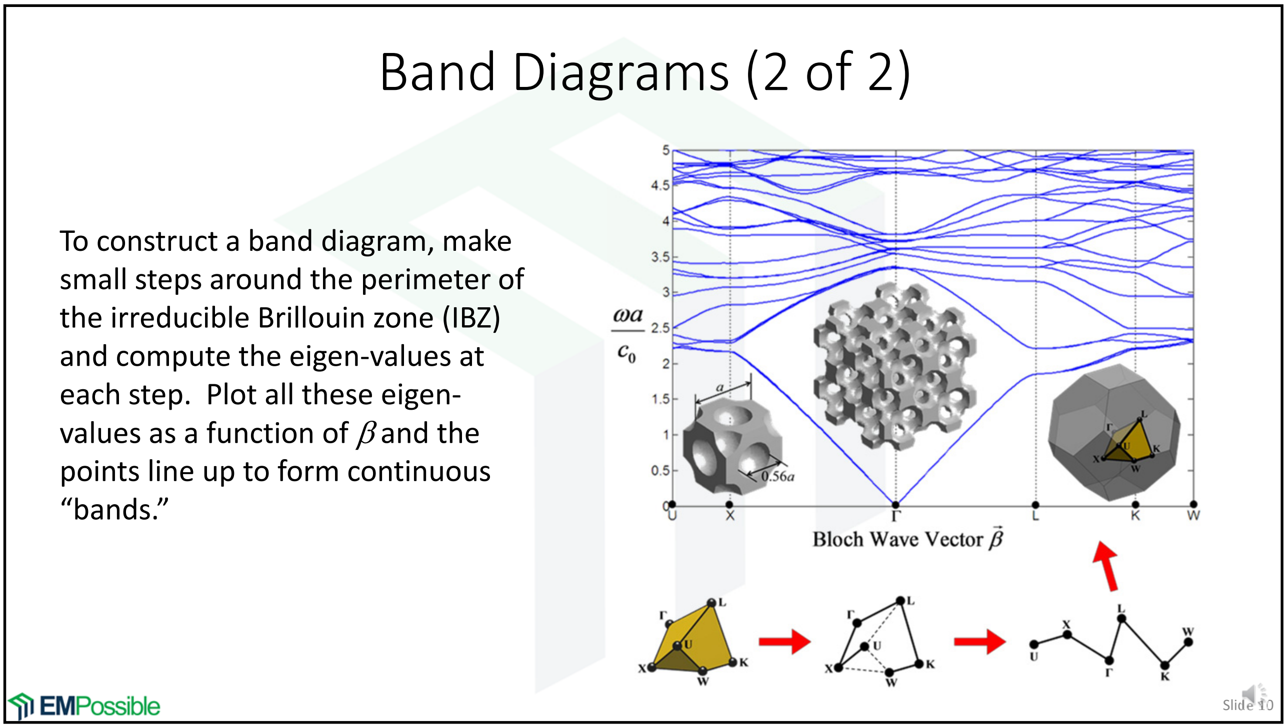
Calculation of Photonic Band Diagrams



Band Diagrams (1 of 2)

Band diagrams are a compact, but incomplete, means of characterizing the electromagnetic properties of a periodic structure. Along the horizontal axis is a list of Bloch wave vectors (direction and period of the Bloch wave). Vertically above each Bloch vector are all of the frequencies which have a mode with that Bloch wave vector.

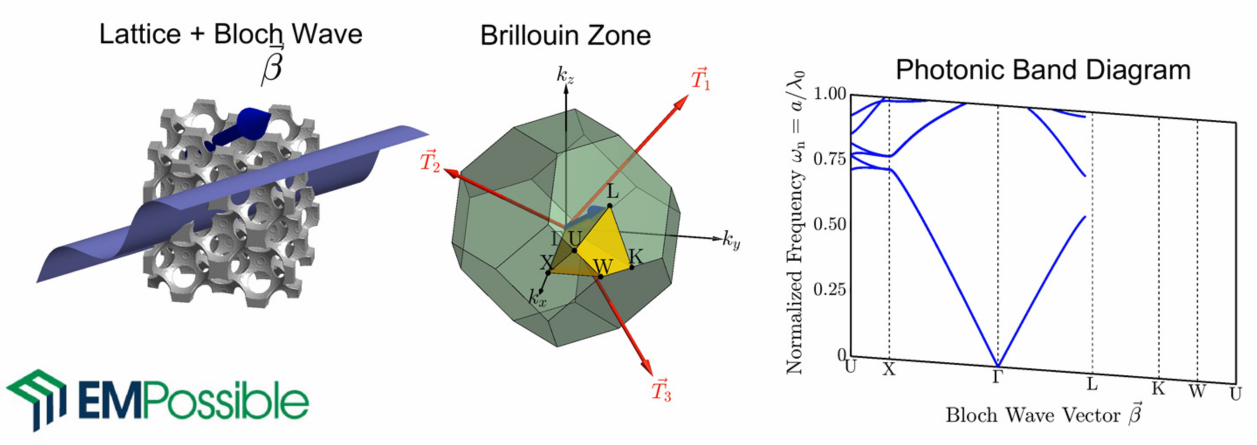
Band Diagram of a Square Lattice



Band Diagrams (2 of 2)

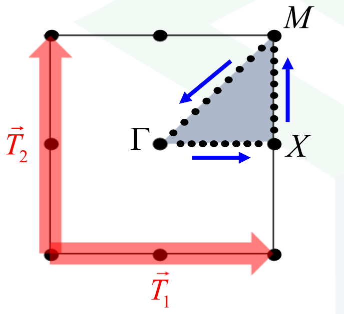
To construct a band diagram, make small steps around the perimeter of the irreducible Brillouin zone (IBZ) and compute the eigen-values at each step. Plot all these eigen-values as a function of β and the points line up to form continuous "bands."

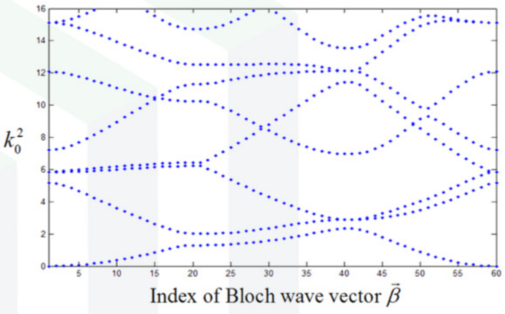
Animation of the Construction of a Band Diagram



List of Bloch Wave Vectors

To calculate a band diagram, it is necessary to generate an array of Bloch wave vectors that march around the perimeter of the IBZ.

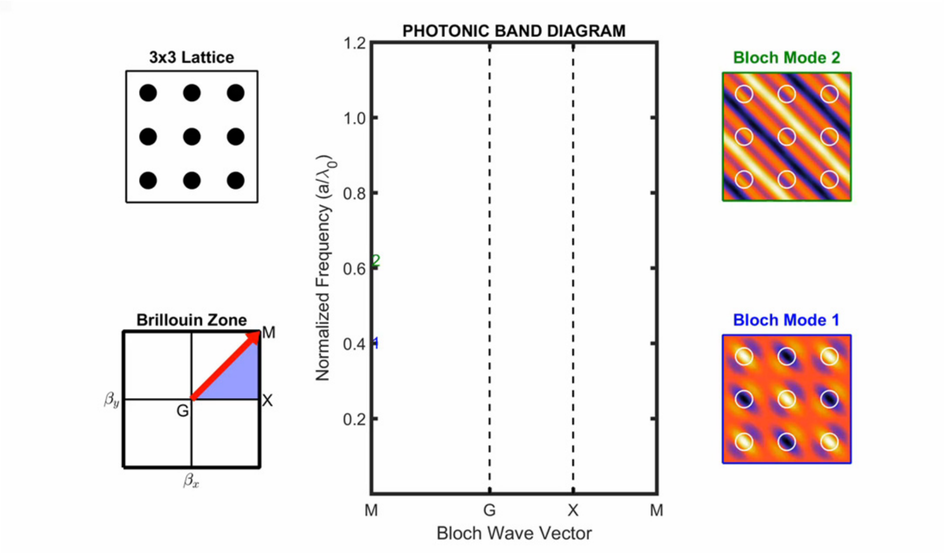




$$\vec{\beta} = \begin{array}{ccccccccccccc} \Gamma & & & & X & & & & M & & & & \Gamma \\ \end{array}$$
$$\vec{\beta} = \begin{bmatrix} 0 & 0.01 & \cdots & 3.13 & 3.14 & 3.14 & \cdots & 3.14 & 3.14 & 3.13 & \cdots & 0.01 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0.01 & \cdots & 3.13 & 3.14 & 3.13 & \cdots & 0.01 & 0 \end{bmatrix}$$

- Use more points in parts of this array that cover longer distances.
- Do not repeat adjacent points.

Animation of Band Calculation & Bloch Waves



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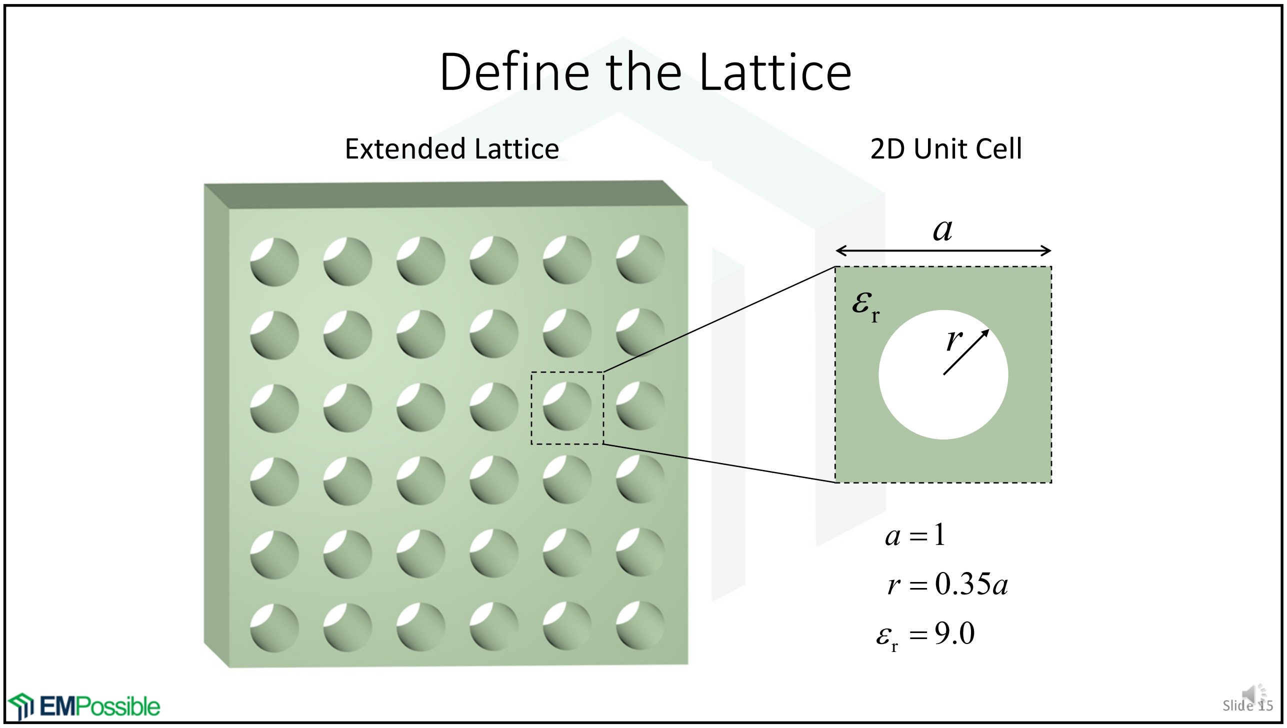
Example – Band Diagram for a 2D EBG with Square Symmetry



Define the Lattice

Extended Lattice

2D Unit Cell

$a = 1$

$r = 0.35a$

$\varepsilon_r = 9.0$

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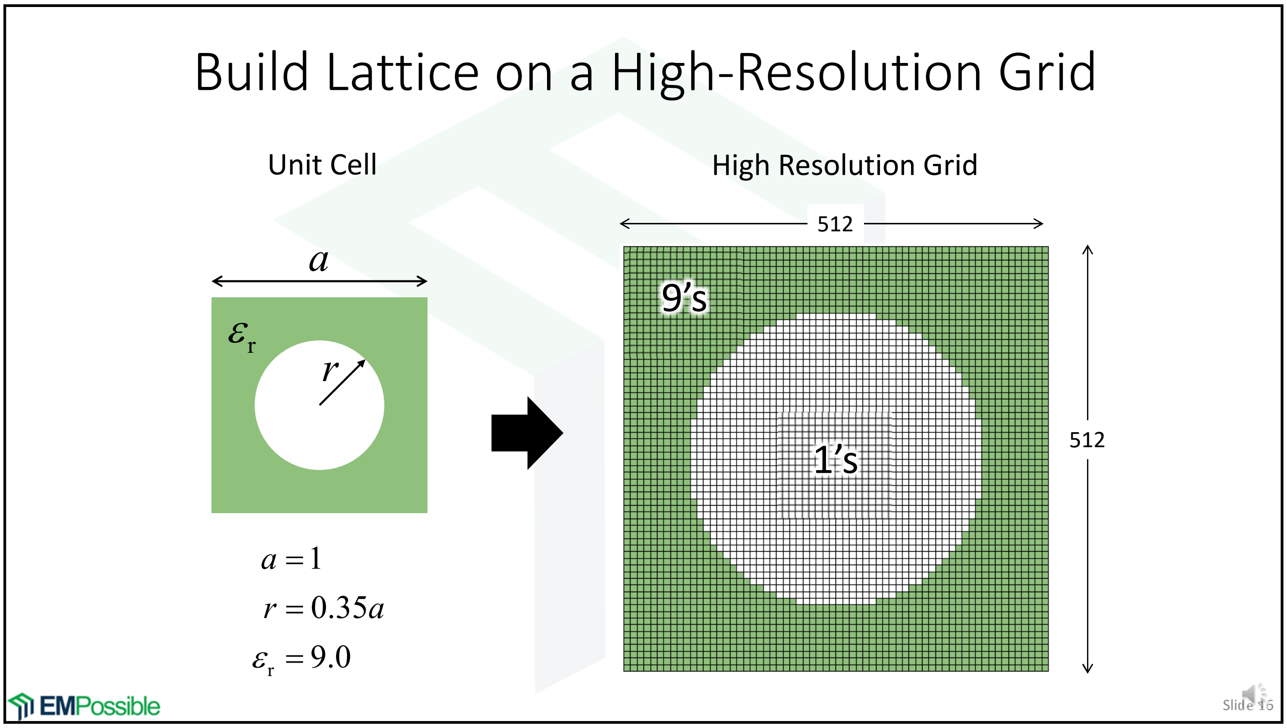

Build Lattice on a High-Resolution Grid

Unit Cell

High Resolution Grid

$a = 1$

$r = 0.35a$

$\varepsilon_r = 9.0$

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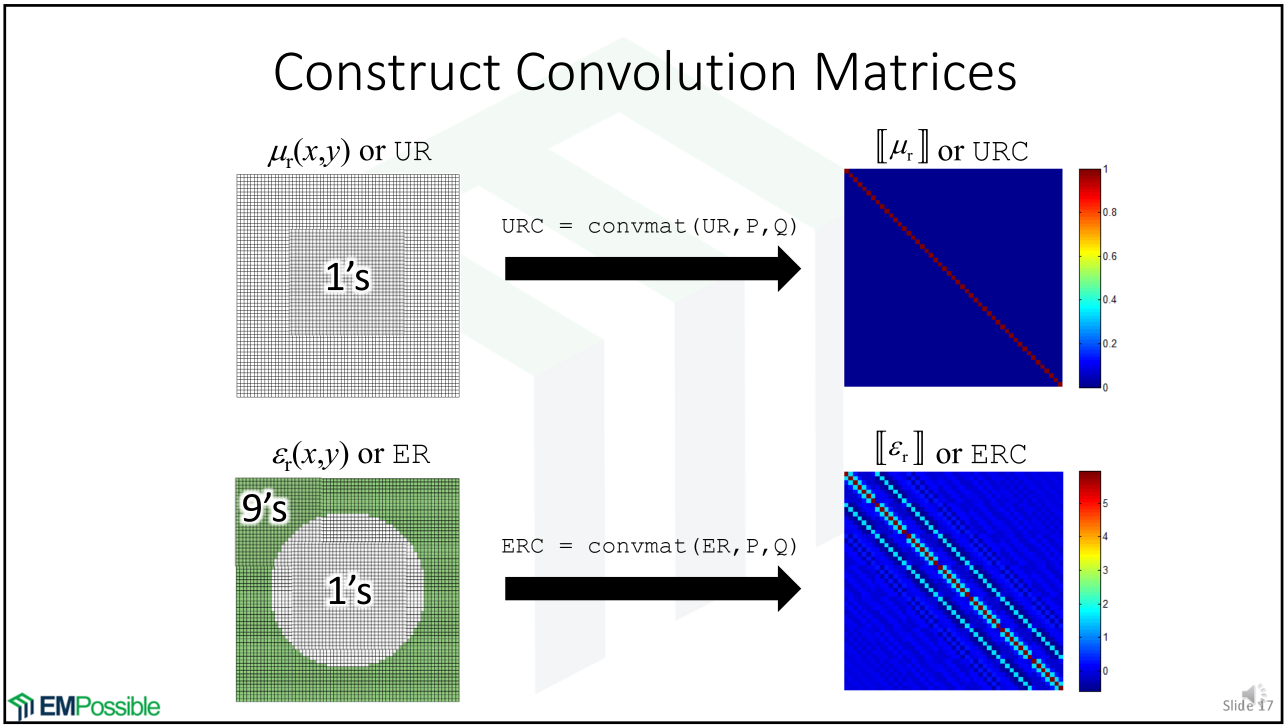

Construct Convolution Matrices

$\mu_r(x,y)$ or UR

1's

`URC = convmat(UR,P,Q)`

$[\![\mu_r]\!]$ or URC

$\varepsilon_r(x,y)$ or ER

9's

1's

`ERC = convmat(ER,P,Q)`

$[\![\varepsilon_r]\!]$ or ERC

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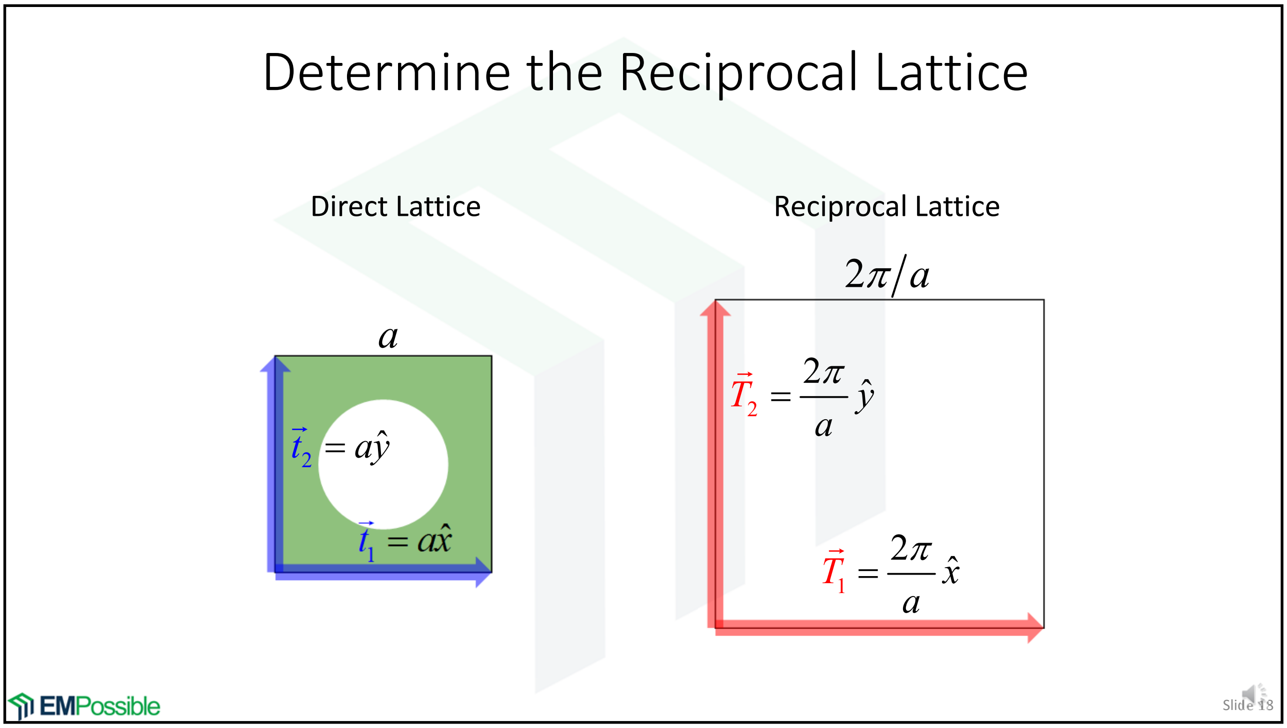

Determine the Reciprocal Lattice

Direct Lattice

Reciprocal Lattice

a

$\vec{t}_2 = a\hat{y}$

$\vec{t}_1 = a\hat{x}$

$2\pi/a$

$\vec{T}_2 = \frac{2\pi}{a}\hat{y}$

$\vec{T}_1 = \frac{2\pi}{a}\hat{x}$

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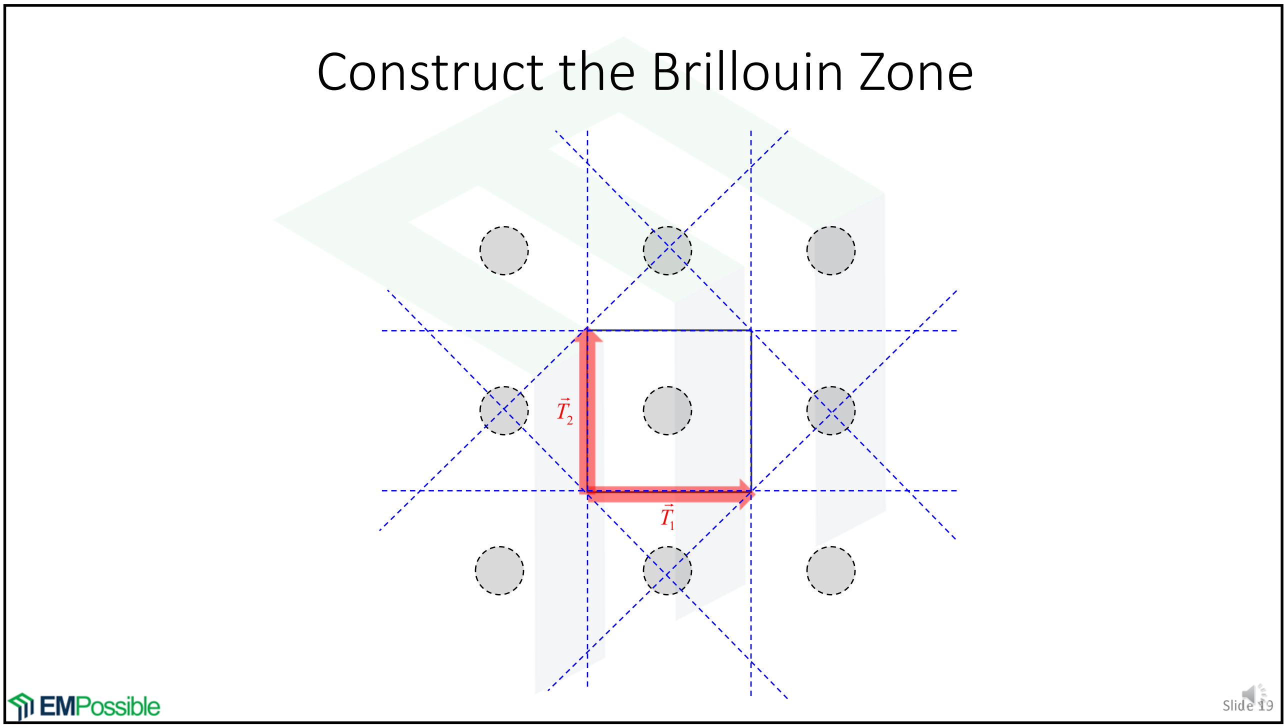
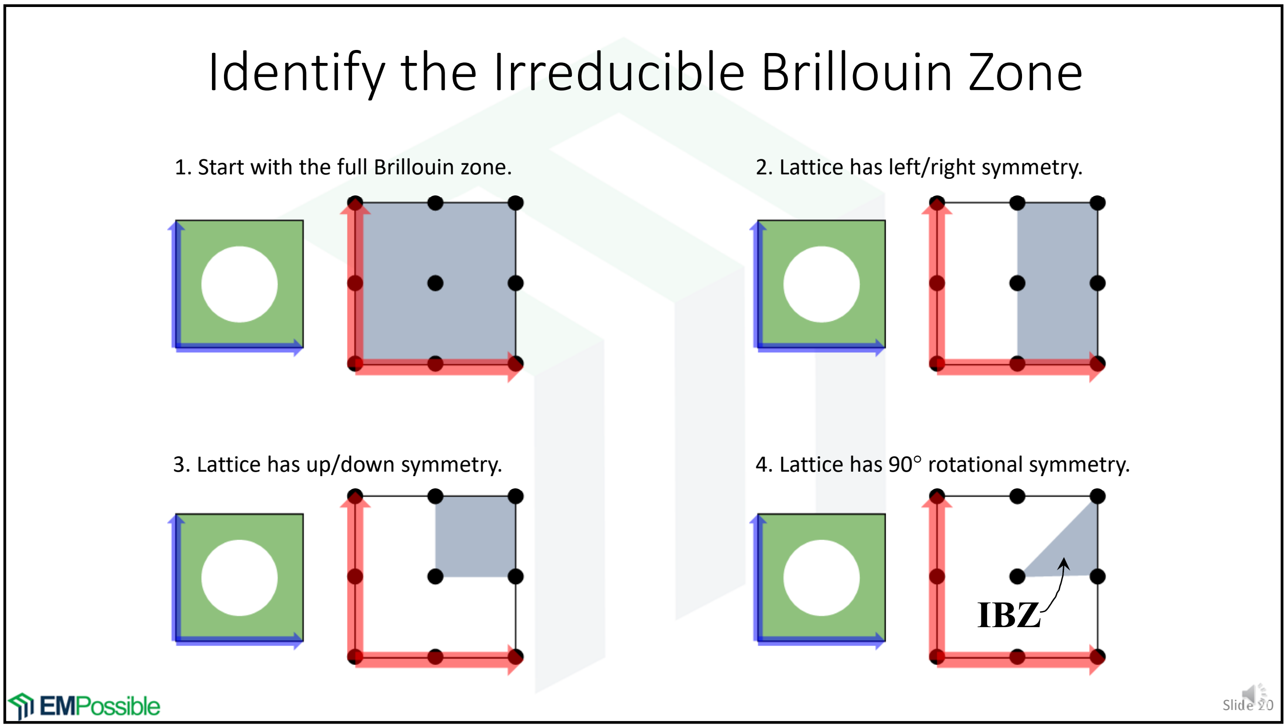


Construct the Brillouin Zone



Identify the Irreducible Brillouin Zone

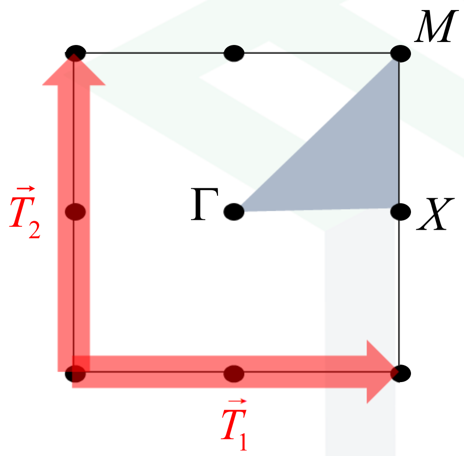
1. Start with the full Brillouin zone.

2. Lattice has left/right symmetry.

3. Lattice has up/down symmetry.

4. Lattice has 90° rotational symmetry.

Identify the Key Points of Symmetry



The key points of symmetry are calculated from a linear combination of the reciprocal lattice vectors.

$$\Gamma = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$X = 0.5\vec{T}_1$$

$$M = 0.5\vec{T}_1 + 0.5\vec{T}_2$$

Formulas for calculating the key points of symmetry along with their naming convention can be found in [M. Lax, *Symmetry Principles in Solid State and Molecular Physics*, (Dover, New York, 1974). See supplemental notes for Lecture 6 “Periodic Structures.”

The Numbers

Typically the lattice constant is normalized to the value of 1.0.

$$a = 1$$

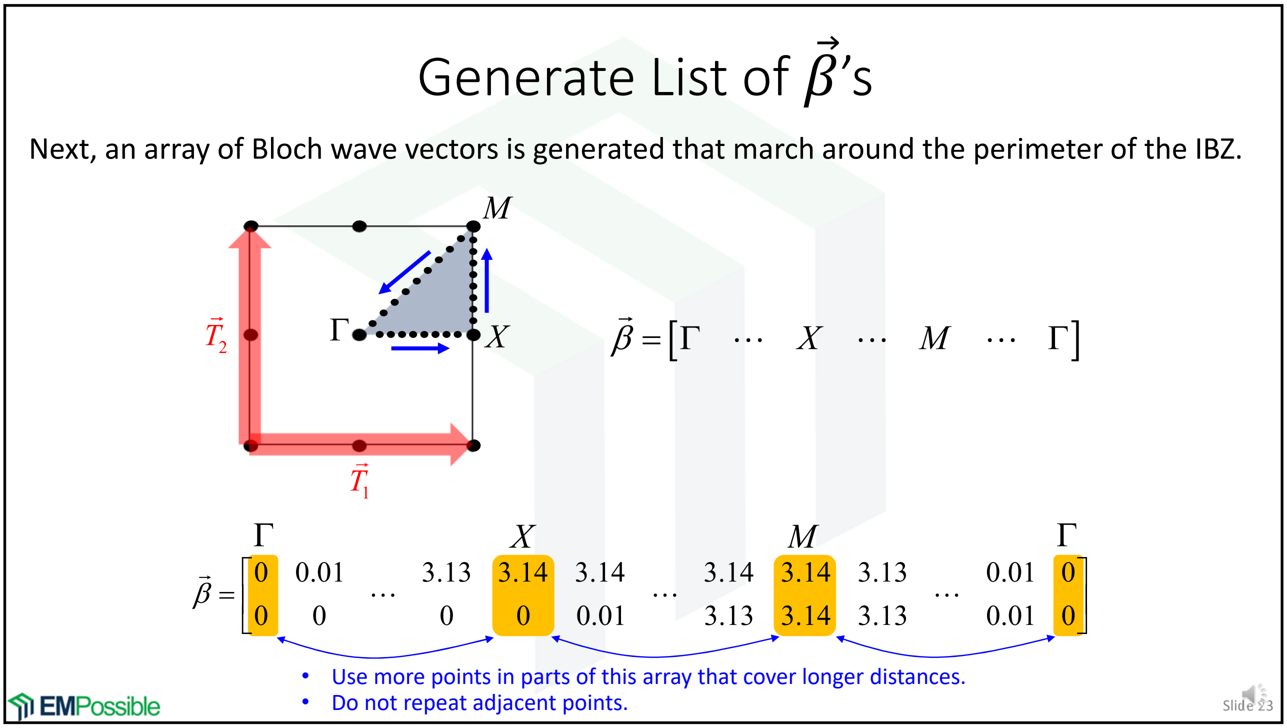
The direct and reciprocal lattice vectors are then

$$\vec{t}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \vec{T}_1 = \begin{bmatrix} 6.28 \\ 0 \end{bmatrix}$$

$$\vec{t}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \qquad \vec{T}_2 = \begin{bmatrix} 0 \\ 6.28 \end{bmatrix}$$

From these, the key points of symmetry are calculated to be

$$\Gamma = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \qquad X = \begin{bmatrix} 3.14 \\ 0 \end{bmatrix} \qquad M = \begin{bmatrix} 3.14 \\ 3.14 \end{bmatrix}$$



Generate List of $\vec{\beta}$'s

Next, an array of Bloch wave vectors is generated that march around the perimeter of the IBZ.

$$\vec{\beta} = [\Gamma \;\; \cdots \;\; X \;\; \cdots \;\; M \;\; \cdots \;\; \Gamma]$$

$$\vec{\beta} = \begin{array}{c}\\ \\ \end{array}\begin{array}{ccccccccccccc} \Gamma & & & & X & & & & M & & & & \Gamma \\ 0 & 0.01 & \cdots & 3.13 & 3.14 & 3.14 & \cdots & 3.14 & 3.14 & 3.13 & \cdots & 0.01 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0.01 & \cdots & 3.13 & 3.14 & 3.13 & \cdots & 0.01 & 0 \end{array}$$

- Use more points in parts of this array that cover longer distances.
- Do not repeat adjacent points.

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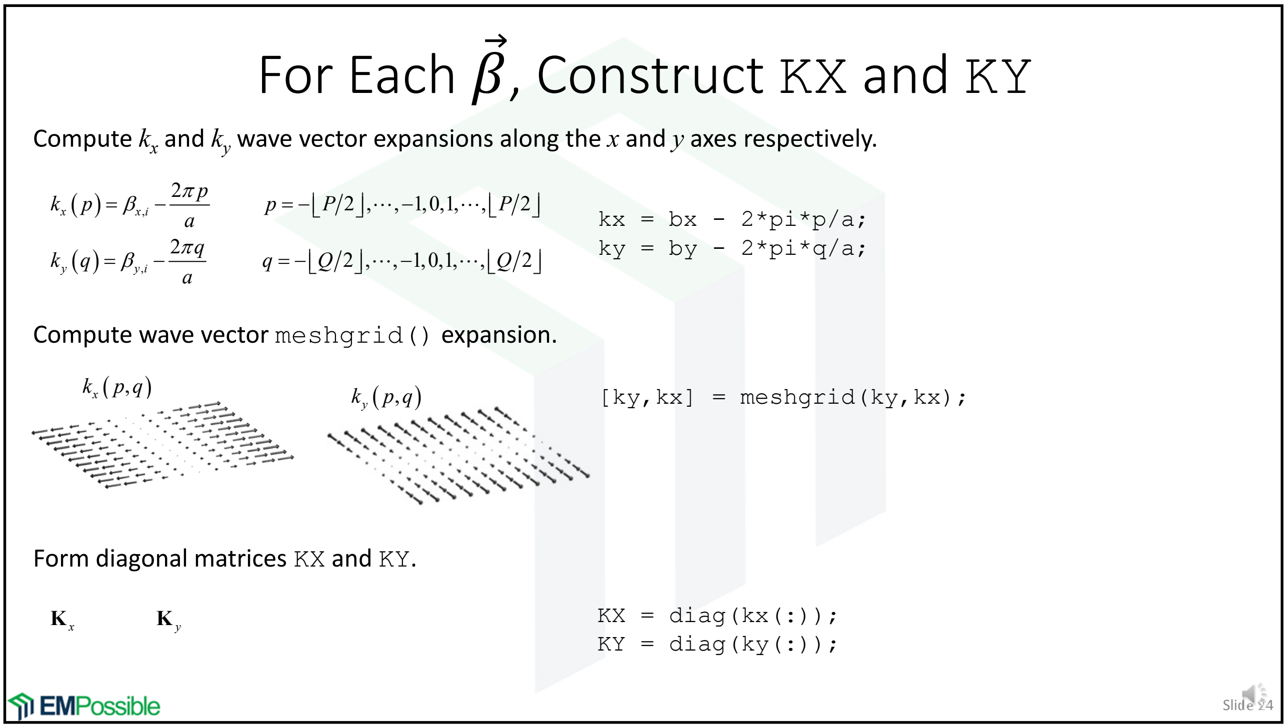

For Each $\vec{\beta}$, Construct KX and KY

Compute k_x and k_y wave vector expansions along the x and y axes respectively.

$$k_x(p) = \beta_{x,i} - \frac{2\pi p}{a} \qquad p = -\lfloor P/2 \rfloor, \cdots, -1, 0, 1, \cdots, \lfloor P/2 \rfloor$$

$$k_y(q) = \beta_{y,i} - \frac{2\pi q}{a} \qquad q = -\lfloor Q/2 \rfloor, \cdots, -1, 0, 1, \cdots, \lfloor Q/2 \rfloor$$

```
kx = bx - 2*pi*p/a;
ky = by - 2*pi*q/a;
```

Compute wave vector `meshgrid()` expansion.

```
[ky,kx] = meshgrid(ky,kx);
```

Form diagonal matrices KX and KY.

$\mathbf{K}_x \qquad \mathbf{K}_y$

```
KX = diag(kx(:));
KY = diag(ky(:));
```

EMPossible

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Solve Eigen-Value Problem for Each β

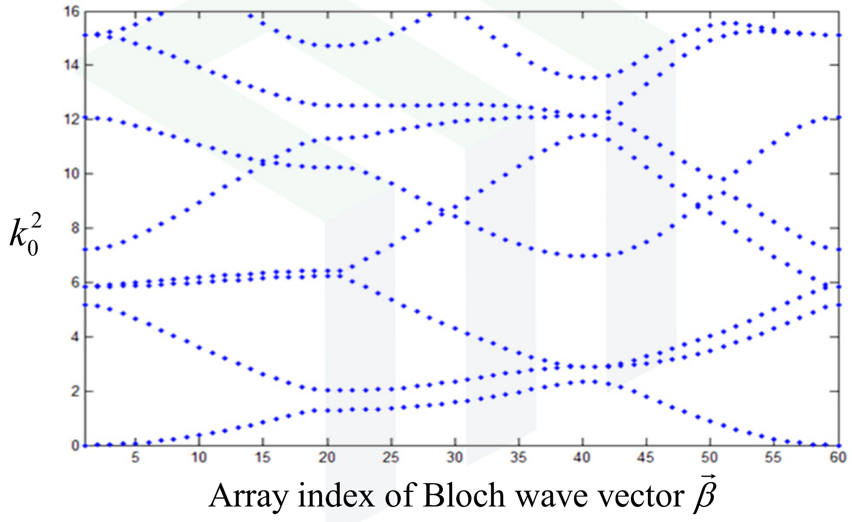
The eigen-values calculated from this problem are:

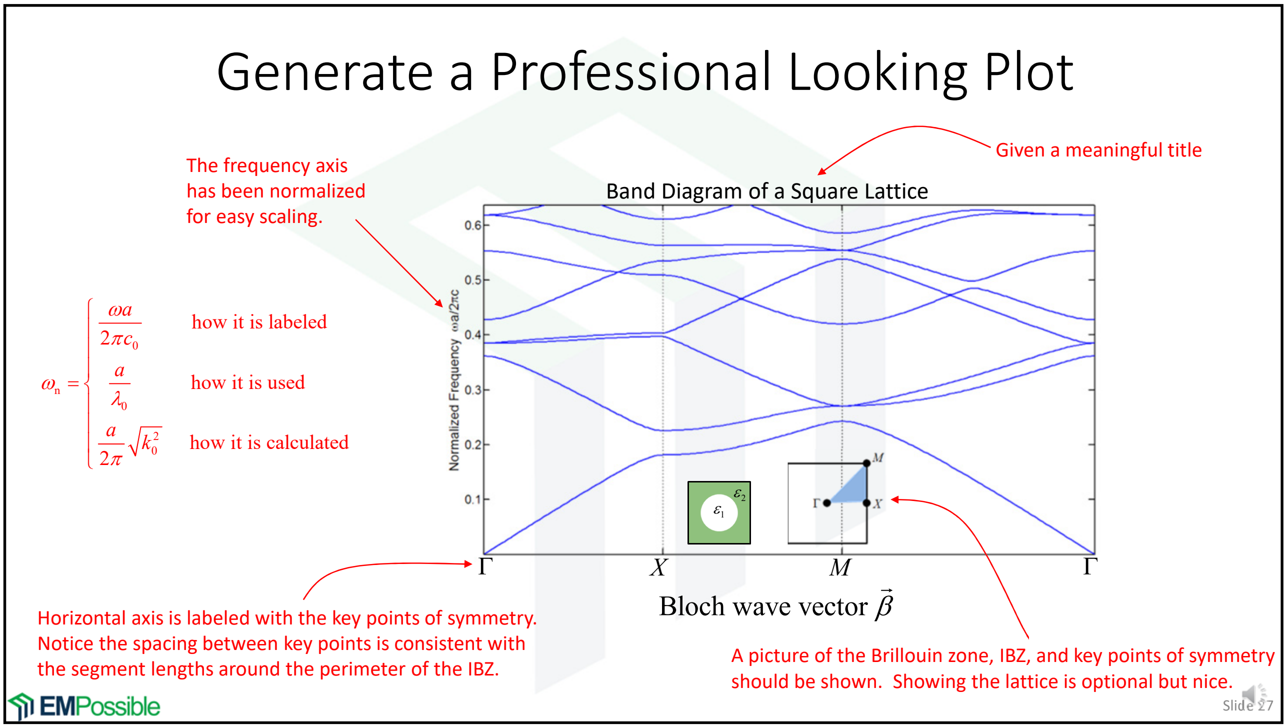
	15.09	15.09		14.72	14.72	14.72		13.53	13.53	13.53		15.09	15.09
	15.09	15.09		12.52	12.52	12.52		12.11	12.11	12.11		15.09	15.09
	12.07	12.07		11.28	11.28	11.28		12.11	12.11	12.11		12.07	12.07
$k_0^2 \rightarrow$	7.22	7.22	$\cdots$	10.22	10.22	10.22	$\cdots$	11.42	11.42	11.42	$\cdots$	7.22	7.22
	5.84	5.84		6.42	6.42	6.42		6.96	6.96	6.96		5.84	5.84
	5.84	5.84		6.22	6.22	6.22		2.89	2.89	2.89		5.84	5.84
	5.16	5.16		2.01	2.01	2.01		2.89	2.89	2.89		5.16	5.16
	0.00	0.00		1.30	1.30	1.30		2.32	2.32	2.32		0.00	0.00

$$\vec{\beta} = \begin{bmatrix} 0.00 & 0.01 & \cdots & 3.13 & 3.14 & 3.14 & \cdots & 3.14 & 3.14 & 3.13 & \cdots & 0.01 & 0.00 \\ 0.00 & 0.00 & \cdots & 0.00 & 0.00 & 0.01 & \cdots & 3.13 & 3.14 & 3.13 & \cdots & 0.01 & 0.00 \end{bmatrix}$$

Γ X M Γ

Plot Eigen-Values Vs. β





Generate a Professional Looking Plot

Given a meaningful title

The frequency axis has been normalized for easy scaling.

$$\omega_n = \begin{cases} \dfrac{\omega a}{2\pi c_0} & \text{how it is labeled} \\ \dfrac{a}{\lambda_0} & \text{how it is used} \\ \dfrac{a}{2\pi}\sqrt{k_0^2} & \text{how it is calculated} \end{cases}$$

Horizontal axis is labeled with the key points of symmetry. Notice the spacing between key points is consistent with the segment lengths around the perimeter of the IBZ.

A picture of the Brillouin zone, IBZ, and key points of symmetry should be shown. Showing the lattice is optional but nice.