



Computational Science:
Introduction to Finite-Difference Time-Domain

Gratings & the Plane Wave Spectrum

1

Lecture Outline

- Review
- Wave vectors
- Phase matching at an interface
- Electromagnetic behavior at an interface
- Diffraction from gratings
- The plane wave spectrum

2

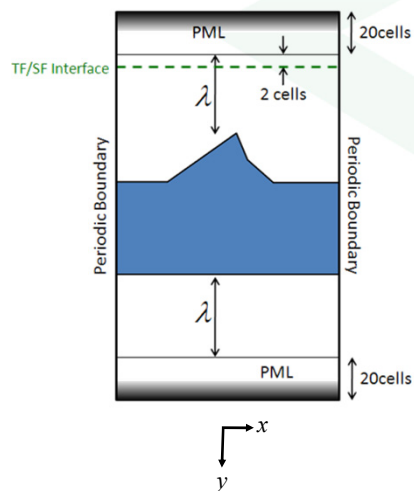
Review

Slide 3

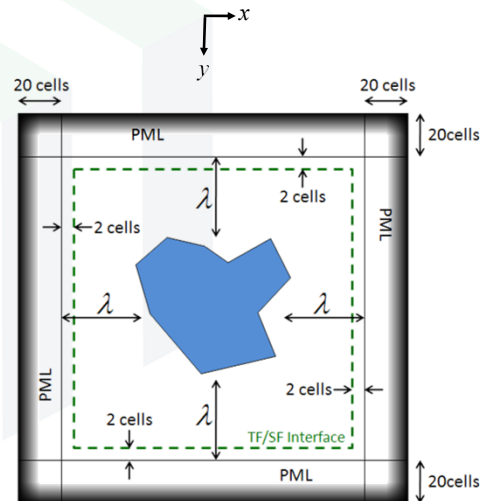
3

Typical 2D FDTD Grid Layouts

For periodic structures



For generalized scattering problems

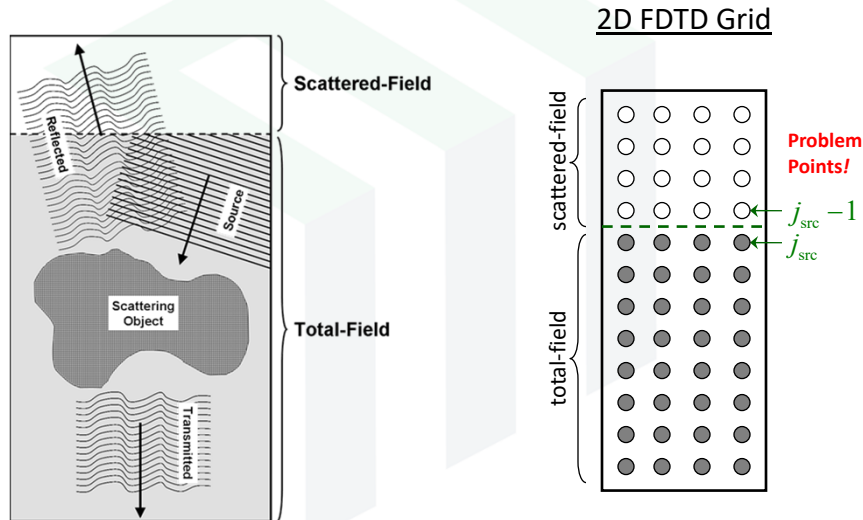


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The Total-Field/Scattered-Field Framework



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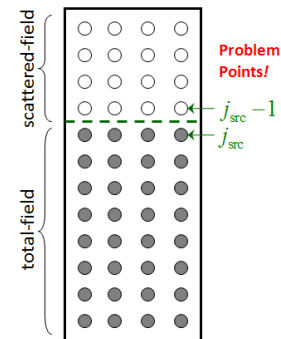
Corrections to Finite-Difference Equations at the Problem Cells (E_z Mode)

On the scattered-field side of the TF/SF interface, the curl equation contains a term from the total-field side. The source must be subtracted from this term to make it look like a scattered-field quantity.

$$C_x^E \Big|_t^{i,j_{src}-1} = \underbrace{\frac{\tilde{E}_z \Big|_t^{i,j_{src}} - \tilde{E}_z \Big|_t^{i,j_{src}-1}}{\Delta y}}_{\text{standard curl equation}} - \frac{1}{\Delta y} E_z^{src} \Big|_t^{i,j_{src}}$$

On the total-field side of the TF/SF interface, the curl equation contains a term from the scattered-field side. The source must be added to this term to make it look like a total-field quantity.

$$C_z^H \Big|_{t+\frac{\Delta t}{2}}^{i,j_{src}} = \underbrace{\frac{H_y \Big|_{t+\frac{\Delta t}{2}}^{i,j_{src}} - H_y \Big|_{t+\frac{\Delta t}{2}}^{i-1,j_{src}}}{\Delta x} - \frac{H_x \Big|_{t+\frac{\Delta t}{2}}^{i,j_{src}} - H_x \Big|_{t+\frac{\Delta t}{2}}^{i,j_{src}-1}}{\Delta y}}_{\text{standard update equation}} + \frac{1}{\Delta y} \tilde{H}_x^{src} \Big|_{t+\frac{\Delta t}{2}}^{i,j_{src}-1}$$



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Calculation of the Source Functions (E_z Mode)

Calculate the electric field as

$$E_z^{\text{src}} \Big|_t^{i,j_{\text{src}}} = g(t)$$

Calculate the magnetic field as

$$\tilde{H}_x^{\text{src}} \Big|_{t+\frac{\Delta t}{2}}^{i,j_{\text{src}}-1} = \sqrt{\frac{\epsilon_{r,\text{src}}}{\mu_{r,\text{src}}}} g \left(t + \frac{n_{\text{src}} \Delta y}{2c_0} + \frac{\Delta t}{2} \right)$$

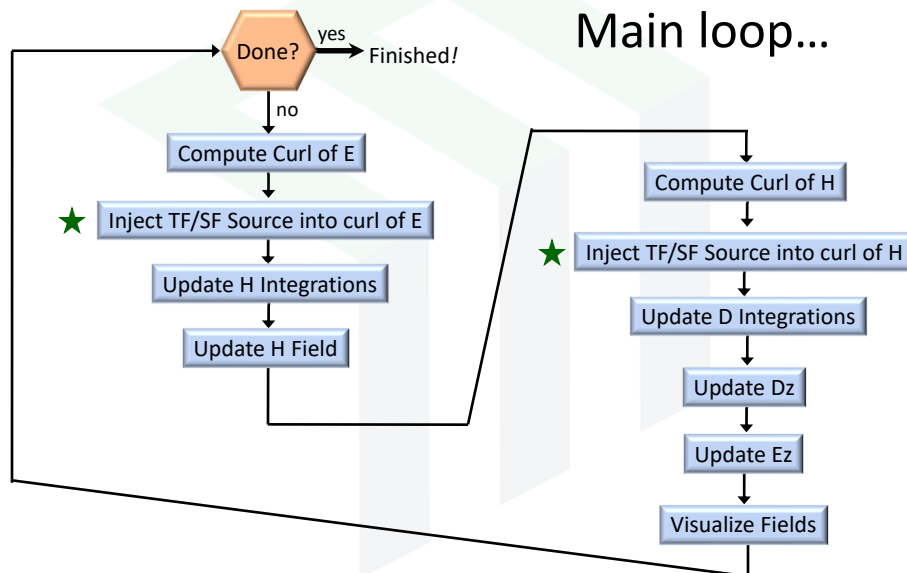
Amplitude due to
Maxwell's equations

Delay through one
half of a grid cell

Half time step
difference

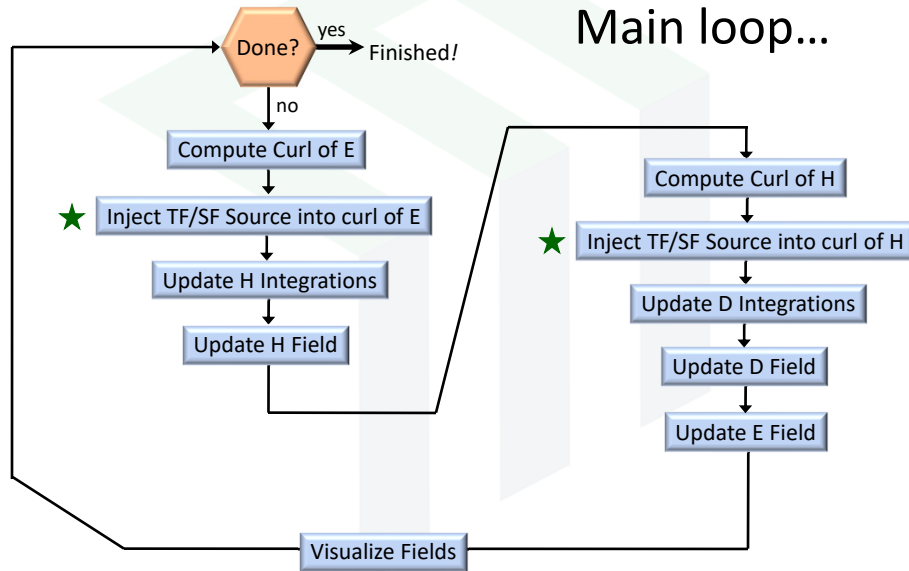
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TF/SF Block Diagram for E_z Mode Main loop...



8

TF/SF Block Diagram for H_z Mode Main loop...



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Wave Vectors

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Wave Vector \vec{k}

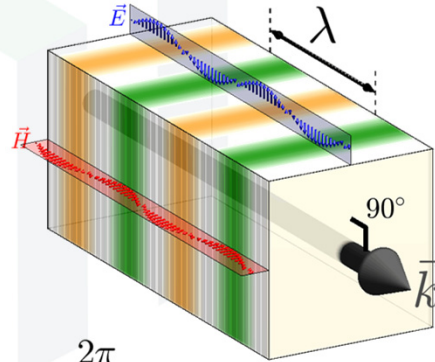
The wave vector \vec{k} conveys two pieces of information: (1) Magnitude conveys the wavelength λ inside the medium, and (2) direction conveys the direction of the wave and is perpendicular to the wave fronts.

$$E(\vec{r}) = E_0 \exp(-j\vec{k} \cdot \vec{r})$$

$$\vec{k} = k_x \hat{a}_x + k_y \hat{a}_y + k_z \hat{a}_z$$

$$\vec{r} = x\hat{x} + y\hat{y} + z\hat{z} \quad \text{position vector}$$

$$|\vec{k}| = \frac{2\pi}{\lambda}$$



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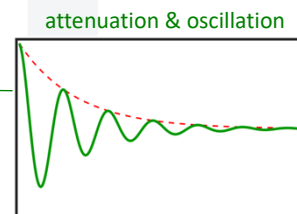
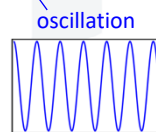
The Complex Wave Number \tilde{k}

A wave travelling in the $+z$ direction can be written in terms of the complex wave number \tilde{k} as

$$\vec{E}(z) = \vec{P}e^{-jkz} \quad k = k' - jk''$$

Substituting $\tilde{k} = k' + jk''$ into the wave solution gives

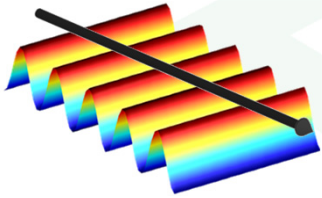
$$\vec{E}(z) = \vec{P}e^{-j(k' - jk'')z} = \vec{P}e^{-k''z} e^{-jk'z}$$



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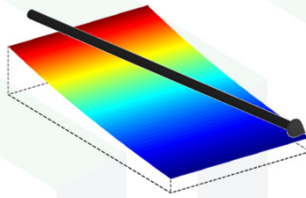
1D Waves with Complex Wave Number \tilde{k}

Purely Real k



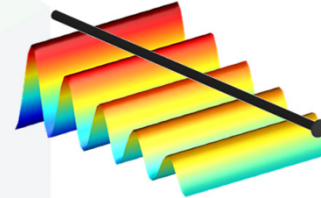
- Uniform amplitude
- Oscillations move power
- Considered to be a propagating wave

Purely Imaginary k



- Decaying amplitude
- No oscillations, no flow of power
- Considered to be evanescent

Complex k

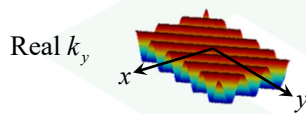


- Decaying amplitude
- Oscillations move power
- Considered to be a propagating wave (not evanescent)

This implies that these are the only 2.5 configurations that electromagnetic fields can take on.

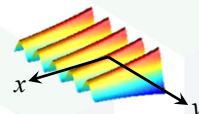
2D Waves with Complex Wave Vector $\vec{\tilde{k}}$

Real k_x

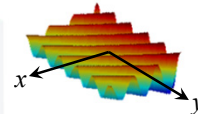


Real k_y

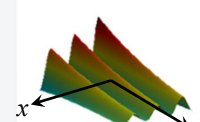
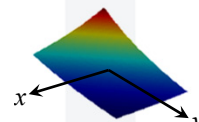
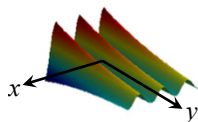
Imaginary k_x



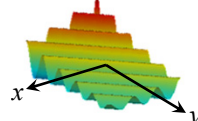
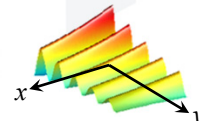
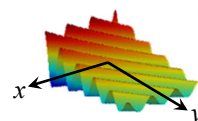
Complex k_x



Imaginary k_y



Complex k_y



Phase Matching at an Interface

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Dispersion Relation and Index Ellipsoids

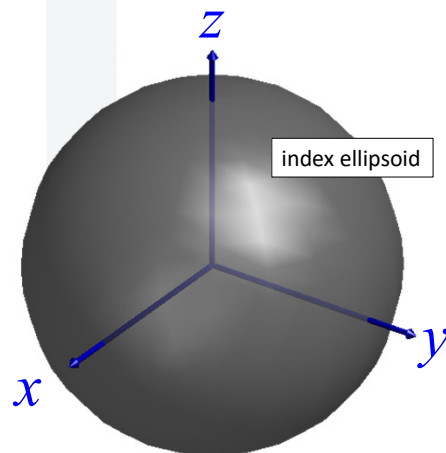
The dispersion relation for a material relates the wave vector to frequency. Essentially, it tells us the refractive index as a function of direction through the material.

For isotropic materials, this is

$$k_x^2 + k_y^2 + k_z^2 = (k_0 n)^2$$

The dispersion relation defines a surface called an “index ellipsoid.” The vector connecting the origin to a point on the sphere is the k -vector for that direction from which refractive index can be calculated.

This surface is a sphere for isotropic materials.



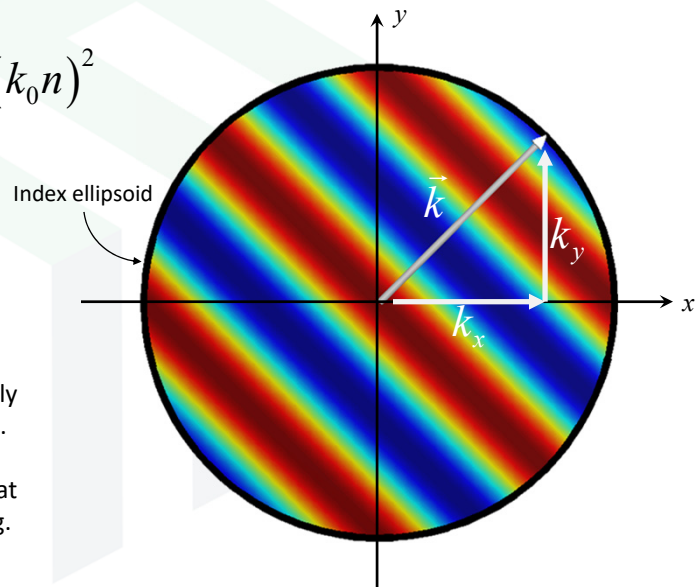
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Geometrical Interpretation of the Dispersion Relation

$$k_x^2 + k_y^2 = |\vec{k}|^2 = (k_0 n)^2$$

The dispersion relation for isotropic materials is essentially just the Pythagorean theorem. It says a wave sees the same refractive index no matter what direction the wave is travelling.

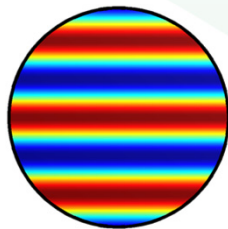


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Index Ellipsoid in Two Different Materials

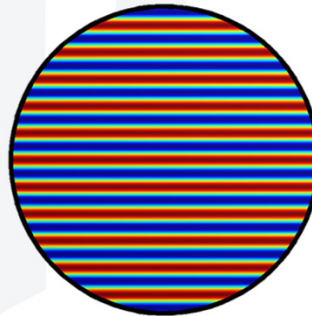
Material 1 (Low n)

$$k_{x,1}^2 + k_{y,1}^2 = |\vec{k}_1|^2 = (k_0 n_1)^2$$



Material 2 (High n)

$$k_{x,2}^2 + k_{y,2}^2 = |\vec{k}_2|^2 = (k_0 n_2)^2$$



$$n_1 < n_2$$

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Phase Matching at the Interface Between Two Materials Where $n_1 < n_2$

$n_1 < n_2$

Material 1

$$k_{x,1}^2 + k_{y,1}^2 = |\vec{k}_1|^2 = (k_0 n_1)^2$$

Material 2

$$k_{x,2}^2 + k_{y,2}^2 = |\vec{k}_2|^2 = (k_0 n_2)^2$$

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Summary of the Phase Matching Trend for $n_1 < n_2$

$n_1 < n_2$

Material 1

$$k_{x,1}^2 + k_{y,1}^2 = |\vec{k}_1|^2 = (k_0 n_1)^2$$

Material 2

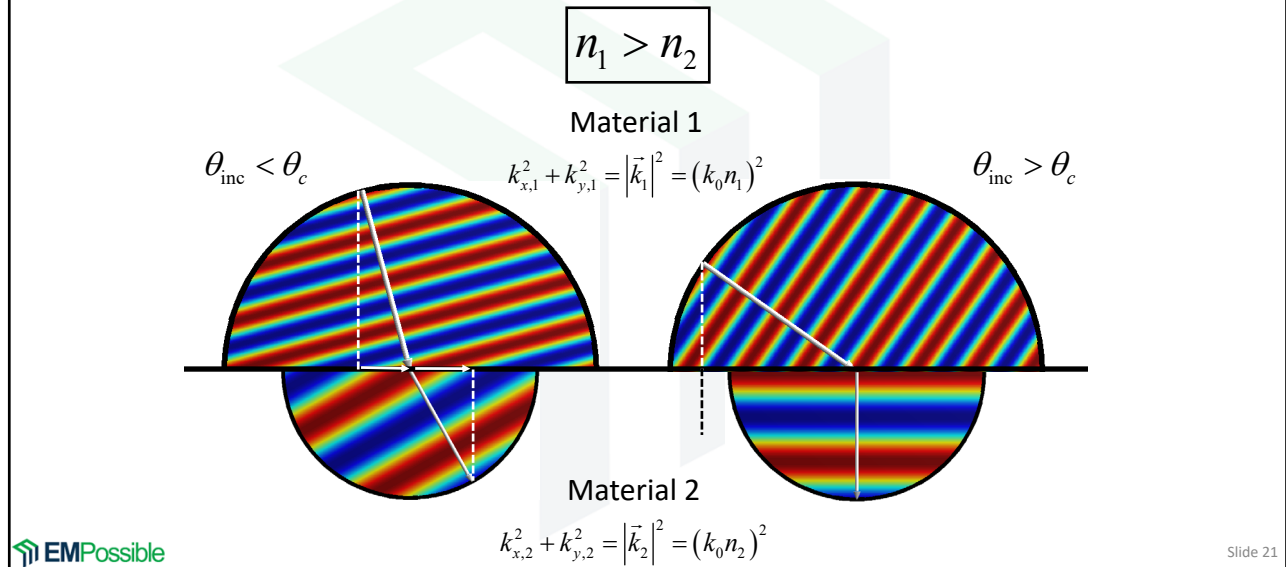
$$k_{x,2}^2 + k_{y,2}^2 = |\vec{k}_2|^2 = (k_0 n_2)^2$$

Properly phased matched at the interface.

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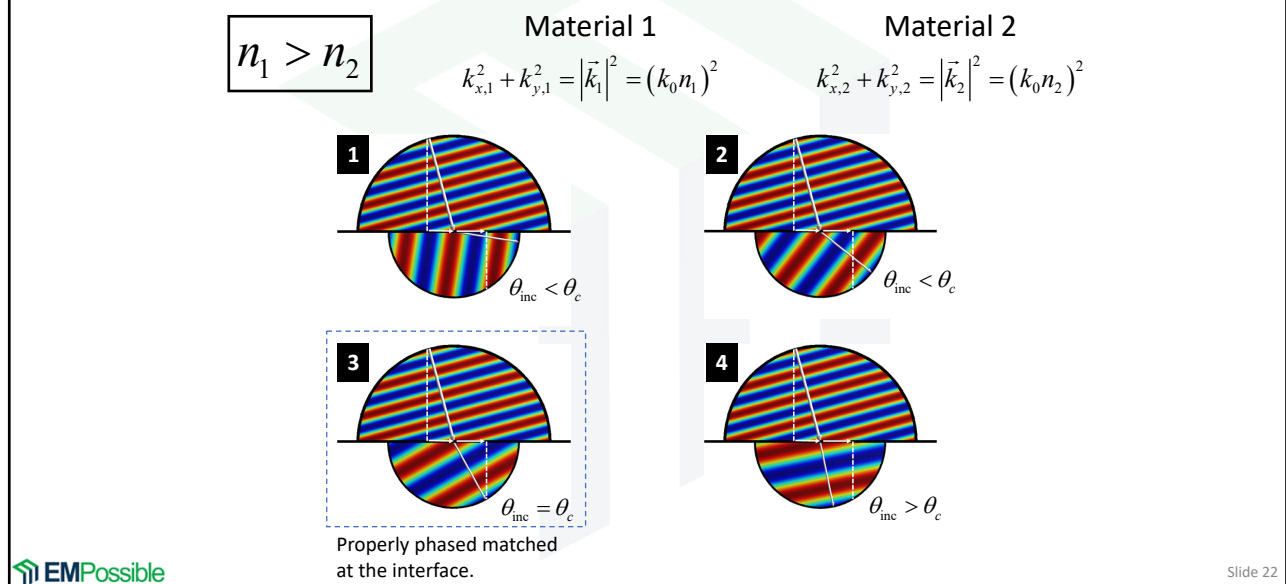
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Phase Matching at the Interface Between Two Materials Where $n_1 > n_2$



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Summary of the Phase Matching Trend for $n_1 > n_2$



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Electromagnetic Behavior at an Interface

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Longitudinal Component of the Wave Vector

1. Boundary conditions require that the tangential component of the wave vector is continuous across the interface.

Assuming k_x is purely real in material 1, k_x will be purely real in material 2.

→ We have oscillations and energy flow in the x direction.

2. Knowing that the dispersion relation must be satisfied, the longitudinal component of the wave vector in material 2 is calculated from the dispersion relation in material 2.

$$k_{x,2}^2 + k_{y,2}^2 = (k_0 n_2)^2$$

$$\downarrow$$

$$k_{y,2} = \sqrt{(k_0 n_2)^2 - k_{x,2}^2}$$

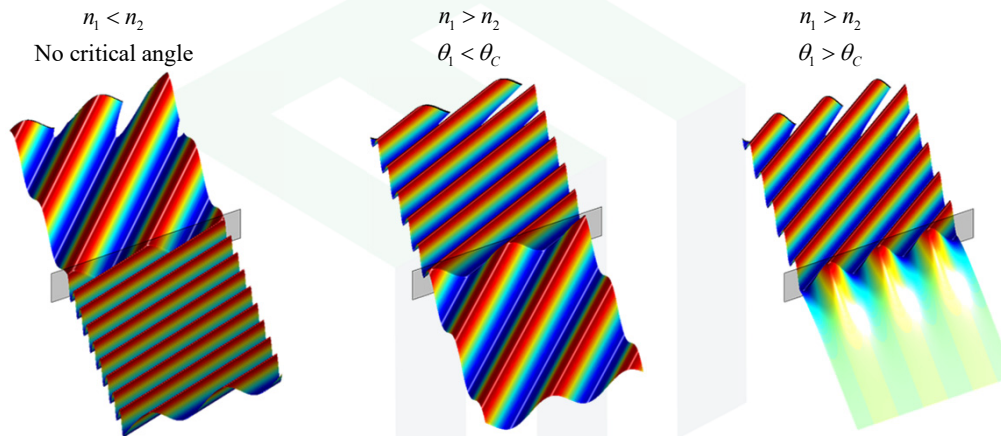
We see that k_y will be purely real if $k_0 n_2 > |k_{x,2}|$.

We see that k_y will be purely imaginary if $k_0 n_2 < |k_{y,z}|$.

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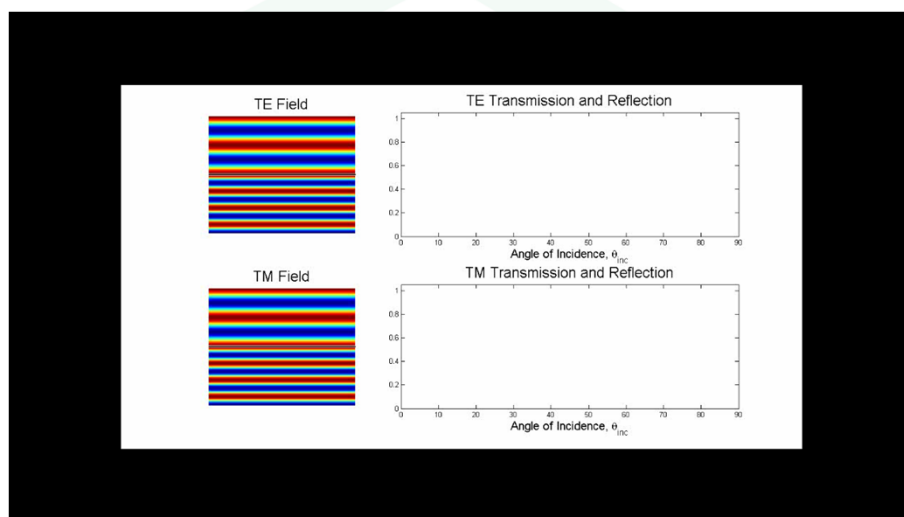
Field at an Interface Above and Below the Critical Angle (Ignoring Reflections)



1. The field always penetrates material 2, but it may not propagate.
2. Above the critical angle, penetration is greatest near the critical angle.
3. Very high spatial frequencies are supported in material 2 despite the dispersion relation.
4. In material 2, energy always flows along x , but not necessarily along y .

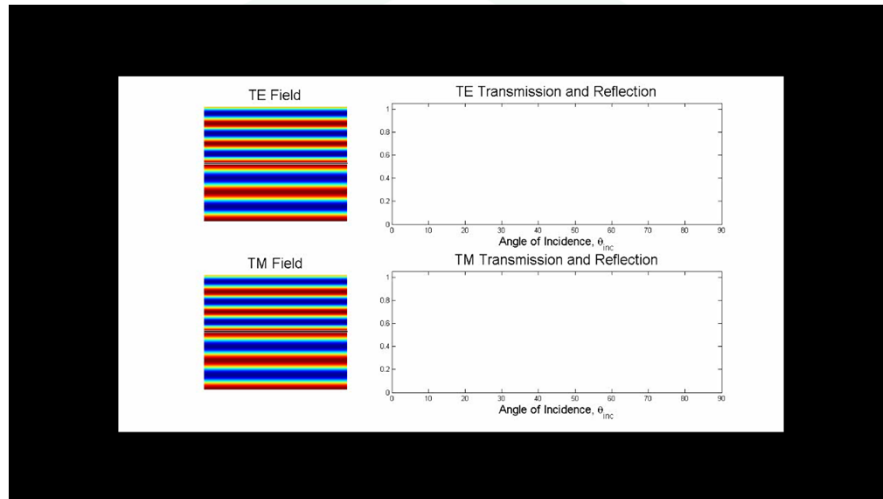
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Simulation of Reflection and Transmission at a Single Interface ($n_1 < n_2$)



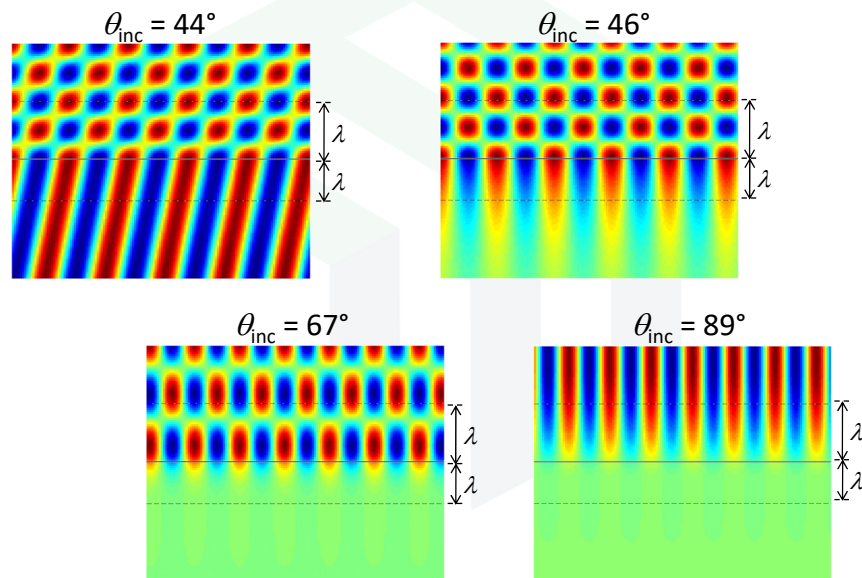
$$n_1=1.0, n_2=1.73 \rightarrow \theta_B=60^\circ$$

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Simulation of Reflection and Transmission at a Single Interface ($n_1 > n_2$)

$$n_1=1.41, n_2=1.0 \rightarrow \theta_c=45^\circ$$

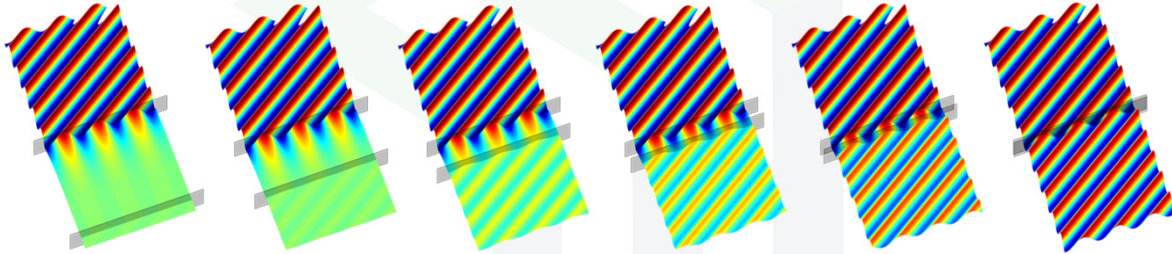
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Field Visualization for $\theta_c=45^\circ$ 

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Electromagnetic Tunneling

If an evanescent field touches a medium with higher refractive index, the field may no longer be cutoff and become a propagating wave.

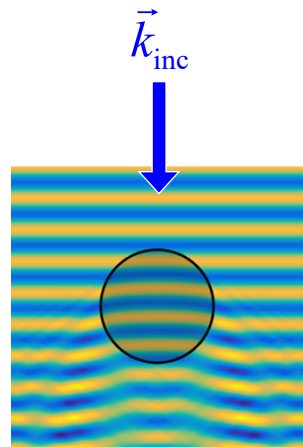


This is a very unusual phenomenon because the evanescent field is contributing to power flow.

This is called electromagnetic tunneling and is analogous to electron tunneling through thin insulators.

Diffraction From Gratings

Fields are Perturbed by Objects



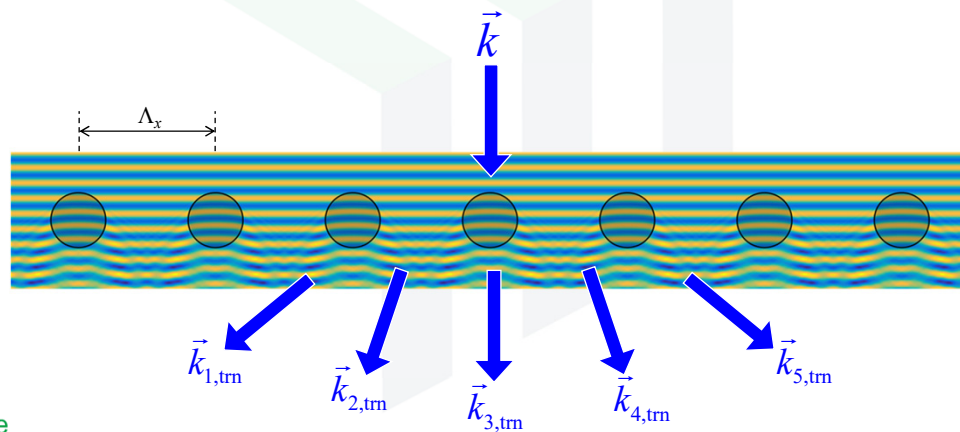
A portion of the wave front is delayed after travelling through the dielectric object.

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Fields in Periodic Structures

Waves in periodic structures take on the same periodicity as their host.



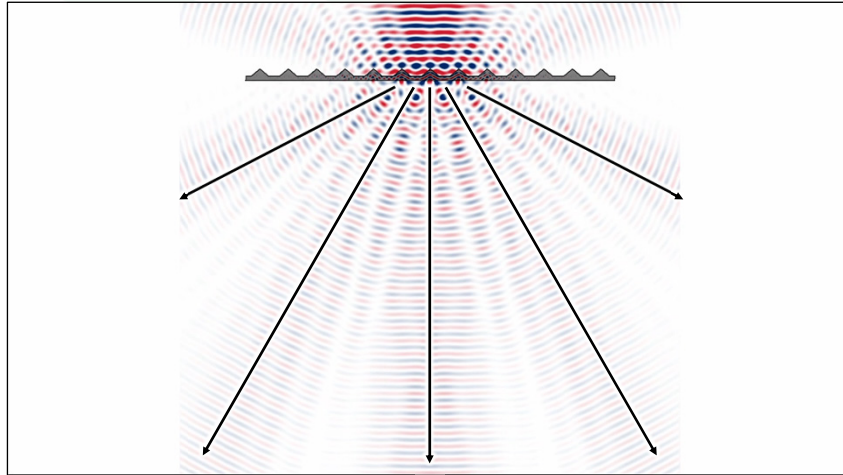
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Diffraction from Gratings

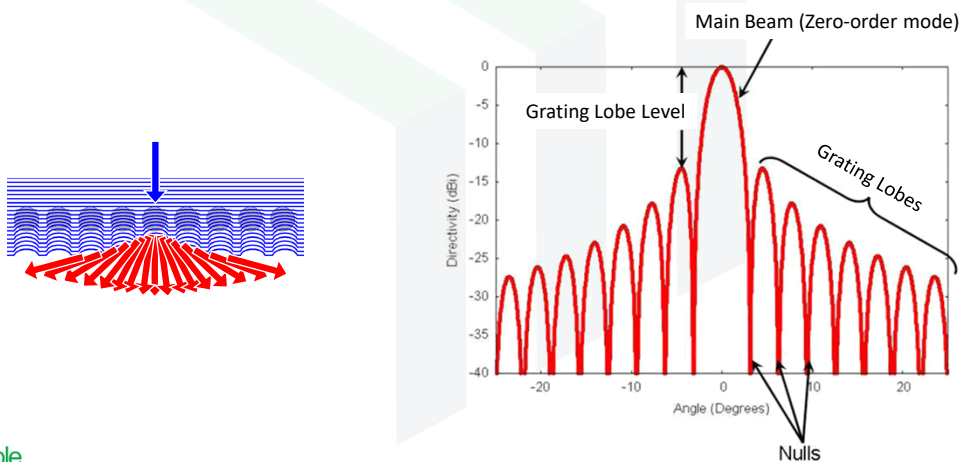
The field is no longer a pure plane wave. The grating “chops” the wave front and sends the power into multiple discrete directions that are called *diffraction orders*.



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Grating Lobes

If we were to plot the power exiting a periodic structure as a function of angle, we would get the following. The power peaks are called *grating lobes* or sometimes *side lobes*. The power minimums are called *nulls*.

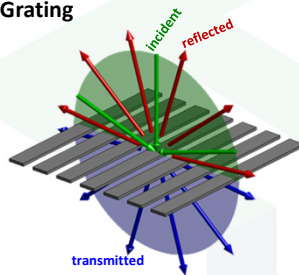


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Diffraction Configurations

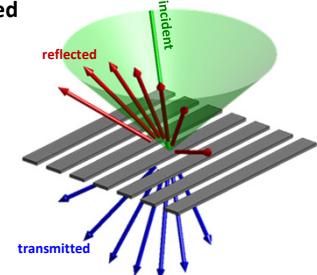
Planar Diffraction from a Ruled Grating

- Diffraction is confined within a plane
- Numerically much simpler than other cases
- E and H modes are independent



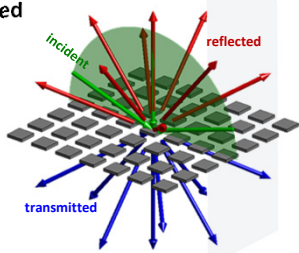
Conical Diffraction from a Ruled Grating

- Diffraction is no longer confined to a plane
- Almost same analytical complexity as crossed grating case, but simpler numerically
- E and H modes are coupled



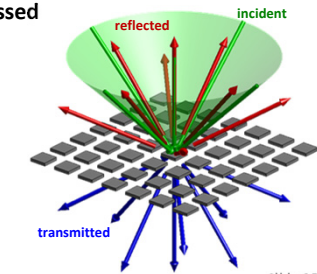
Conical Diffraction from a Crossed Grating with Planar Incidence

- Diffraction occurs in all directions
- Almost same numerical complexity as next case
- E and H modes are coupled



Conical Diffraction from a Crossed Grating

- Diffraction occurs in all directions
- Most complicated case numerically
- E and H modes are coupled
- Essentially the same as previous case



Grating Equation for Planar Diffraction

The angles of the diffracted modes are related to the wavelength and grating period through the grating equation.

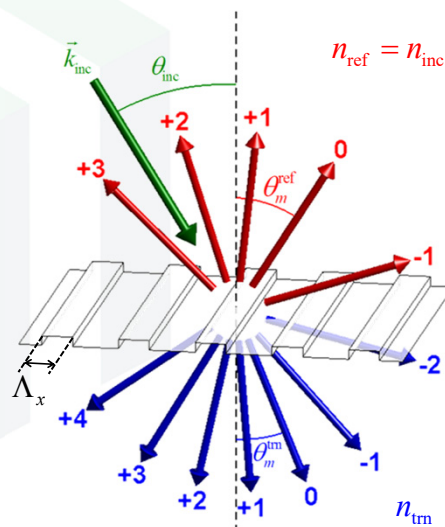
The grating equation only predicts the directions of the modes, not how much power is in them.

Reflection Region

$$n_{\text{ref}} \sin \theta_m = n_{\text{inc}} \sin \theta_{\text{inc}} - m \frac{\lambda_0}{\Lambda_x}$$

Transmission Region

$$n_{\text{tm}} \sin \theta_m = n_{\text{inc}} \sin \theta_{\text{inc}} - m \frac{\lambda_0}{\Lambda_x}$$



Effect of Grating Periodicity

Subwavelength Grating

$\Lambda_x < \frac{\lambda_0}{n_{avg}}$

"Subwavelength" Grating

$\frac{\lambda_0}{n_{avg}} < \Lambda_x < \frac{\lambda_0}{n_{inc}}$

Low Order Grating

$\Lambda_x > \frac{\lambda_0}{n_{inc}}$

High Order Grating

$\Lambda_x \gg \frac{\lambda_0}{n_{inc}}$

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Animation of Grating Diffraction (1 of 3)

$n_1 = 1.0$

$n_2 = 2.0$

$\frac{\Lambda}{\lambda_1} = 0.30$

$\frac{\Lambda}{\lambda_2} = 0.60$

$\lambda_1 = \frac{\lambda_0}{n_1}$

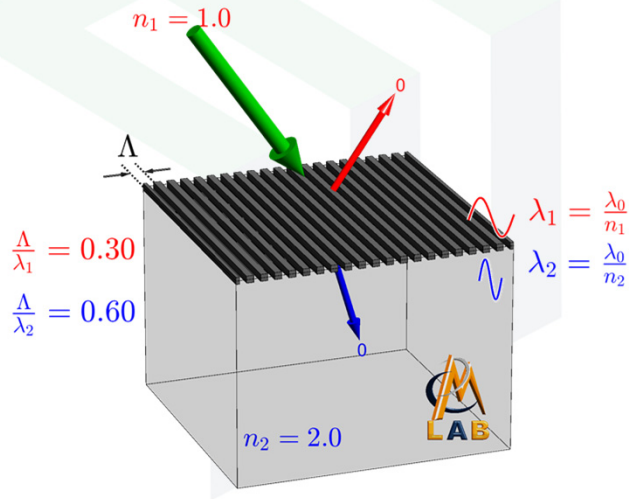
$\lambda_2 = \frac{\lambda_0}{n_2}$

LAB

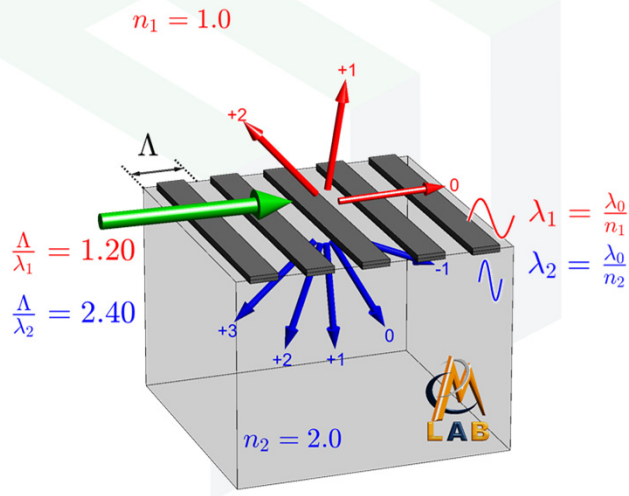
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Animation of Grating Diffraction (2 of 3)



Animation of Grating Diffraction (3 of 3)

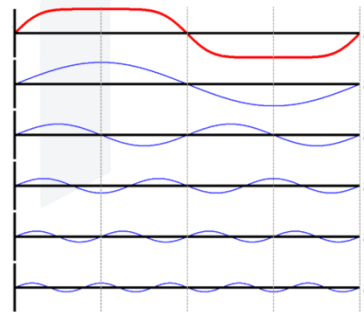
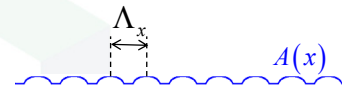
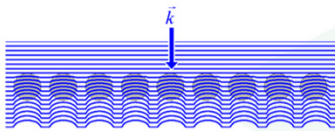


The Plane Wave Spectrum

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Periodic Functions Can Be Expanded into a Fourier Series



Waves in periodic structures obey Bloch's equation

$$E(x, y) = A(x) e^{j\vec{\beta} \cdot \vec{r}}$$

The envelope $A(x)$ is periodic along x with period Λ_x so it can be expanded into a complex Fourier series.

$$A(x) = \sum_{m=-\infty}^{\infty} S(m) e^{-j \frac{2\pi m x}{\Lambda_x}}$$

$$S(m) = \frac{1}{\Lambda} \int_{\Lambda} A(x) e^{j \frac{2\pi m x}{\Lambda_x}} dx$$

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Rearrange the Fourier Series (1 of 2)



A periodic field can be expanded into a Fourier series.

$$\begin{aligned}
 E(x, y) &= A(x) e^{j\vec{\beta} \cdot \vec{r}} \\
 &= \left[\sum_{m=-\infty}^{\infty} S(m) e^{-j \frac{2\pi m x}{\Lambda_x}} \right] e^{j\vec{\beta} \cdot \vec{r}} \\
 &= \sum_{m=-\infty}^{\infty} S(m) e^{j\vec{\beta} \cdot \vec{r}} e^{-j \frac{2\pi m x}{\Lambda_x}} \\
 &= \sum_{m=-\infty}^{\infty} S(m) e^{j\beta_x x} e^{j\beta_y y} e^{j\beta_z z} e^{-j \frac{2\pi m x}{\Lambda_x}}
 \end{aligned}$$

Here the plane wave term $e^{j\vec{\beta} \cdot \vec{r}}$ is brought inside of the summation.

Rearrange the Fourier Series (2 of 2)



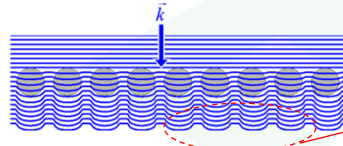
β_x can be combined with the last complex exponential.

$$\begin{aligned}
 E(x, y) &= \sum_{m=-\infty}^{\infty} S(m) e^{j\beta_x x} e^{j\beta_y y} e^{j\beta_z z} e^{-j \frac{2\pi m x}{\Lambda_x}} \\
 &= \sum_{m=-\infty}^{\infty} S(m) e^{j\beta_y y} e^{j\beta_z z} e^{j \left(\beta_x - \frac{2\pi m}{\Lambda_x} \right) x}
 \end{aligned}$$

Now let $k_{x,m} = \beta_x - \frac{2\pi m}{\Lambda_x}$ and $k_{y,m} = \beta_y, k_{z,m} = \beta_z$

$$E(x, y) = \sum_{m=-\infty}^{\infty} S(m) e^{j\vec{k}(m) \cdot \vec{r}} \quad \vec{k}(m) = \left(\beta_x - \frac{2\pi m}{\Lambda_x} \right) \hat{a}_x + \beta_y \hat{a}_y + \beta_z \hat{a}_z$$

The Plane Wave Spectrum



$$E(x, y) = \sum_{m=-\infty}^{\infty} S(m) e^{j\vec{k}^{(m)} \cdot \vec{r}}$$

Terms were rearranged to show that a periodic field can also be thought of as an infinite sum of plane waves at different angles. This is the “plane wave spectrum” of a periodic field.



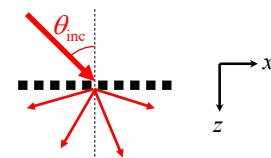
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Longitudinal Wave Vector Components of the Plane Wave Spectrum

The wave incident on a grating can be written as

$$E_{\text{inc}}(x, y) = E_0 e^{j(k_{x,\text{inc}}x + k_{z,\text{inc}}z)}$$

$$\begin{aligned} k_{x,\text{inc}} &= k_0 n_{\text{inc}} \sin \theta_{\text{inc}} \\ k_{y,\text{inc}} &= 0 \\ k_{z,\text{inc}} &= k_0 n_{\text{inc}} \cos \theta_{\text{inc}} \end{aligned}$$



Phase matching into the grating leads to

$$k_x(m) = k_{x,\text{inc}} - m \frac{2\pi}{\Lambda_x} \quad m = \dots, -2, -1, 0, 1, 2, \dots$$

Note: k_x is always real.

Each wave must satisfy the dispersion relation.

$$k_x^2(m) + k_z^2(m) = (k_0 n_{\text{grat}})^2$$

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$$k_z(m) = \sqrt{(k_0 n_{\text{grat}})^2 - k_x^2(m)}$$

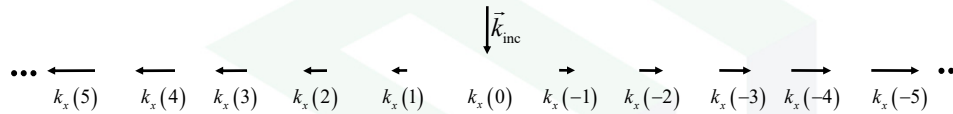
There are two possible solutions here.

1. Purely real k_z
2. Purely imaginary k_z

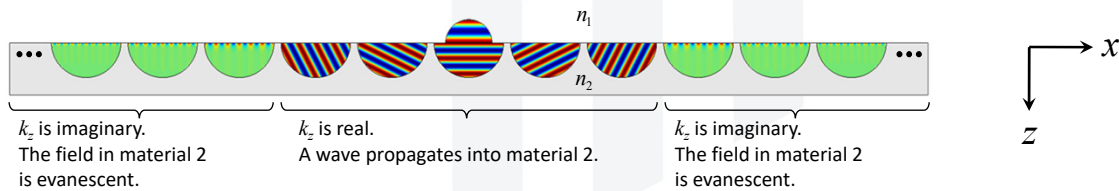
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Visualizing Phase Matching into the Grating

The wave vector expansion for the first 11 modes can be visualized as...



Each of these is phase matched into material 2. The longitudinal component of the wave vector is calculated using the dispersion relation in material 2.



Note: The “evanescent” fields in material 2 are not completely evanescent. They have a purely real k_x so power flows in the transverse direction.

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Conclusions About the Plane Wave Spectrum

- Fields in periodic media take on the same periodicity as the media they are in.
- Periodic fields can be expanded into a Fourier series.
- Each term of the Fourier series represents a spatial harmonic (plane wave).
- Since there are an infinite number of terms in the Fourier series, there are an infinite number of spatial harmonics.
- Only a few of the spatial harmonics are actually propagating waves. Only these can carry power away from a device. Tunneling is an exception.

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