Computational Photonics

Basics of grating theories - interface problem

Field expansion inside the grating

→ can be unambiguously written down, e.g., for E_x

$$E_x(x,y,z) = \sum_{l=1}^{2N_0} \{A_l \exp[i\beta_l z] + B_l \exp[-i\beta_l (z-h)]\} \times \sum_{m,n} E_{xmnl} \exp[i(k_{mn,x} x + k_{mn,y} y)]$$

- plane wave expansion of the l^{th} eigenmode
- E_{xmnl} eigenvectors from the eigenvalue problem
- $\exp[\pm i\beta_l z]$ forward / backward propagating eigenmodes
- A_l / B_l unknown amplitudes of the eigenmodes

  → have to be determined from boundary conditions

Field expansion inside the grating

⟹ for completeness, the same expansion holds for all fields

$$E_x(x,y,z) = \sum_{l=1}^{2N_0} \{A_l \exp[i\beta_l z] + B_l \exp[-i\beta_l (z-h)]\} \times \sum_{m,n} E_{xmnl} \exp[i(k_{mn,x} x + k_{mn,y} y)]$$

$$E_y(x,y,z) = \sum_{l=1}^{2N_0} \{A_l \exp[i\beta_l z] + B_l \exp[-i\beta_l (z-h)]\} \times \sum_{m,n} E_{ymnl} \exp[i(k_{mn,x} x + k_{mn,y} y)]$$

for the electric field

Field expansion inside the grating

⇒ for completeness, the same expansion holds for all fields

$$H_x(x,y,z) = k\sum_{l=1}^{2N_0}\{A_l\exp[i\beta_l z] - B_l\exp[-i\beta_l(z-h)]\} \times \sum_{m,n} H_{xmnl}\exp[i(k_{mn,x}x + k_{mn,y}y)]$$

$$H_y(x,y,z) = k\sum_{l=1}^{2N_0}\{A_l\exp[i\beta_l z] - B_l\exp[-i\beta_l(z-h)]\} \times \sum_{m,n} H_{ymnl}\exp[i(k_{mn,x}x + k_{mn,y}y)]$$

for the magnetic field

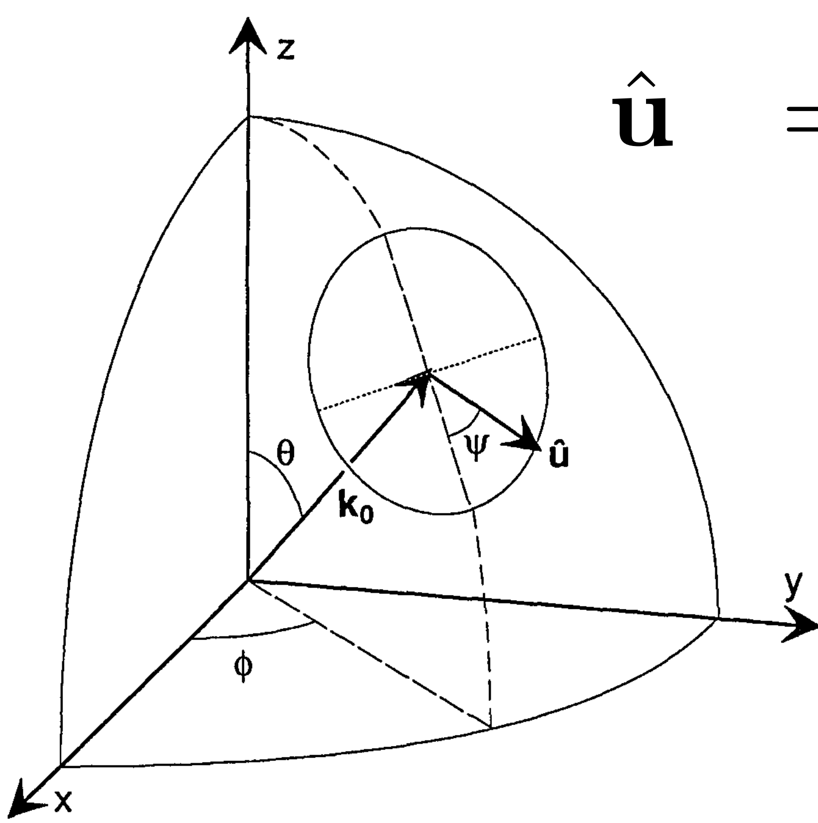
Incident field in the Fourier space

➡ assuming plane wave illumination

(arbitrary wave fields in space and time are decomposed)

$$\mathbf{E}_I(\mathbf{r}) = \hat{\mathbf{u}} e^{i\mathbf{k_0}\cdot\mathbf{r}}$$

$$\mathbf{k_0} = k_{0x}\hat{\mathbf{x}} + k_{0y}\hat{\mathbf{y}} + k_{0z}\hat{\mathbf{z}}$$



$$\begin{aligned}\hat{\mathbf{u}} \quad = \quad & (\cos\psi\cos\theta\cos\phi - \sin\psi\sin\phi)\,\hat{\mathbf{x}} \\ & + (\cos\psi\cos\theta\sin\phi + \sin\psi\cos\phi)\,\hat{\mathbf{y}} \\ & - \cos\psi\sin\theta\hat{\mathbf{z}}\end{aligned}$$

Reflected/transmitted field in the Fourier space

$$\mathbf{E}_R(\mathbf{r}) = \sum_{m,n} \mathbf{R}_{mn} e^{i\mathbf{k}_{1mn}\cdot\mathbf{r}}$$

$$\mathbf{E}_T(\mathbf{r}) = \sum_{m,n} \mathbf{T}_{mn} e^{i\mathbf{k}_{2mn}\cdot(\mathbf{r}-h\hat{\mathbf{z}})}$$

$$\mathbf{k}_{1mn} = k_{mn,x}\hat{\mathbf{x}} + k_{mn,y}\hat{\mathbf{y}} - k^{I}_{mn,z}\hat{\mathbf{z}}$$

$$\mathbf{k}_{2mn} = k_{mn,x}\hat{\mathbf{x}} + k_{mn,y}\hat{\mathbf{y}} + k^{II}_{mn,z}\hat{\mathbf{z}}$$

$$k^{I/II}_{mn,z} = \sqrt{k_0^2\epsilon_{I/II} - k^2_{mn,x} - k^2_{mn,y}}$$

Enforcing interface conditions

- matching eigenmodes with same tangential wave vector in the entire structure (omitting the terms $\exp[i(k_{mn,x}x + k_{mn,y}y)]$)

- continuity of the tangential electrical field at the interface between the illuminating space and the grating ($z = 0$)

$$u_x \delta_{m0} \delta_{n0} + R_{xmn} = \sum_l \left[A_l + B_l \exp(i\beta_l h) \right] E_{xmnl}$$

- x-component of the illuminating field *(term 1)*
- x-component of the reflected field field *(term 2)*
- sum over forward and backward propagating plane wave contributions to eigenmodes with same k_{mn} *(term 3)*

- four similar equations for all tangential components

Enforcing interface conditions at z=0

$$u_x\delta_{m0}, \delta_{n0} + R_{xmn} = \sum_l \left[A_l + B_l \exp(i\beta_l h)\right] E_{xmnl}$$

$$u_y\delta_{m0}, \delta_{n0} + R_{ymn} = \sum_l \left[A_l + B_l \exp(i\beta_l h)\right] E_{ymnl}$$

$$(k_{0y}u_z - k_{0z}u_y)\delta_{m0}, \delta_{n0} + k_{mn,y}R_{zmn} + k^I_{mn,z}R_{ymn}$$

$$= k\sum_l \left[A_l - B_l \exp(i\beta_l h)\right] H_{xmnl}$$

$$(k_{0z}u_x - k_{0x}u_z)\delta_{m0}\delta_{n0} - k^I_{mn,z}R_{xmn} - k_{mn,x}R_{zmn}$$

$$= k\sum_l \left[A_l - B_l \exp(i\beta_l h)\right] H_{ymnl}$$

Enforcing interface conditions at z=h

→ same interface conditions for the back interface

$$\sum_l \left[A_l \exp(i\beta_l h) + B_l\right] E_{xmnl} \quad = \quad T_{xmn}$$

$$\sum_l \left[A_l \exp(i\beta_l h) + B_l\right] E_{ymnl} \quad = \quad T_{ymn}$$

$$k \sum_l \left[A_l \exp(i\beta_l h) - B_l\right] H_{xmnl} \quad = \quad k_{mn,y} T_{zmn} - k^{II}_{mn,z} T_{ymn}$$

$$k \sum_l \left[A_l \exp(i\beta_l h) - B_l\right] H_{ymnl} \quad = \quad k^{II}_{mn,z} T_{xmn} - k_{mn,x} T_{zmn}$$

→ eight linear independent equations with eight unknown variables

$$A_l,\ B_l,\ R_{xmn},\ R_{ymn},\ R_{zmn},\ T_{xmn},\ T_{ymn},\ \text{and}\ T_{zmn}$$

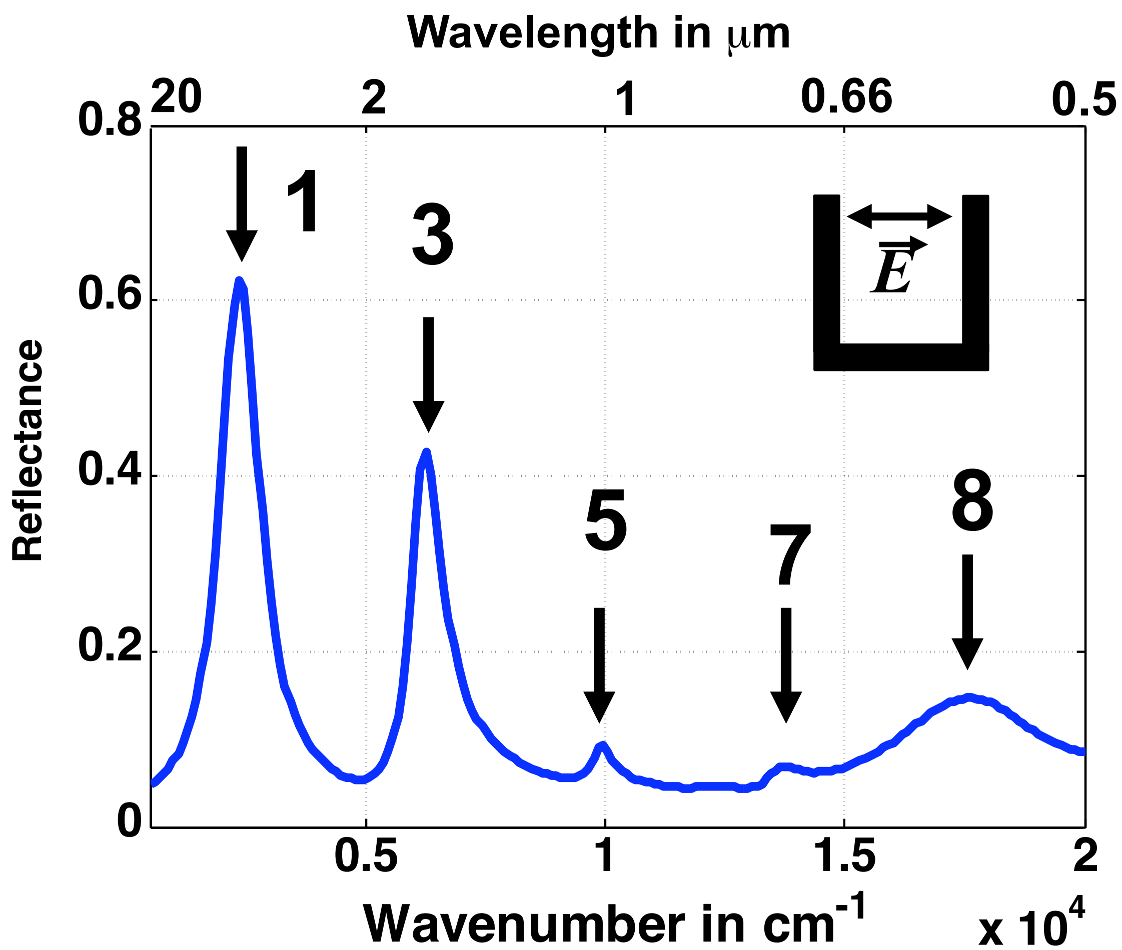
→ unique solution

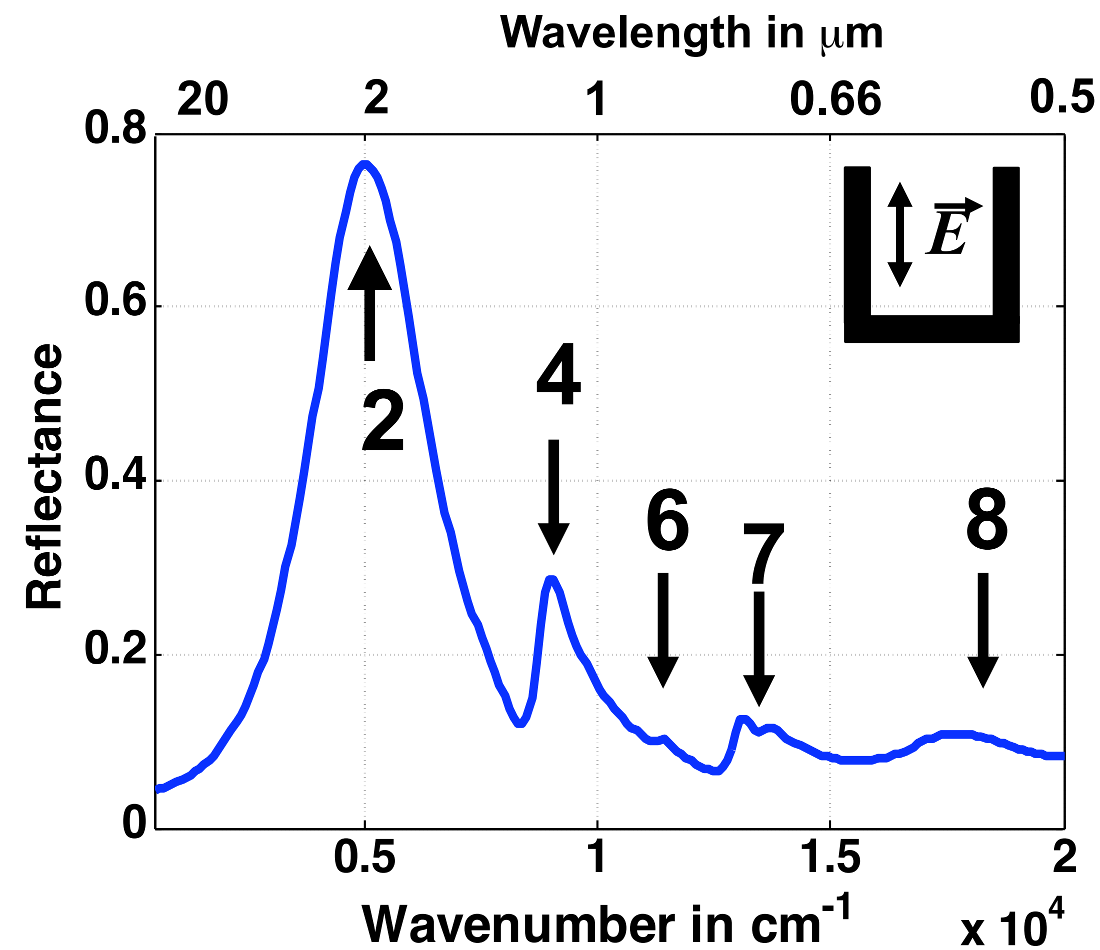
(Noponen et al., JOSA A, Vol. 11, 2494 1994)

Summary of the algorithm

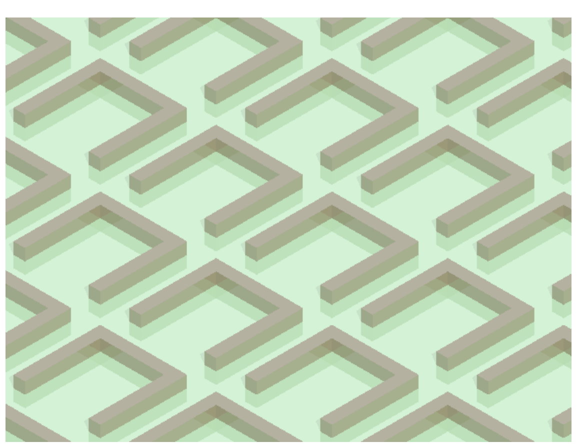
- calculate all wave vector components of interest
- Fourier transforming the permittivity distribution
- calculating eigenvalues and eigenvectors of eigenmodes supported by the structure in Fourier space
- solving the system of linear equations that provide the amplitude of all relevant field components
    - calculating quantities of interest, such as diffraction efficiency and/or field distributions in regions of interest
    - note that the algorithm thus far requires invariance of the structure in the propagation direction

Application examples





$(l_\perp = l_{||} = 400\ \mathrm{nm},\ \Lambda = 500\ \mathrm{nm},\ h = 20\ \mathrm{nm},\ w = 60\ \mathrm{nm},\ \mathrm{Au})$

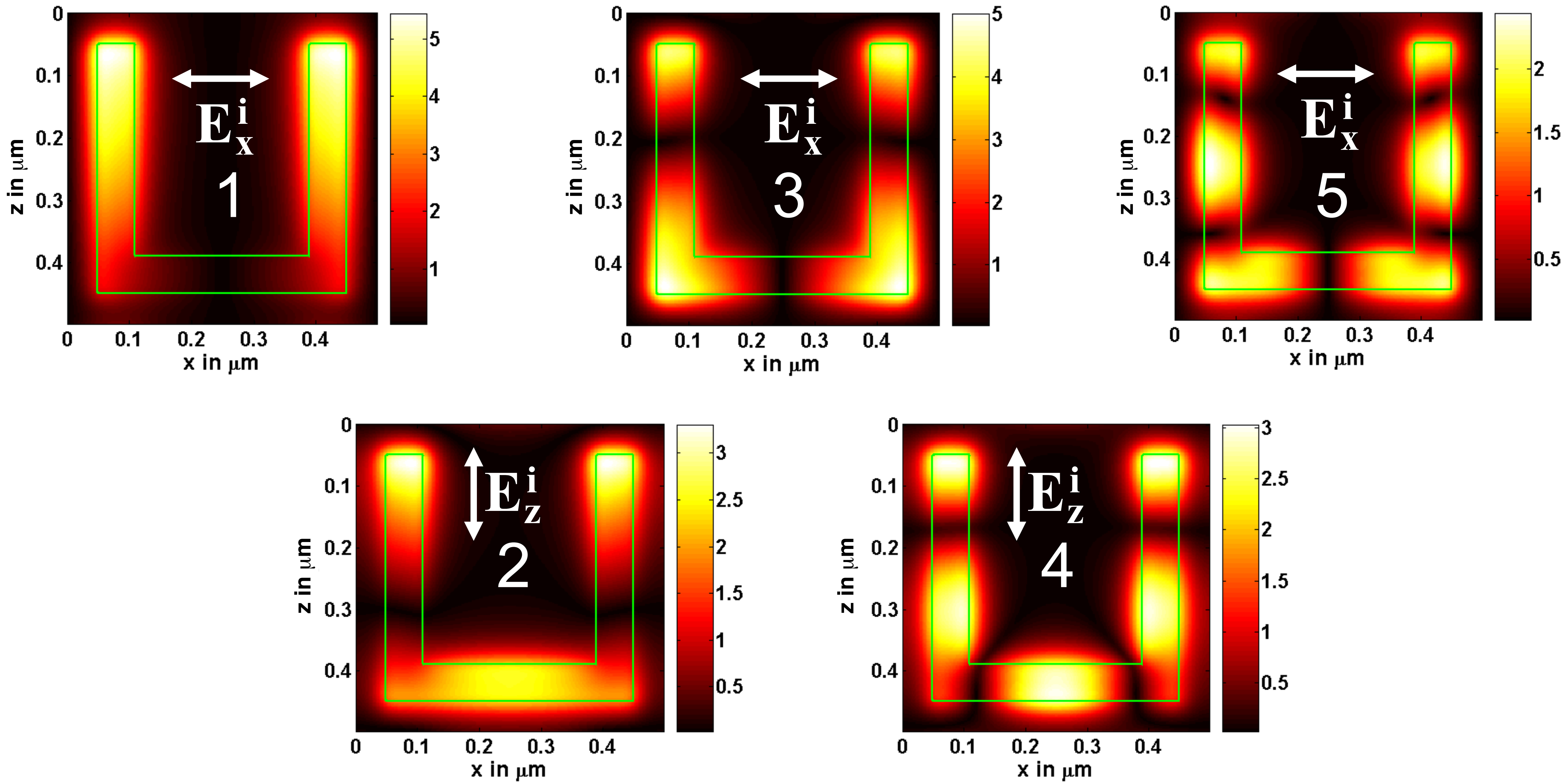


(1-6) plasmonic eigenmodes of the SRR

(7) wood anomaly

(8) plasmonic resonance of the cylinder

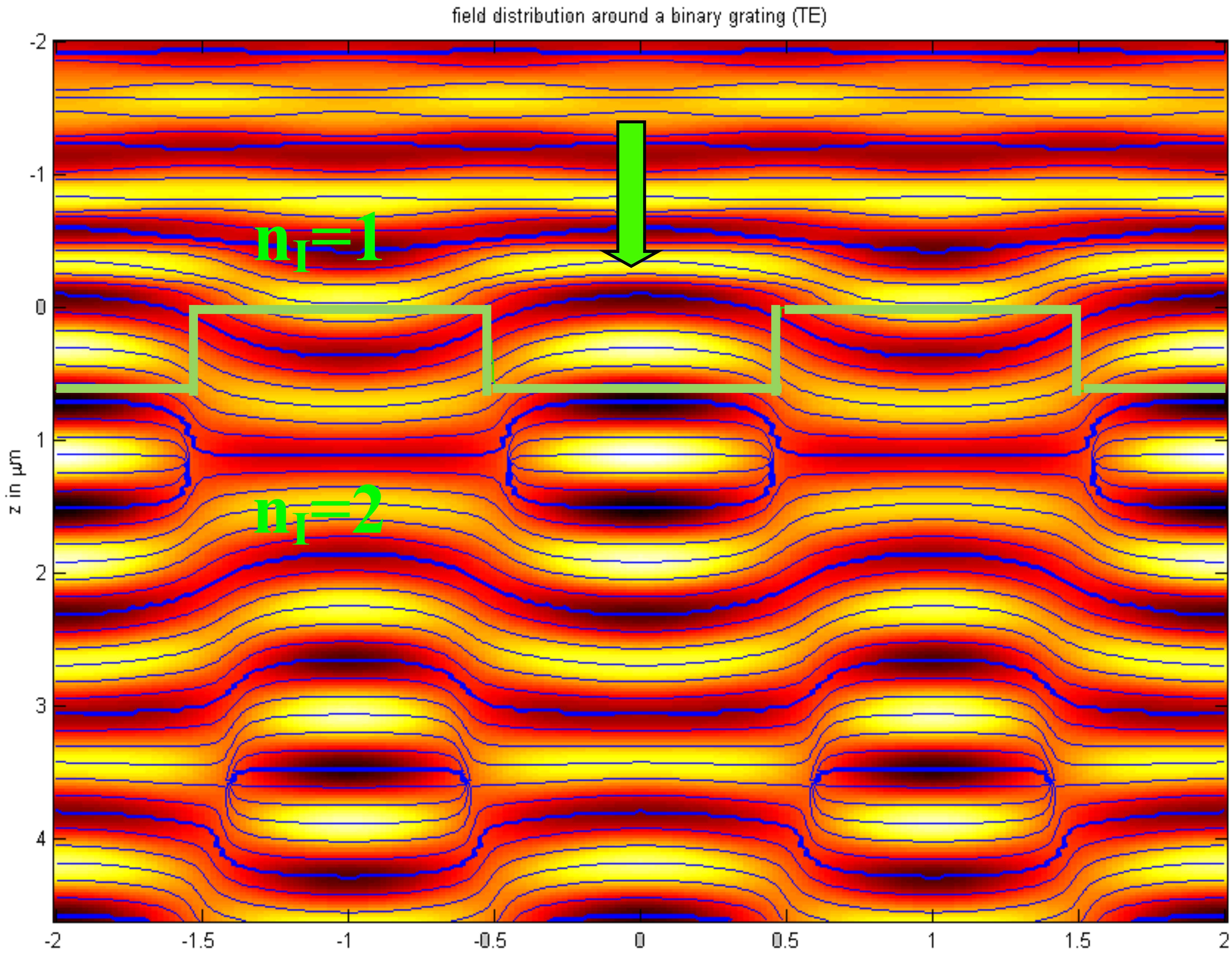
Application examples



- **E**-field component ⊥ to the SRR used for resonance labelling

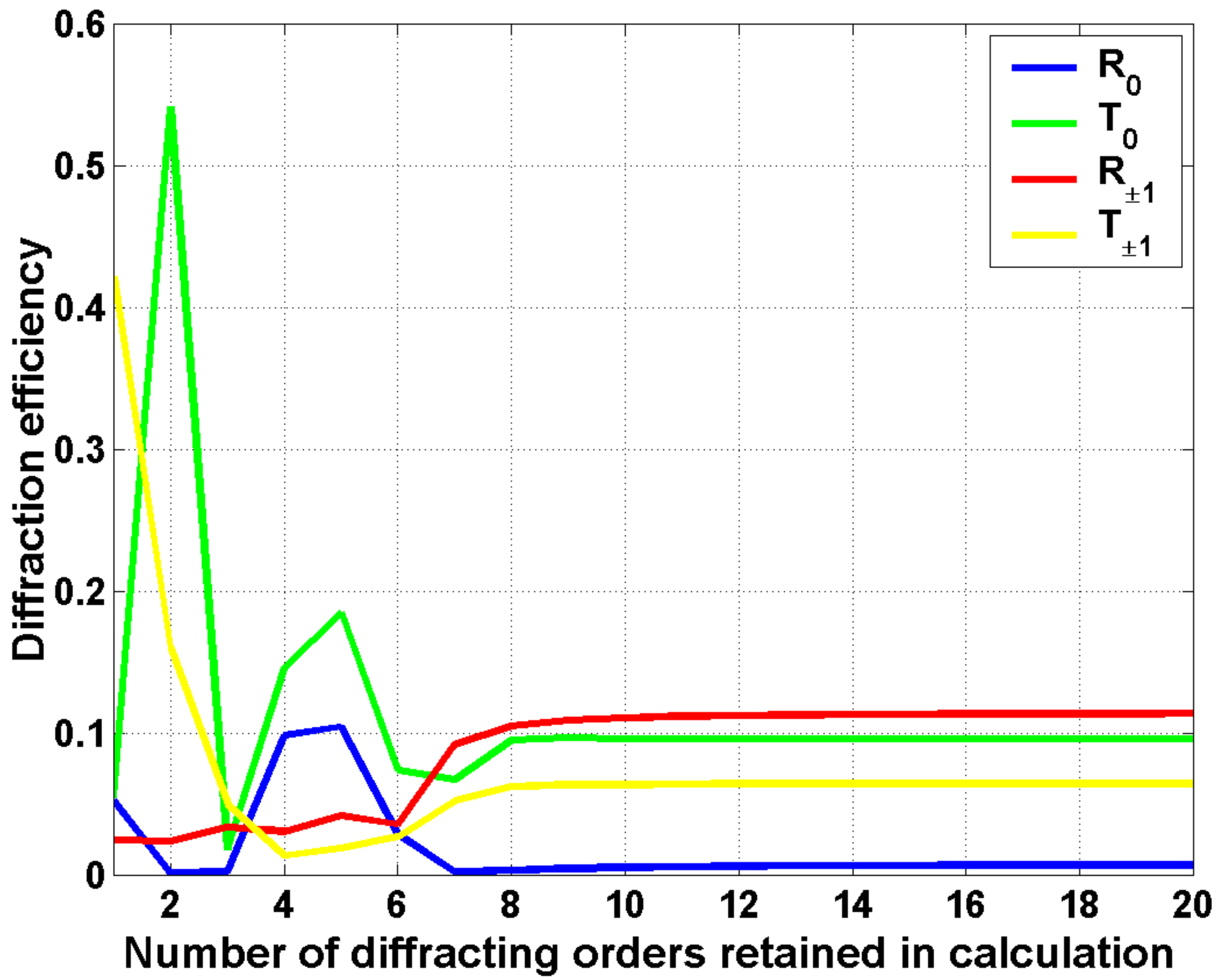
→ *E_y amplitude 20 nm above the SRR is shown*

Numerical peculiarities - truncation of the orders



Numerical peculiarities - truncation of the orders

→ for keeping the system of equation treatable in a computer, we have to limit the number of diffraction orders retained in the calculation



(Λ=2.5λ, h=λ, n_I=1, n_G=3, n_{II}=2, TE, sinusoidal)

- rule of thumb: number of propagating orders plus 10 evanescent orders
- convergence has to be always ensured (*increasing the number of orders shall have no effect on the diffraction efficiencies)*
- energy conservation for loss-less materials

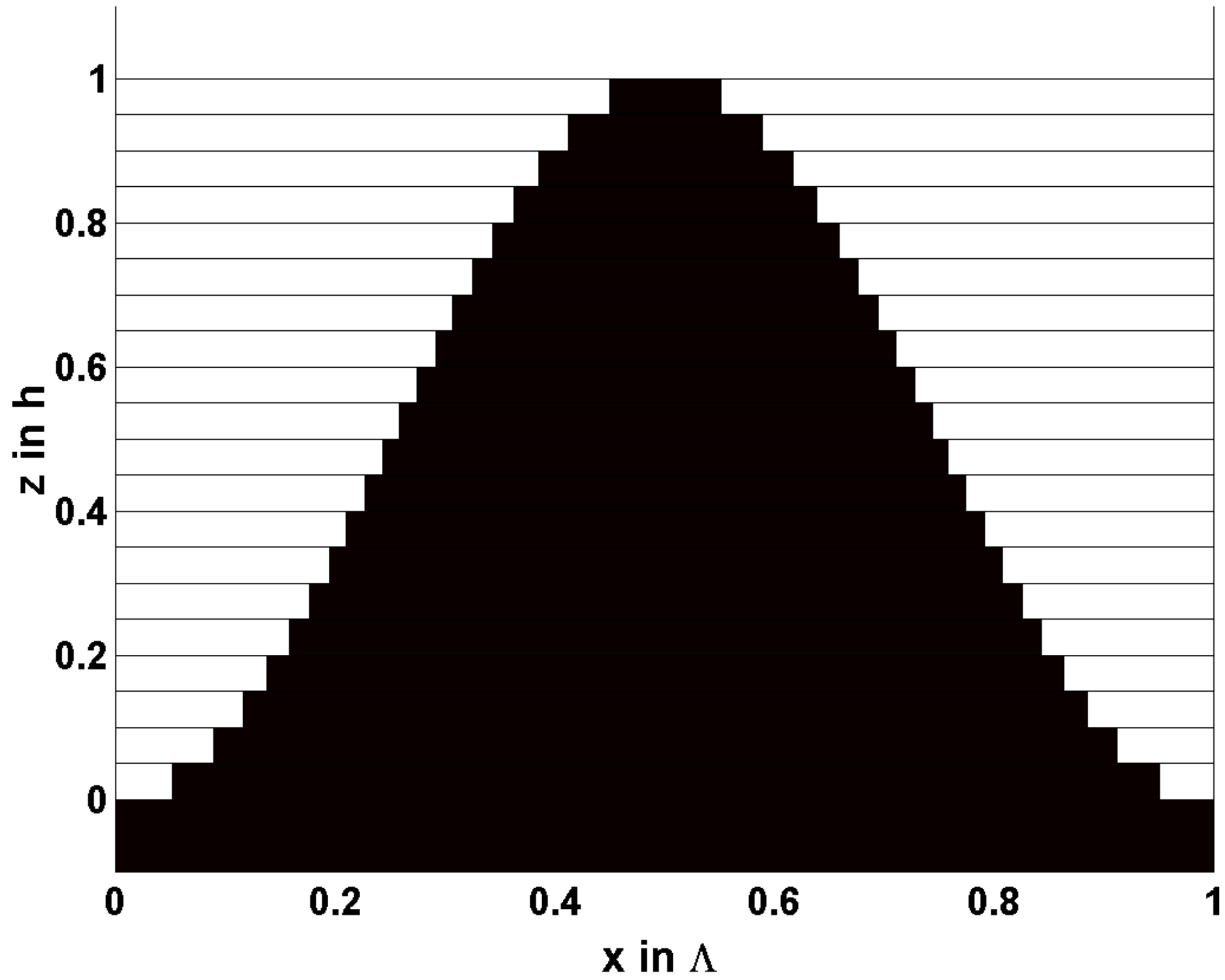
$$\sum_n \eta_{R,n} + \eta_{T,n} = 1$$

How to handle non-binary gratings

Remember

assumption: no variation of the dielectric function in z-direction

⇨ slicing continuous surface profile into a sufficient number of invariant layers



- field is expanded in each layer and additional equations for the boundary conditions are established

- for sufficient convergence a proper number of slices has to be made taken into account

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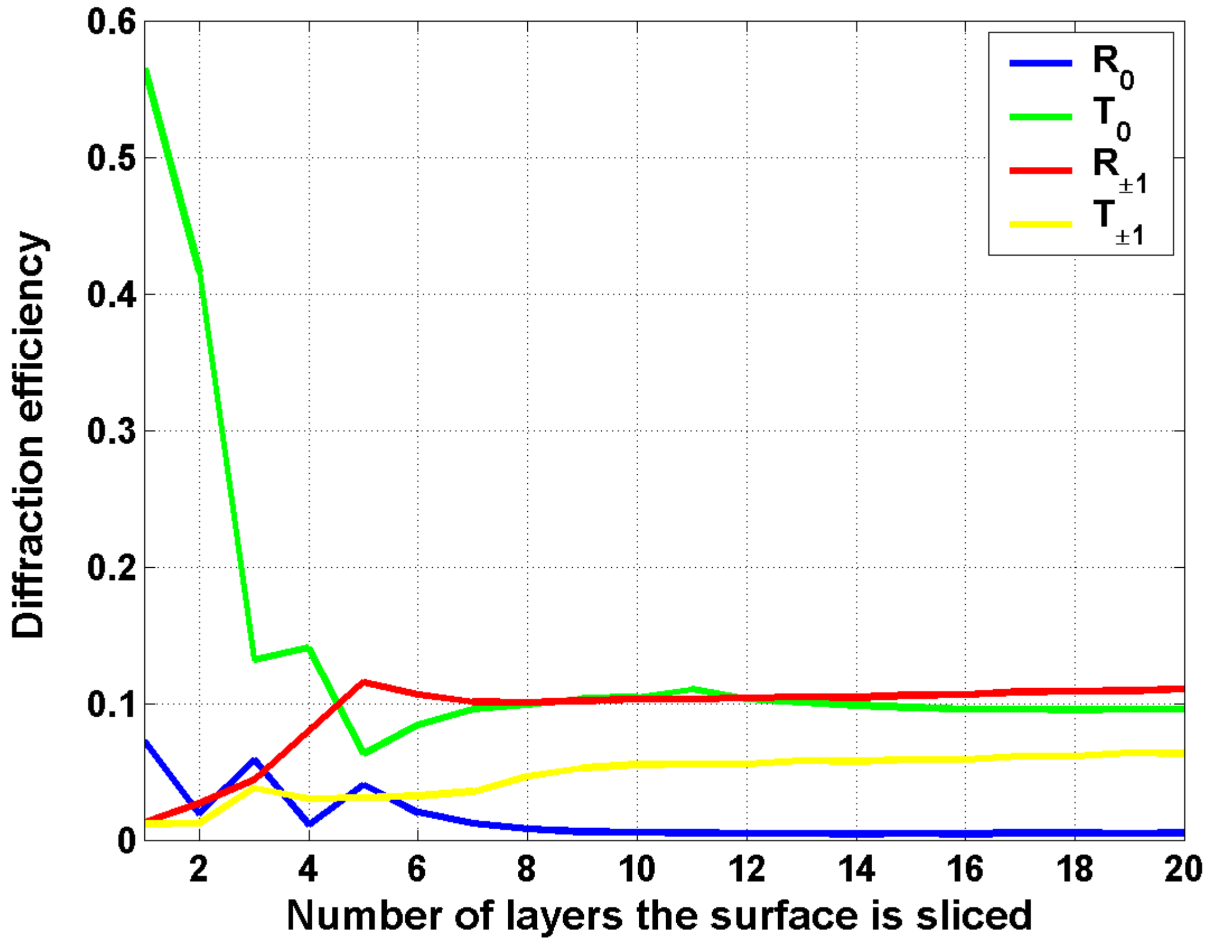

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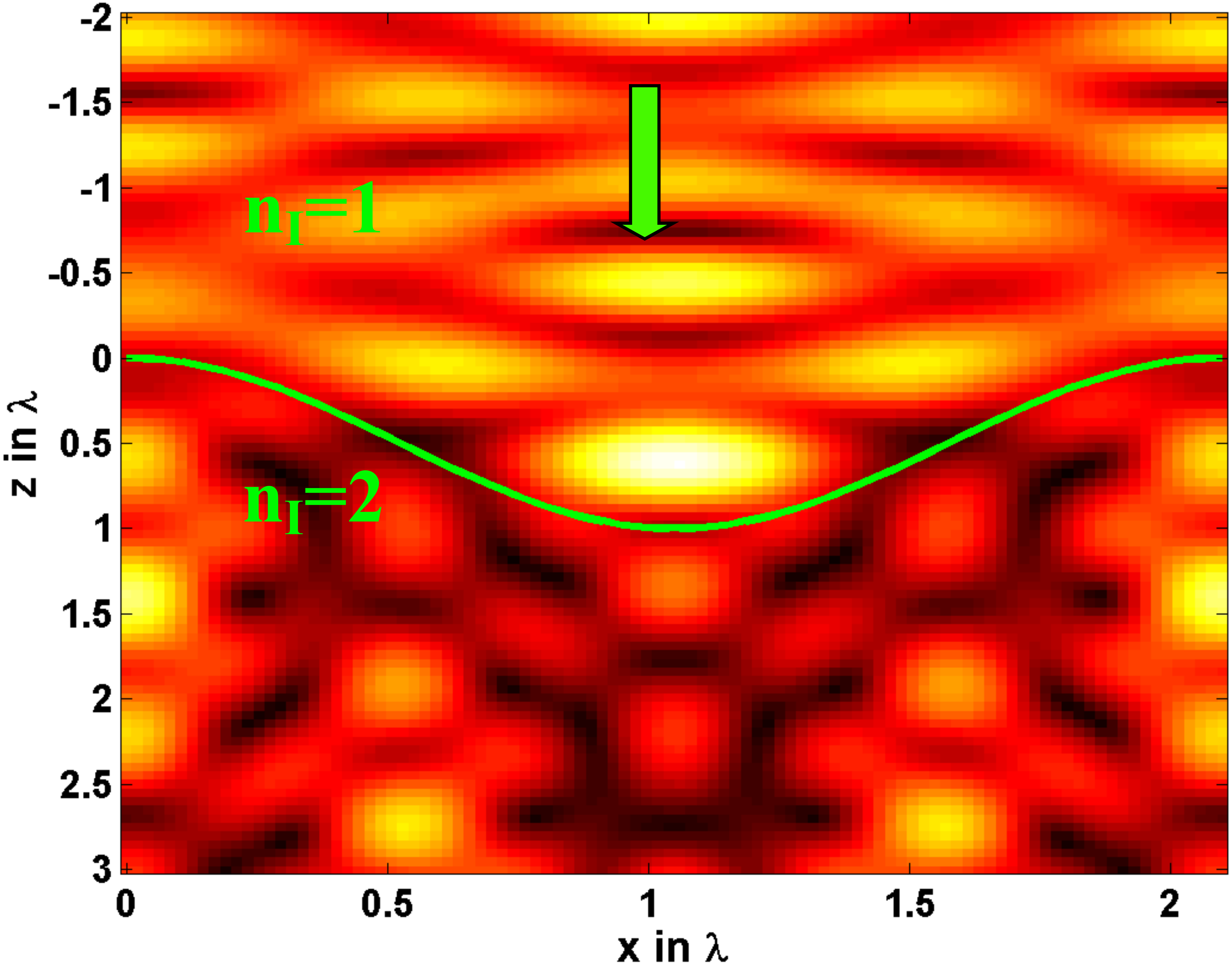


Eigenmodes of a periodic media

- Maxwell's equations transform to:

$$i\frac{\partial}{\partial z}\mathbf{X}(z)=\hat{\mathrm{M}}(z;\alpha,\beta,\omega)\mathbf{X}(z) \quad \text{with} \quad \mathbf{X}(z)=(\tilde{E}_x,\tilde{E}_y,\tilde{H}_x,\tilde{H}_y)$$

- Solution: $\mathbf{X}(z)=\underline{\underline{\hat{\mathrm{T}}(z)}}\mathbf{X}(0)$

Transfermatrix

- Addional imposure of Bloch condition in the propagation direction

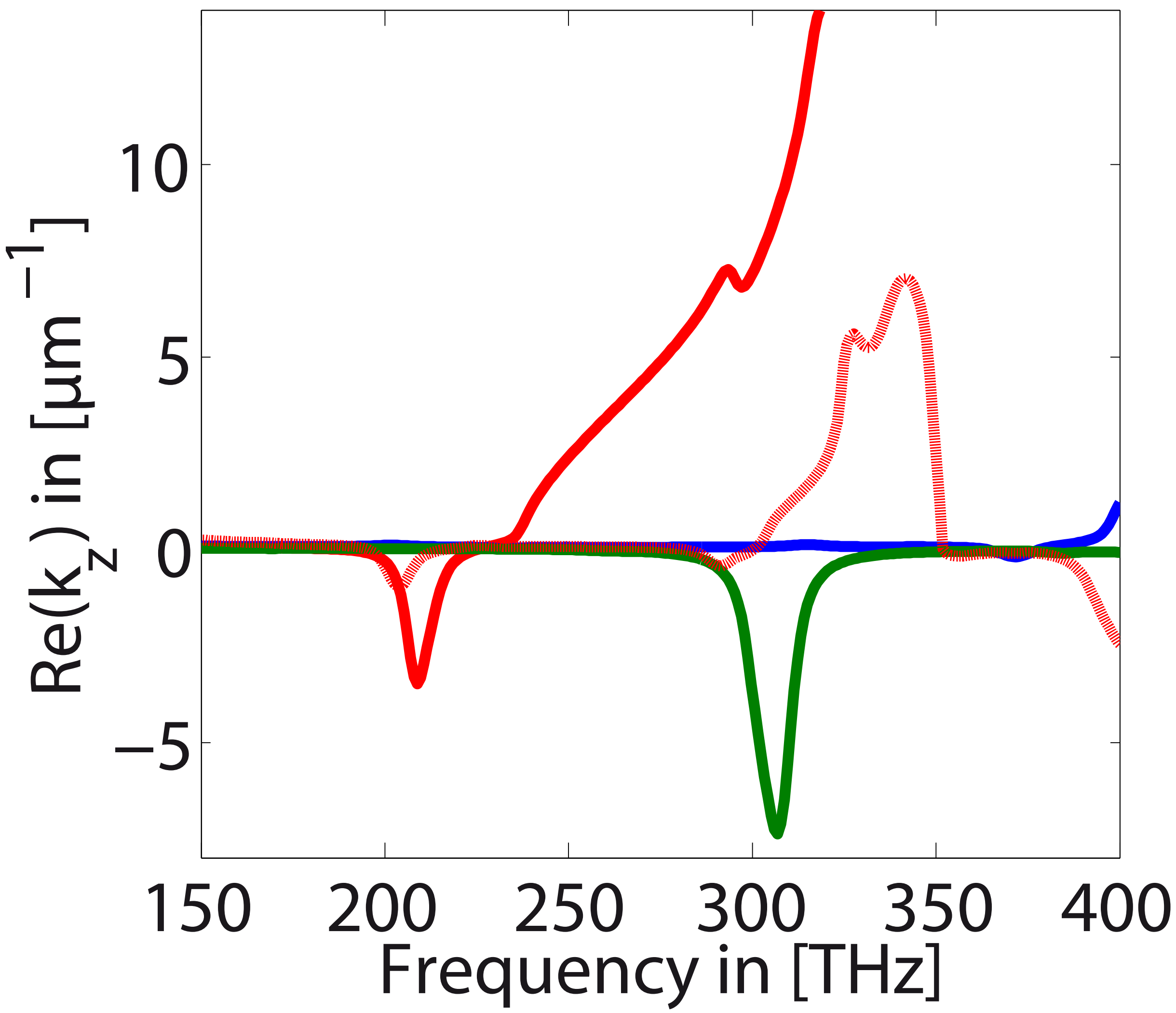
$$\mathbf{X}(\Lambda_z)=\hat{\mathrm{T}}(\Lambda_z)\mathbf{X}(0)=\exp(ik_z\Lambda_z)\mathbf{X}(0)$$

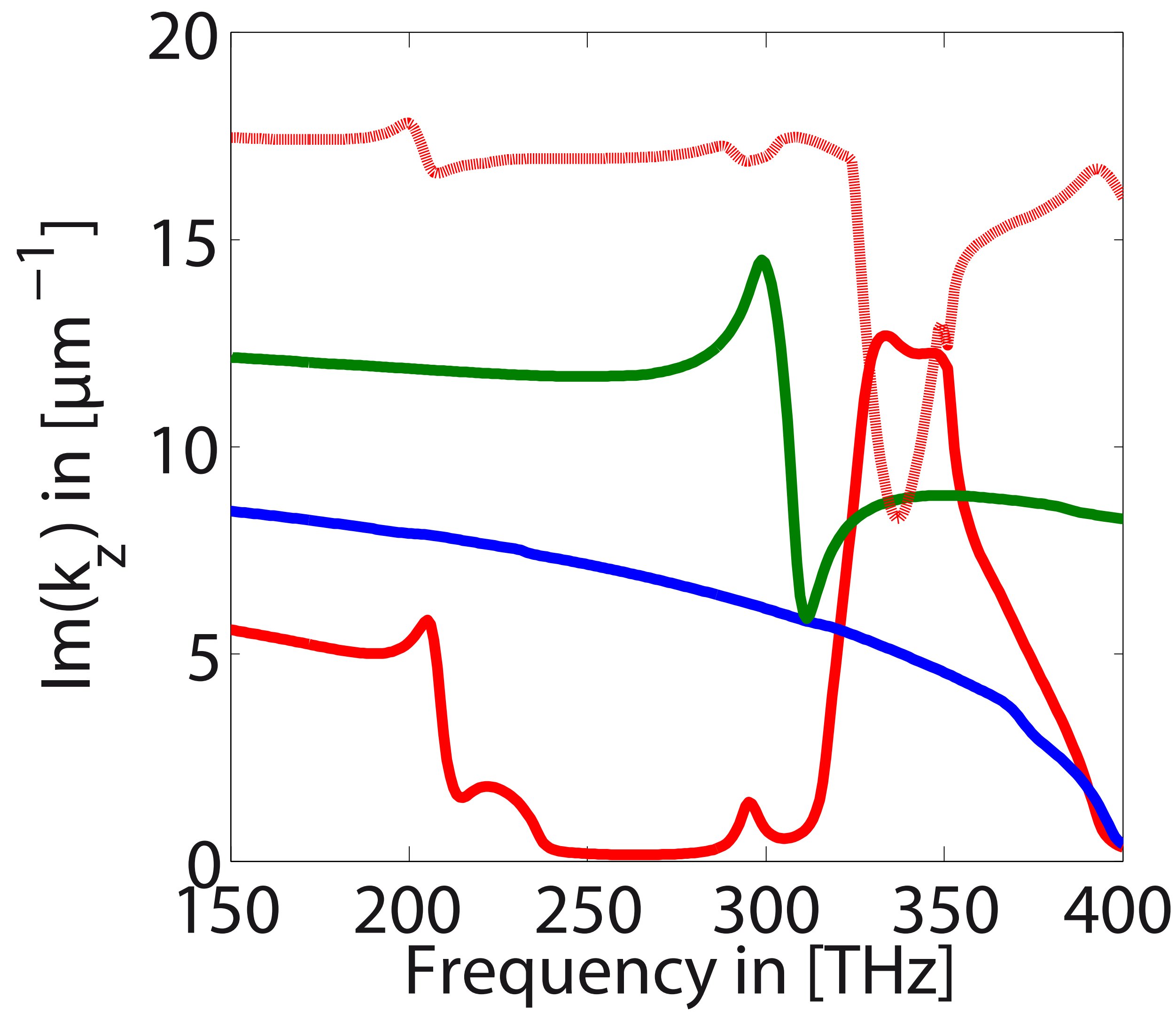
- Solution provides a discrete set of modes

$$\boxed{k_z=k_{z,p}(\alpha,\beta,\omega)\in\mathbb{C}} \qquad \text{with} \quad p\in\mathbb{N} \quad \text{and} \quad (\alpha,\beta)\in 1.\mathrm{BZ}$$

Referential example: the fishnet

- Frequency dispersion for a high symmetry direction ($\alpha=\beta=0$)

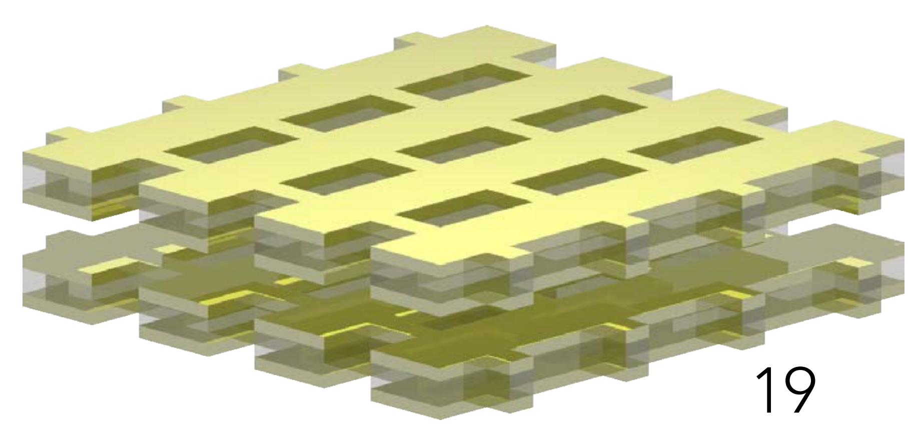




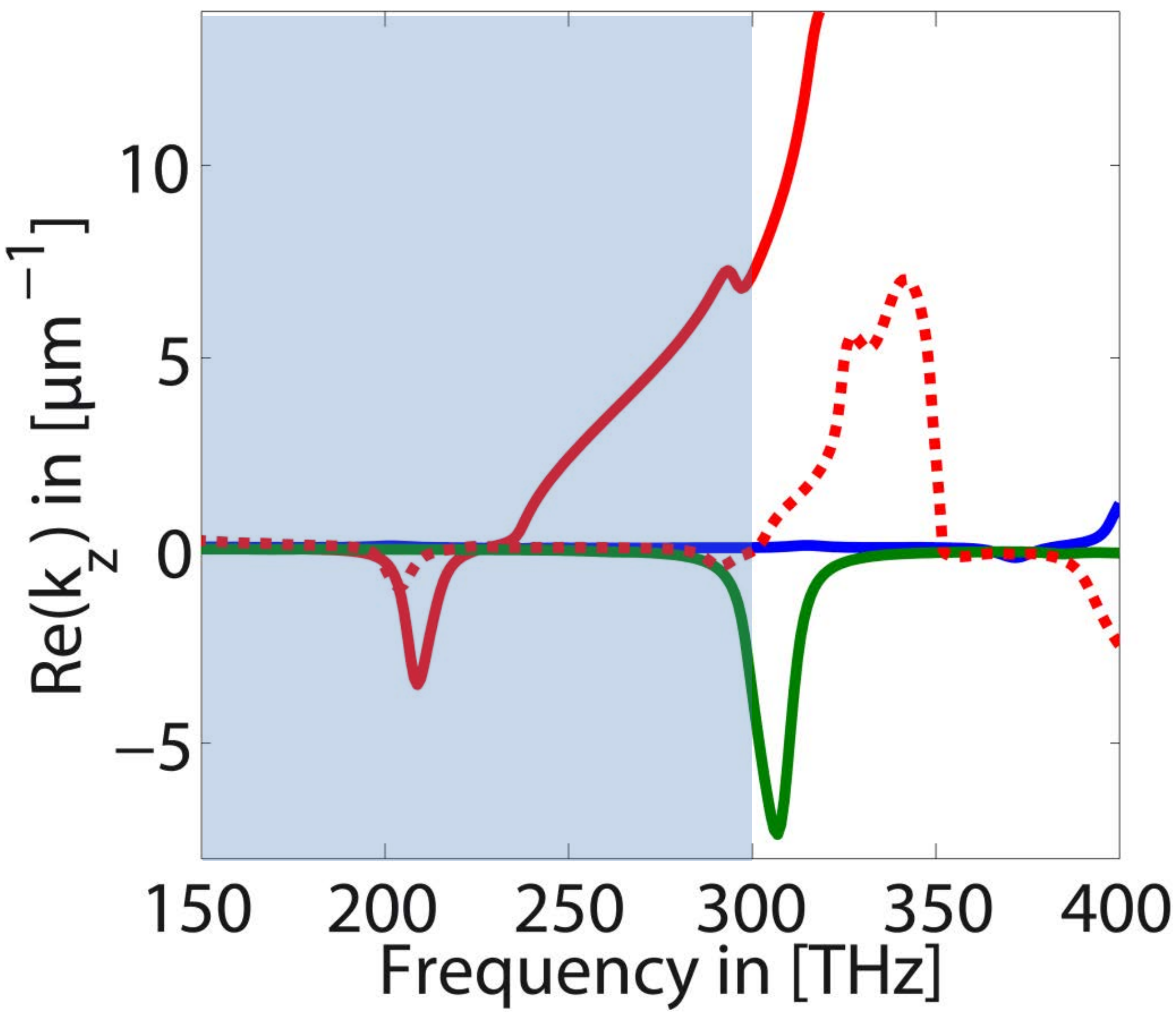
Excitable with a predominantly y-polarized wave

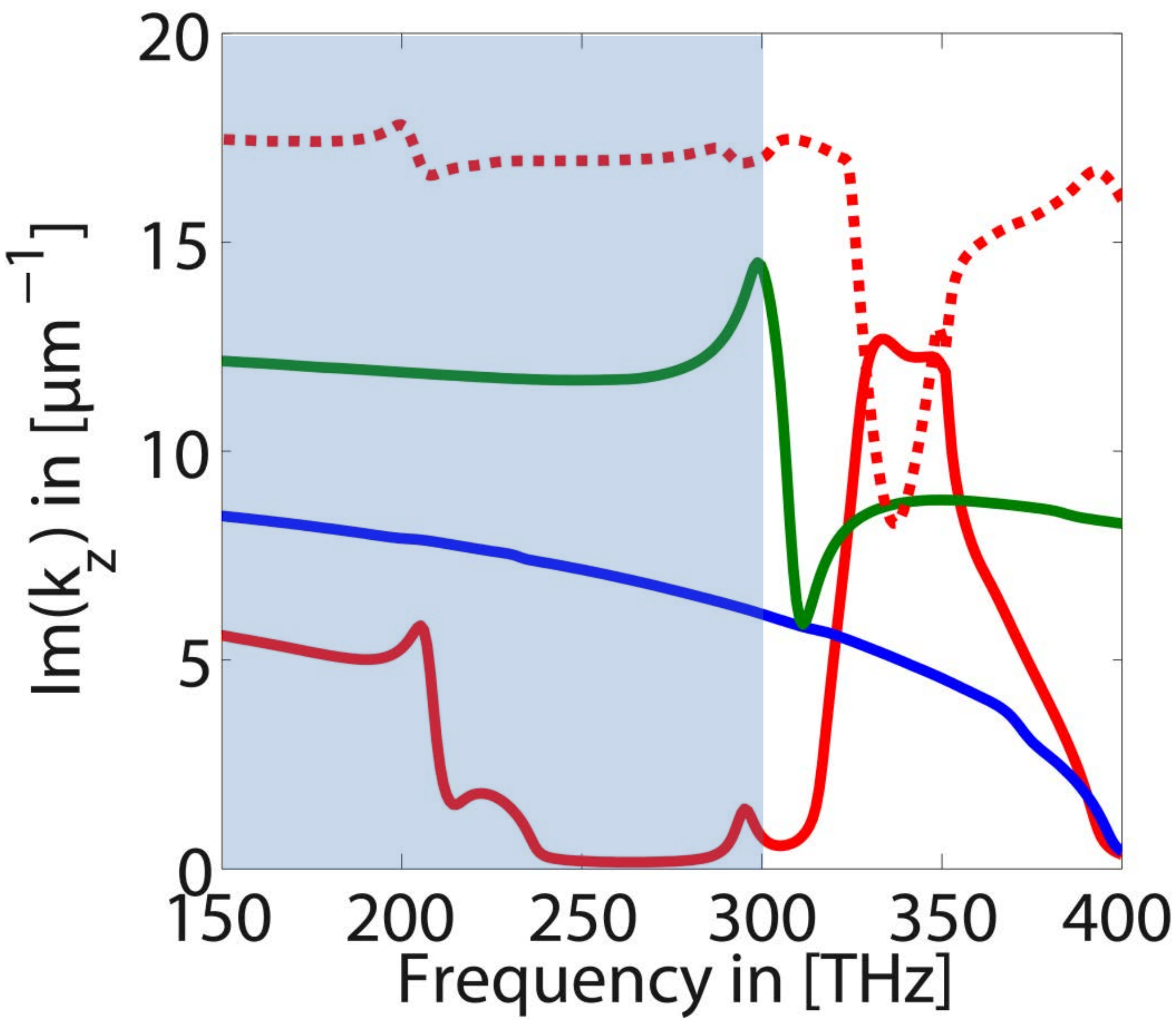
Excitable with a predominantly x-polarized wave

Not excitable due to symmetry constraints



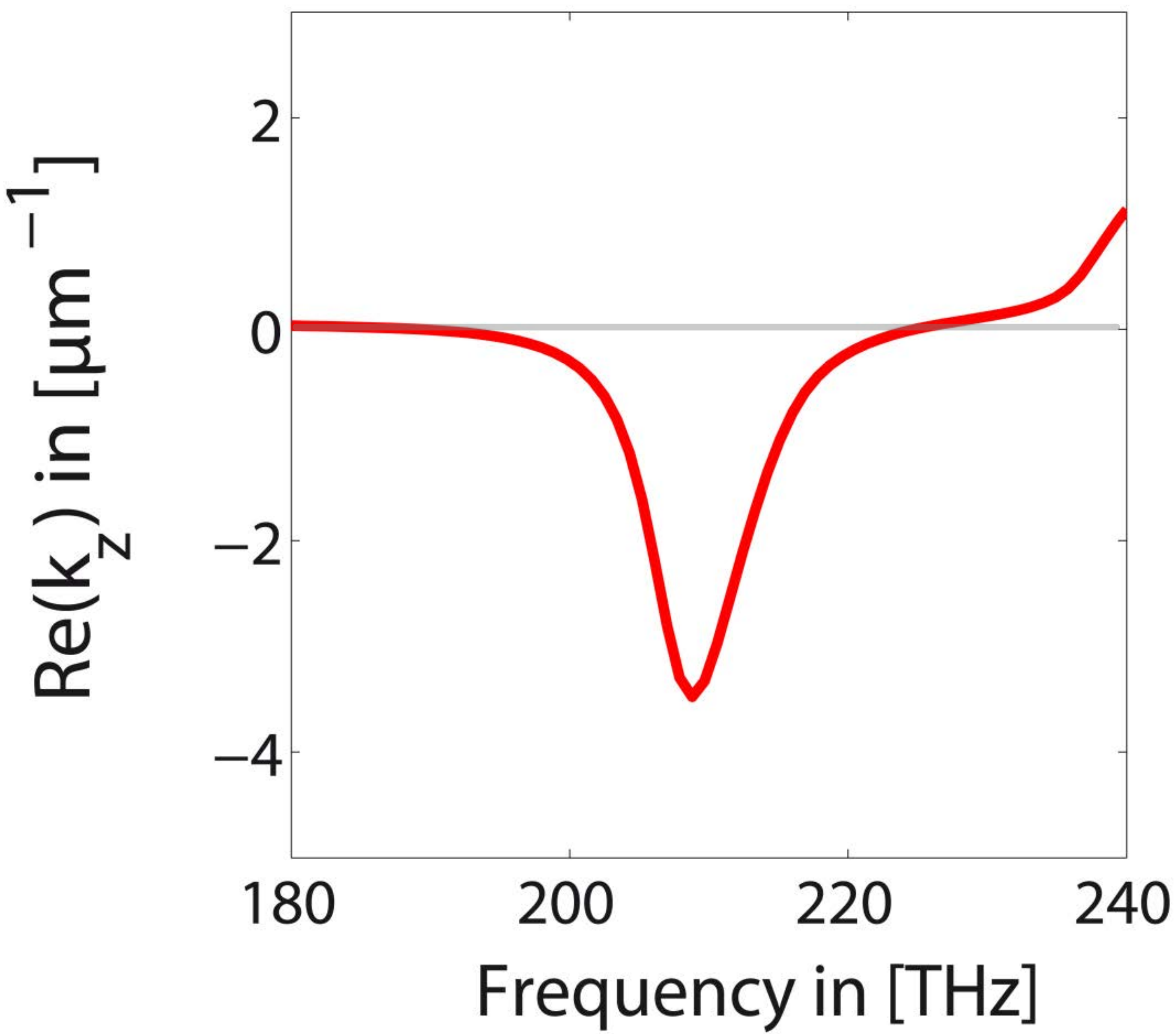
Referential example: the fishnet

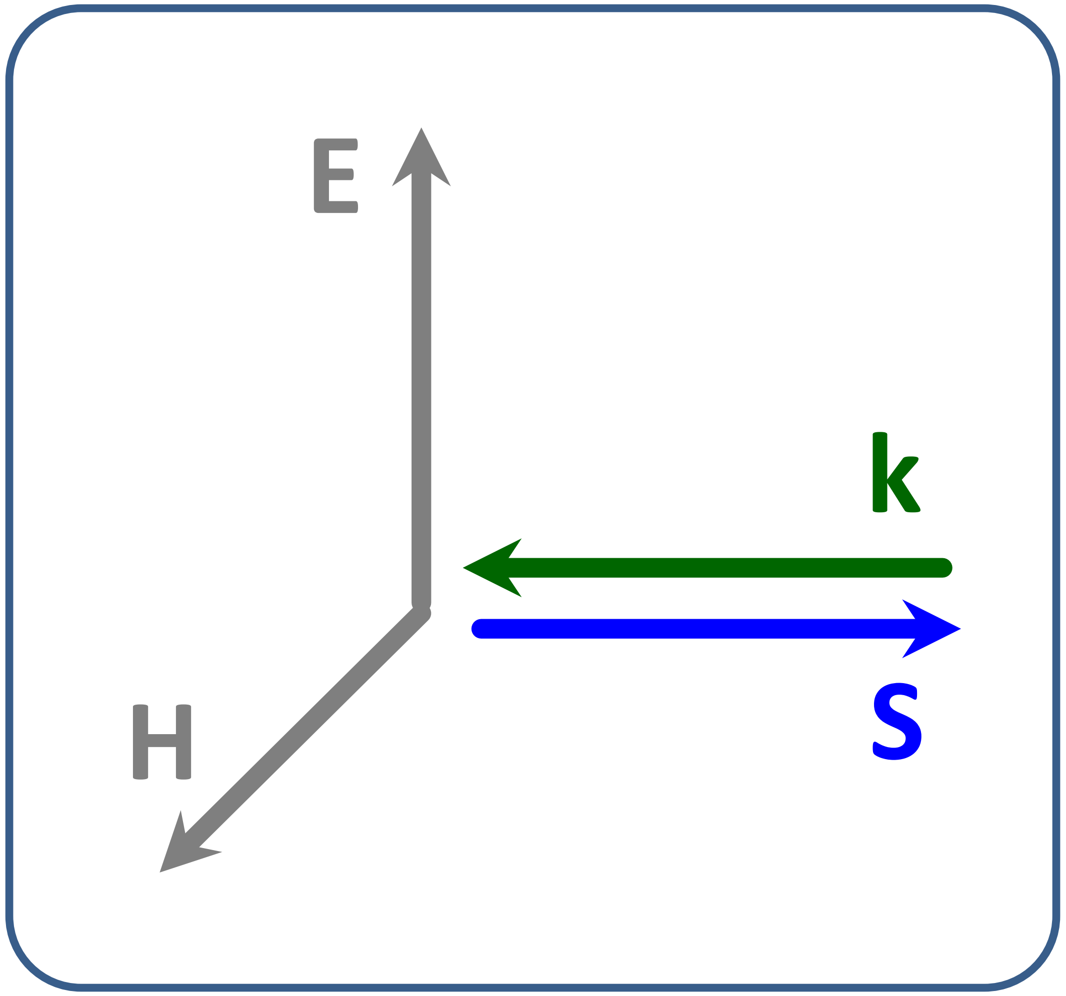




Fundamental mode classified by **min[Im(k_z)]**

Referential example: the fishnet





The fundamental mode is **left handed**

Propagation of bundles

- Bundle as a superposition of eigenmodes

$$\mathbf{E}(\mathbf{r}) = \sum_p \int_{\mathrm{BZ}} d\alpha\, A_p(\alpha) \underline{\underline{\mathbf{e}_p(\mathbf{r};\alpha)}} \exp[i(\alpha x + k_{z,p} z)]$$

$$\approx e(\not{r}, \alpha)$$

- Restriction to the fundamental mode

$$\mathbf{E}(\mathbf{r}) = \mathbf{e}_0(\mathbf{0};\alpha) \int_{\mathrm{BZ}} d\alpha\, A_0(\alpha) \exp[i(\alpha x + k_{z.0} z)]$$

$$k_z = k_z(\alpha, \omega) = \eta_0 + \eta_1(\alpha - \alpha_0) + \tfrac{\eta_2}{2}(\alpha - \alpha_0)^2 + \ldots$$

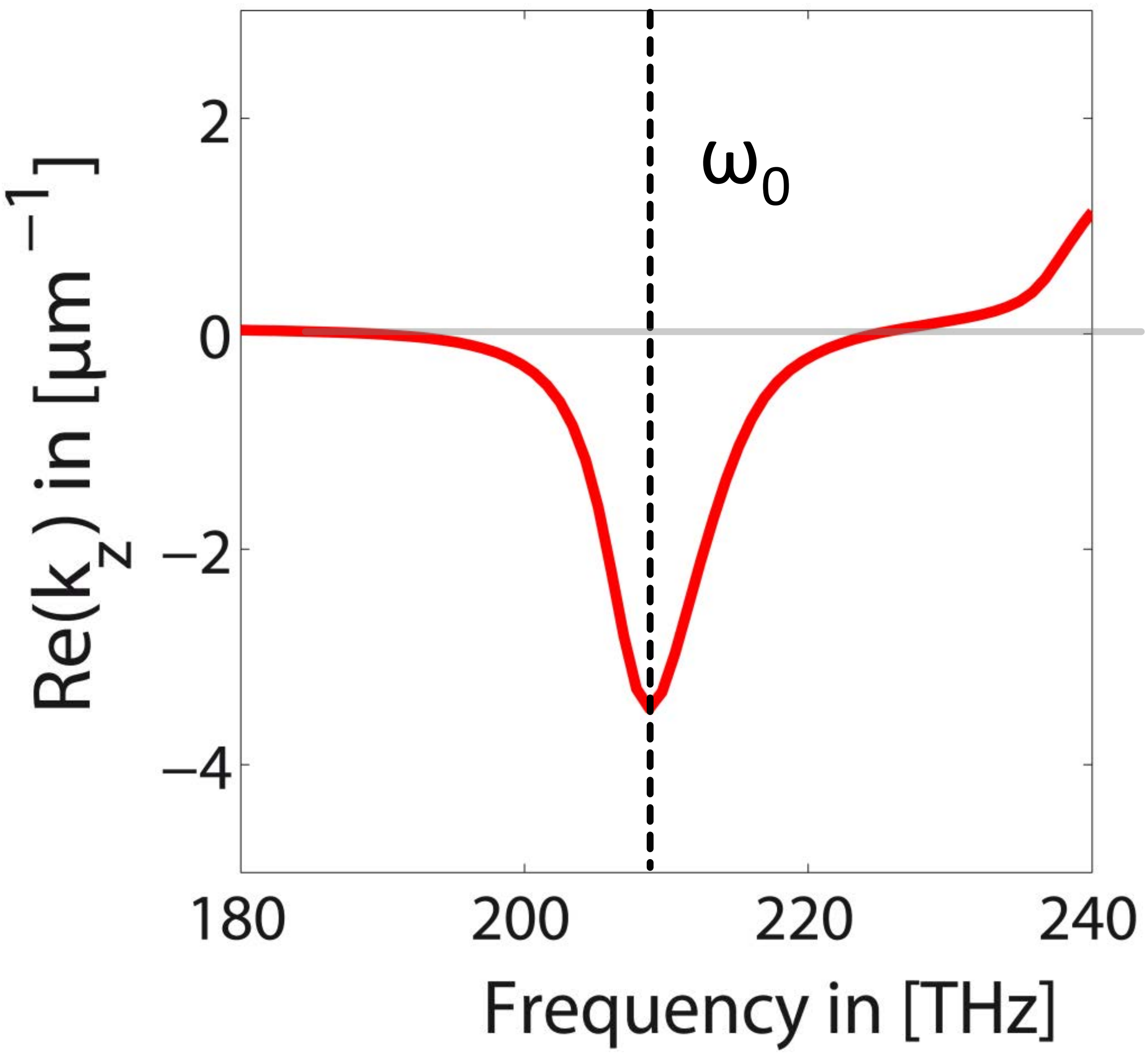
- Paraxial approximation of k_z

$$\left[i\frac{\partial}{\partial z} + \eta_0 - i\eta_1 \frac{\partial}{\partial x} - \frac{\eta_2}{2} \frac{\partial^2}{\partial x^2} \right] \overline{\mathbf{E}}(x,z) = 0$$

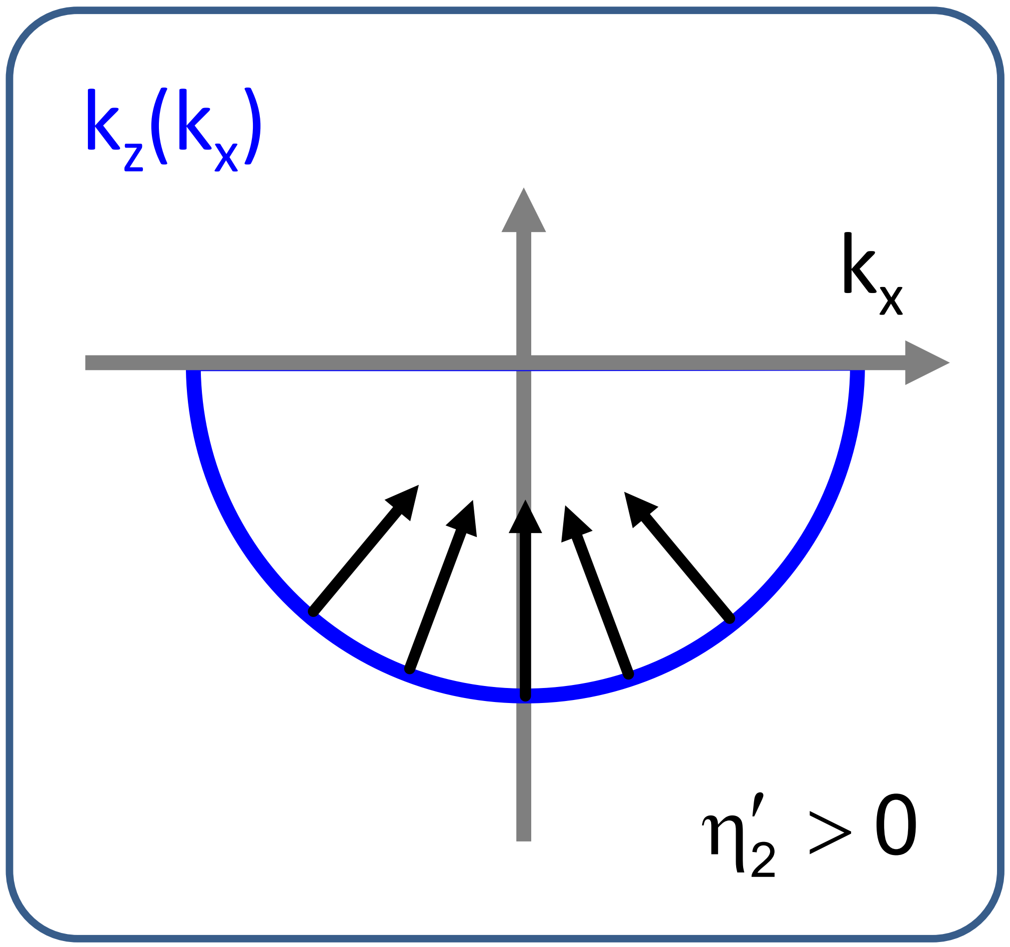
$$\overline{\mathbf{E}}(x,z) = \mathbf{E}(x,z)\exp(-i\alpha_0 x)$$

Referential example: the fishnet

Reminder: **frequency dispersion**

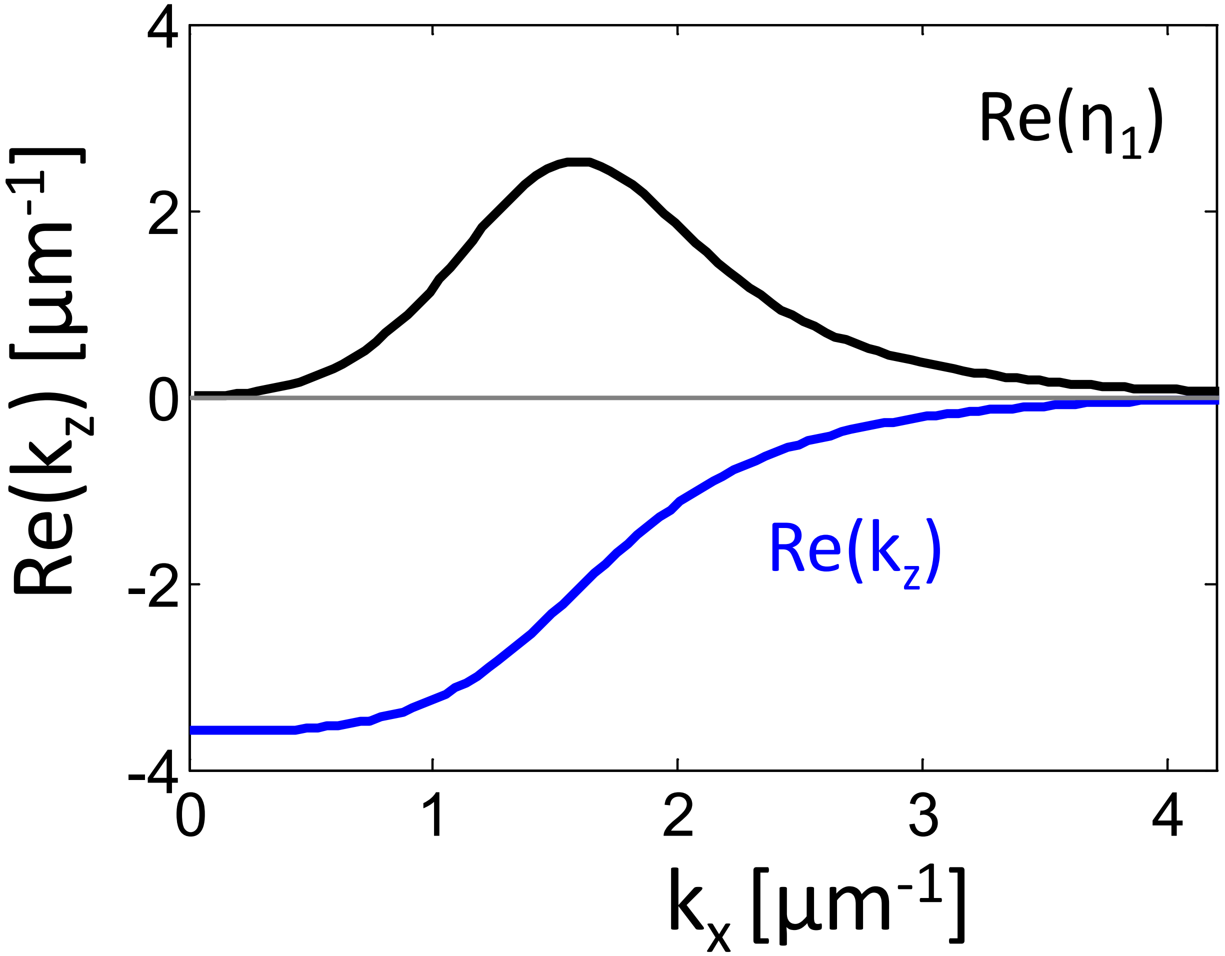


Reminder: **angular dispersion**

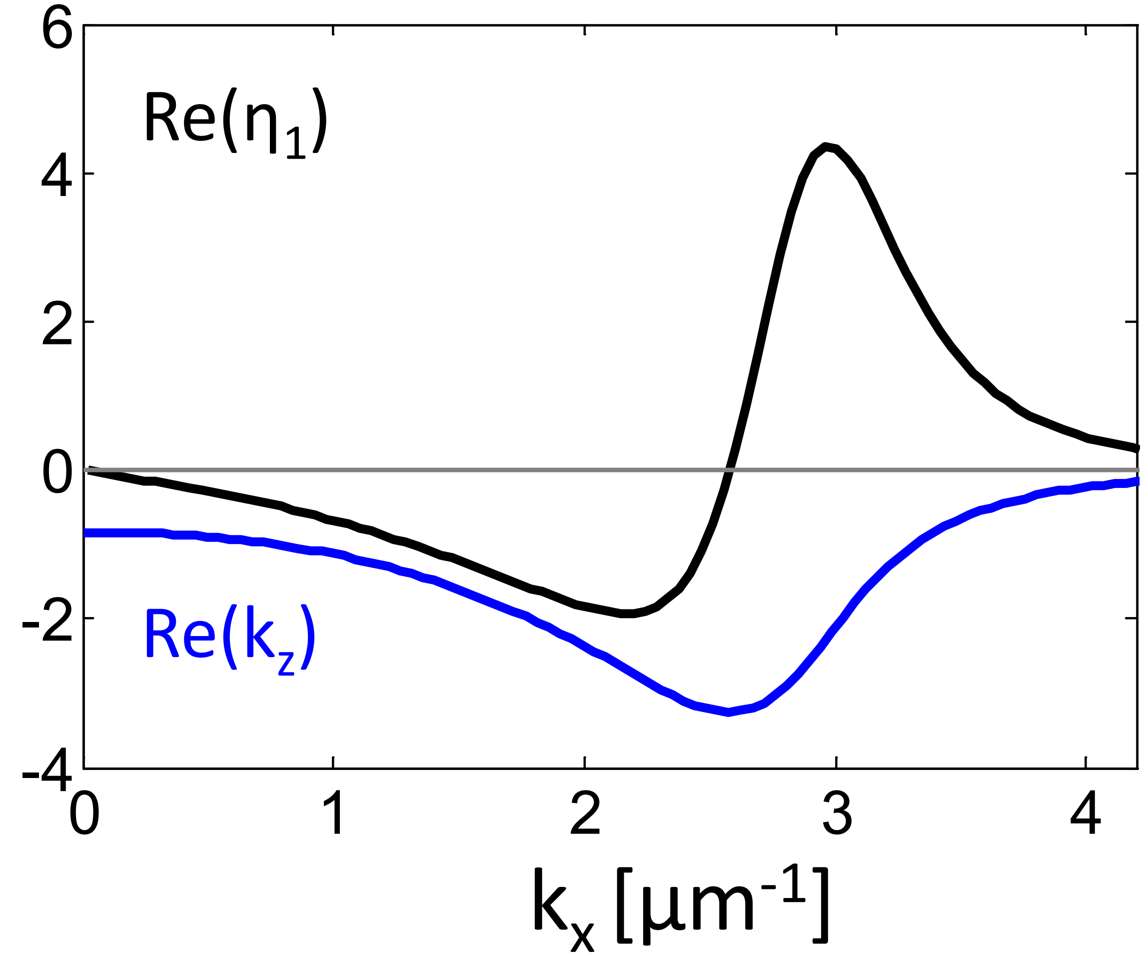


Angular dispersion

- $\omega = \omega_0$



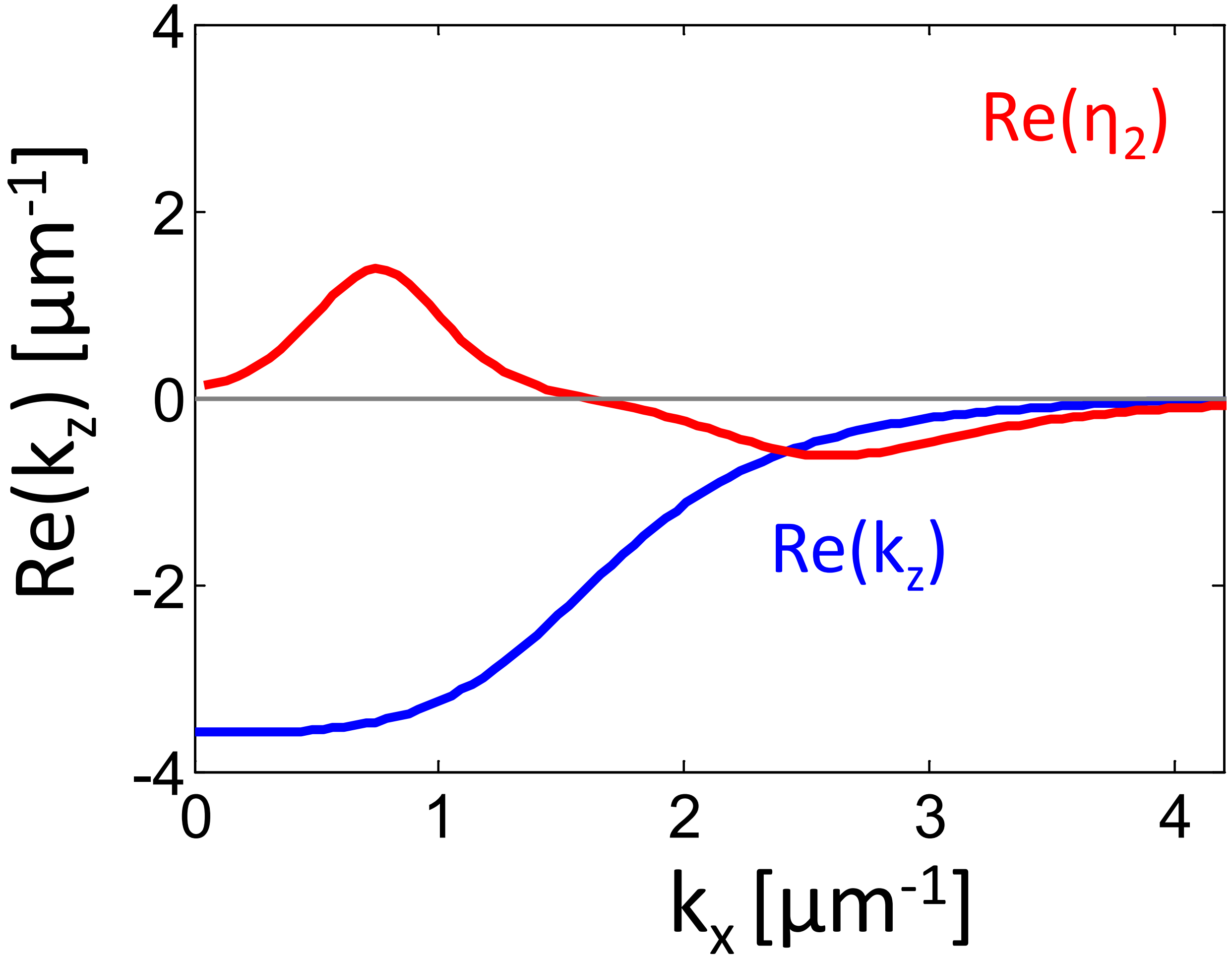
- $\omega > \omega_0$ ($\Delta\lambda \approx 50$nm)



- Negative refraction
- Positive refraction up to $k_x = 2.5\mu m^{-1}$

Angular dispersion

- $\omega = \omega_0$



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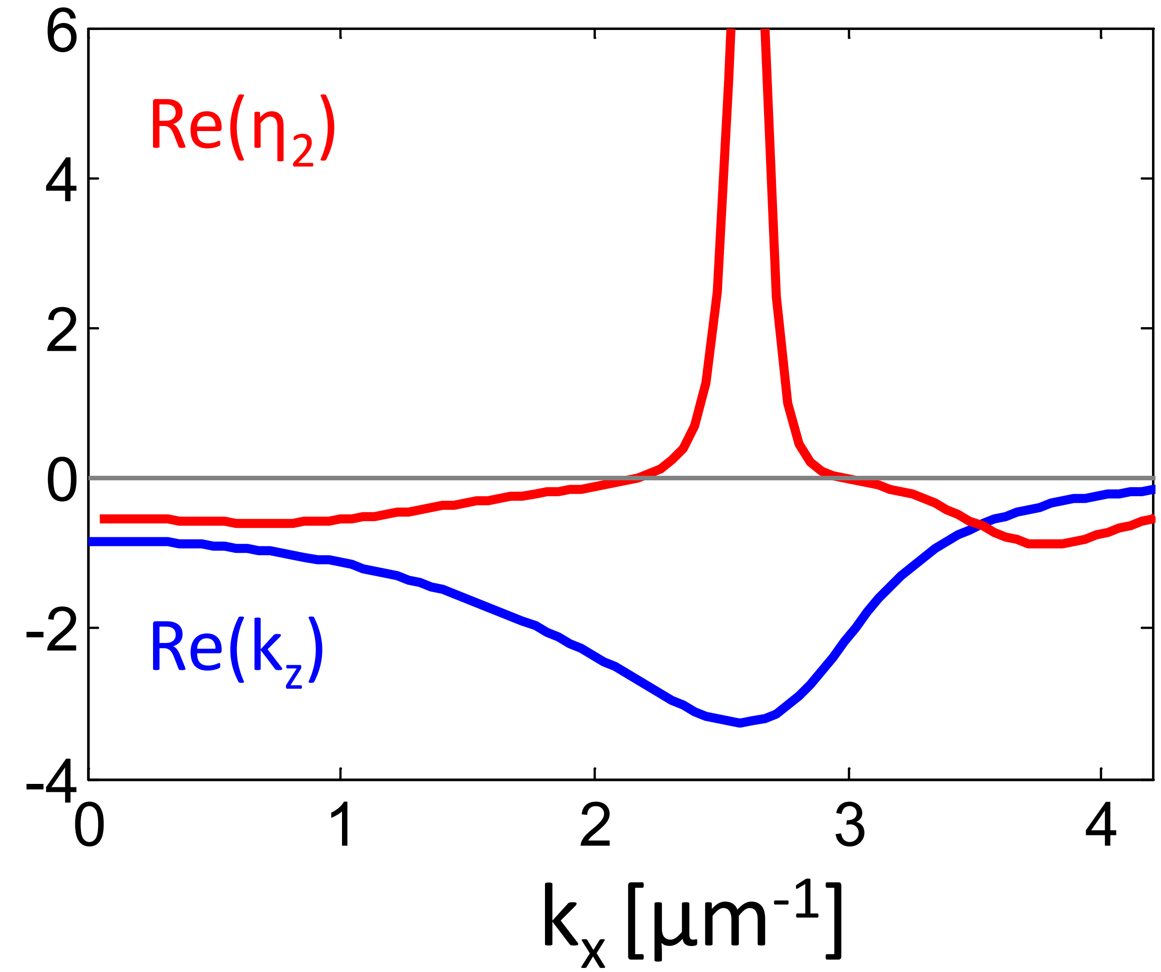

- Negative refraction
- Anomalous diffraction around $k_x=0$

- Positive refraction
- Normal diffraction around $k_x=0$

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