Modeling Electromagnetic Wave Interactions with Ferroelectric Vortex Lattices in the Sub-THz Regime

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Abstract

A frequency response in the sub-THz regime of strained ferroelectric materials forming chiral polar ferroelectric vortex-antivortex lattices (FVL) in a meta-stable state has been observed experimentally. In this contribution, we discuss the physics of the interactions in the sub-THz regime and aim at a corresponding numerical full-wave model.

1 Introduction

Conventional bulk ferroelectric materials have been used in electronic and optical devices for decades. The recent discovery of strained ferroelectric materials forming chiral polar ferroelectric vortex-antivortex lattices (FVL) in a meta-stable state and the experimental observation of a frequency response in the sub-THz regime [1] point to the potential of such materials to be used in electronic devices operating in the sub-THz regime. However, to understand the underlaying physics and to exploit the full potential of these materials, analytical and numerical models of their electromagnetic wave interaction are required but have yet to be developed.

2 Modeling

A schematical view of a FVL is shown in Fig. 1. The structure is invariant along the z-direction and the distance between the (anti-) periodic polar vortices is d and $2d$ in the x and y direction, respectively. One prominent candidate of such a strucutre consists of alternating perovskite layers of strontium titanate (STO) and lead titanate (PTO) grown on a dysprosium scandium oxide (DSO) substrate [not shown in the figure], where d is on the order of 10 nm [1]. Based on these size parameters in conjunction with Bloch's theorem, one assumes a frequency response in the optical regime. However, although counterintuitive, the experimental observation of a frequency response in the sub-THz regime, where the wavelength is on the order of 1 mm and thus drastically exceeds the size parameters of the FVL, has been reported [1]. The reason for this is a coupling of the electromagnetic wave with the polarization vortices, as given by the Maxwell equations

$$\nabla \times \mathbf{E} = -\mu_0 \frac{\partial \mathbf{H}}{\partial t}, \qquad (1a) \qquad\qquad \nabla \times \mathbf{H} = \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} + \frac{\partial \mathbf{P}}{\partial t}, \qquad (1b)$$

where $\mathbf{E}$, $\mathbf{H}$, and $\mathbf{P}$ are the electric field, magnetic field, and polarization density, respectively, and ε_0 and μ_0 are the vacuum permittivity and permeability. It should be noted that the polarization density $\mathbf{P}$ is a superposition of dielectric polarization density $\mathbf{P}_\mathrm{d}$ and spontaneous polarization density $\mathbf{P}_\mathrm{s}$ where the former describes the dielectric response of the material (usually

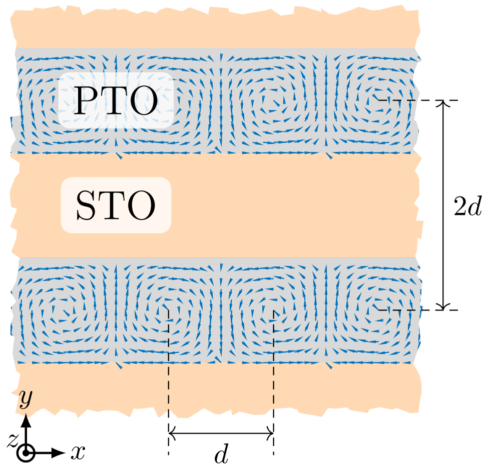

Figure 1: Cross-sectional view of a ferroelectric vortex lattice composed of alternating layers of PTO and STO. The spontaneous polarization $\mathbf{P}_s$ is indicated by the arrows and evolves predominantly in the PTO material. The distance between the polar vortices is d and $2d$ in x and y direction, respectively. The structure is assumed to be invariant along the z-direction.

taken into account via a relative permittivity ε_r) and the latter refers to the vortex lattice structure. Microscopically, the spontaneous polarization density is caused by discrete dipoles, indicated by the arrows in Fig. 1. Once an electromagnetic wave interacts [cf. (1a) and (1b)] with a FVL, the dipoles' steady state is slightly perturbed yielding a restoring force towards the steady state and subsequently an oscillation. This is the case for a transversal electric (with the axis of invariance) polarized wave, when the electric field lies in the same plane as the polarisation vortices. As experimental [1] and numerical [2] observations show, the eigenfrequency of these oscillations is in the sub-THz regime explaining the frequency response in this spectral regime. Contrary, in the case of a transversal magnetic wave, the electric field is perpendicular to the polarisation vortices, and hence no first-order (linear) interaction occurs [2].

To further investigate these interactions, rigorous numerical models are required. The core of these models is the description of the dipole dynamics in the FVL based on a second-order time-dependent Landau-Ginzburg-Devonshire (LGD) equation [3] minimizing the free energy of the system

$$\alpha_k \ddot{P}_i + \frac{1}{L}\dot{P}_i = -\frac{\delta F}{\delta P_i}, \tag{2}$$

where α_k and L are kinetic coefficients, index i indicates the directional components of a vector and F is the free energy functional of the system taking into account strain, depolarization, gradient energy effects and mechanical displacement.

The interaction with the electromagnetic wave in a full-wave manner is then described by solving the system of coupled differential equations (1a), (1b), and (2).

Acknowledgements

This work was supported by the Deutsche Forschungsgemeinschaft (DFG) through CRC/TRR 196 MARIE (287022738) under project M03.

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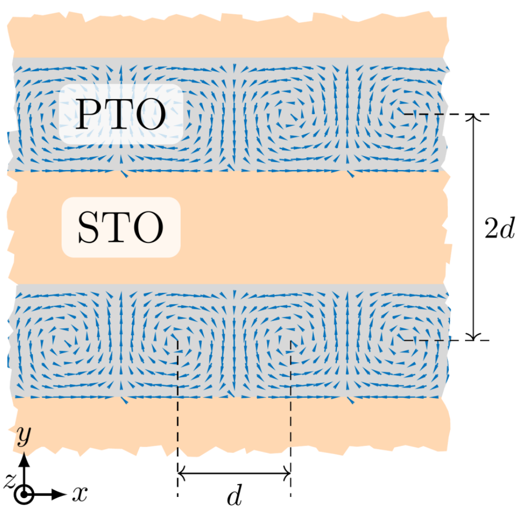
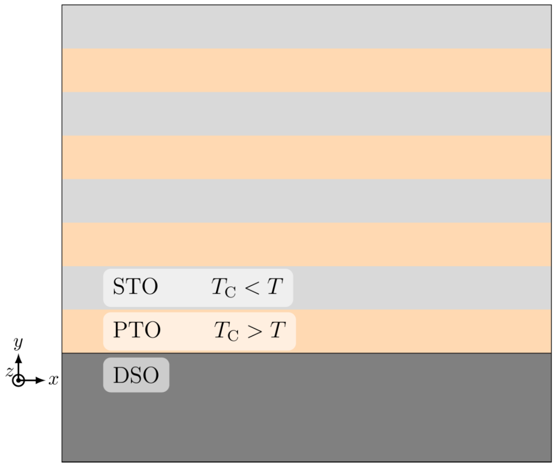
Outline

- Introduction
- EM-Wave-FVL-Interaction
  - Rotator model & Bloch mode analysis
  - Rigorous coupled wave method
  - T-matrix method and lattice sums (LS)-technique
- Model Including Ferroelectric Dynamics
  - FDTD-approach
  - Reductive perturbation method
- Conclusion and outlook



Introduction

- Strained alternating perovskite layers of ferroelectric materials
  - $T_{\mathrm{C,STO}} < T$ (Paraelectric)
  - $T_{\mathrm{C,PTO}} > T$ (Ferroelectric)
- Meta-stable state: polarization vortex-antivortex lattice



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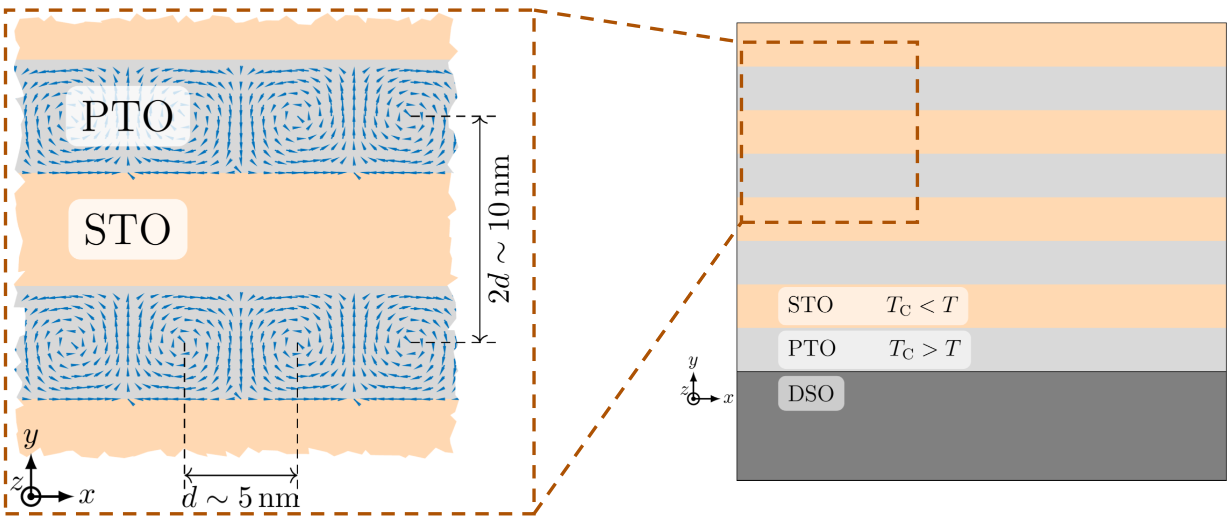

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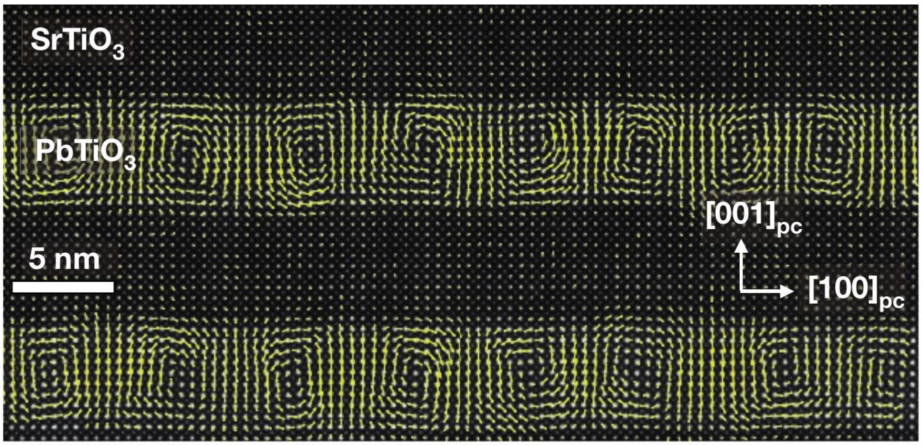

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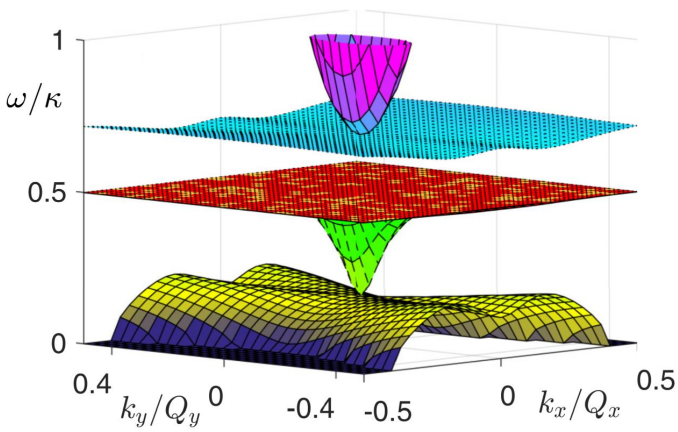
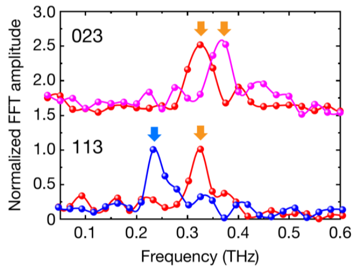
Introduction



[2] R. Khomeriki et al., „Photonic ferroelectric vortex lattice," *Phys. Rev. B*, vol. 109, no. 4, p. 045428, Jan. 2024.

- Period length: Frequency response in the optical range?
- Experimental [1] and numerical [2] observations: Frequency response in the sub-THz regime



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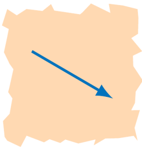
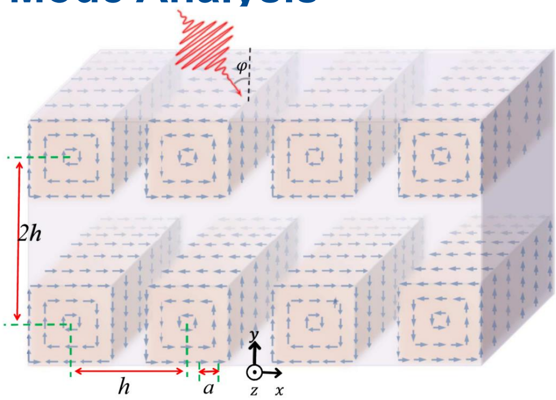
EM-Wave-FVL-Interaction – Bloch Mode Analysis

- Rotator-model

$$\hat{\mathbf{I}}\ddot{\boldsymbol{\alpha}} = \mathbf{d}\times\mathbf{E} + \mu_0 \boldsymbol{l}\times(\dot{\mathbf{d}}\times\mathbf{H})$$
$$\mathbf{d} = \mathbf{d}_0 + \delta\mathbf{d}(t); \quad \delta\mathbf{d} = \boldsymbol{\alpha}\times\mathbf{d}_0$$
$$\hat{\mathbf{I}}\delta\ddot{\mathbf{d}} = -\mathbf{d}_0\times(\mathbf{d}_0\times\mathbf{E})$$





$$\rightarrow \hat{\chi} = \begin{pmatrix} -\frac{d_{0y}^2}{\varepsilon_0\omega^2 I_z} & \cancel{\frac{d_{0y}d_{0x}}{\varepsilon_0\omega^2 I_z}} & 0 \\ \cancel{\frac{d_{0y}d_{0x}}{\varepsilon_0\omega^2 I_z}} & -\frac{d_{0x}^2}{\varepsilon_0\omega^2 I_z} & 0 \\ 0 & 0 & -\frac{d_{0x}^2+d_{0y}^2}{\varepsilon_0\omega^2 I_x} \end{pmatrix}$$

[2] R. Khomeriki et al., „Photonic ferroelectric vortex lattice," *Phys. Rev. B*, vol. 109, no. 4, p. 045428, Jan. 2024.

$$\hat{\varepsilon} = \begin{pmatrix} \varepsilon_x & 0 & 0 \\ 0 & \varepsilon_y & 0 \\ 0 & 0 & \varepsilon_z \end{pmatrix}$$

Fourier series →

$$\varepsilon_x = \varepsilon_y = \varepsilon_0 - \frac{\varepsilon_0\kappa^2}{4\,\omega^2}\left(1+\frac{4}{\pi}\cos\left(\frac{Q\,y}{2}\right)+\cdots\right)\left(1+\frac{4}{\pi}\cos(Q\,x)+\cdots\right)$$

EM-Wave-FVL-Interaction – Bloch Mode Analysis

$$\hat{\boldsymbol{\varepsilon}} = \begin{pmatrix} \varepsilon_x & 0 & 0 \\ 0 & \varepsilon_y & 0 \\ 0 & 0 & \varepsilon_z \end{pmatrix}$$

Fourier series →

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$$\varepsilon_z = \varepsilon_0 - \frac{\varepsilon_0(\kappa')^2}{2\,\omega^2}\left(1+\frac{4}{\pi}\cos\left(\frac{Q\,y}{2}\right)+\cdots\right)$$

- Wave equation:

$$\Delta\mathbf{E} - \nabla(\nabla\cdot\mathbf{E}) = -\frac{\omega^2\hat{\boldsymbol{\varepsilon}}\cdot\mathbf{E}}{c^2\varepsilon_0}$$

→

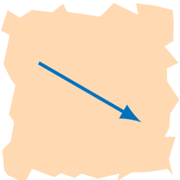
$$\left(\frac{\omega^2}{c^2}-\frac{\kappa^2}{4\,c^2}-k_y^2\right)E_{\mathbf{k}}^x + k_x k_y E_{\mathbf{k}}^y = \sum_s\left(\frac{\kappa_s^x}{c^2}\,E_{\mathbf{k}+\mathbf{Q}_s}^x\right)$$
$$\left(\frac{\omega^2}{c^2}-\frac{\kappa^2}{4\,c^2}-k_x^2\right)E_{\mathbf{k}}^y + k_x k_y E_{\mathbf{k}}^x = \sum_s\left(\frac{\kappa_s^y}{c^2}\,E_{\mathbf{k}+\mathbf{Q}_s}^y\right)$$
$$\left(\frac{\omega^2}{c^2}-\frac{(\kappa')^2}{2\,c^2}-k_x^2-k_y^2\right)E_{\mathbf{k}}^z = \frac{(\kappa')^2}{\pi c^2}\left(E_{\mathbf{k}+\mathbf{Q}_y}^z + E_{\mathbf{k}-\mathbf{Q}_y}^z\right)$$

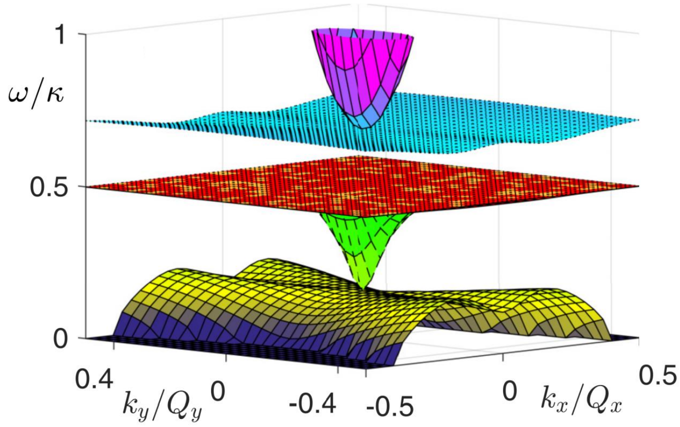
EM-Wave-FVL-Interaction – Bloch Mode Analysis

$$\hat{\boldsymbol{\varepsilon}} = \begin{pmatrix} \varepsilon_x & 0 & 0 \\ 0 & \varepsilon_y & 0 \\ 0 & 0 & \varepsilon_z \end{pmatrix}$$

- Wave equation:

$$\Delta \mathbf{E} - \nabla(\nabla \cdot \mathbf{E}) = -\frac{\omega^2 \hat{\boldsymbol{\varepsilon}} \cdot \mathbf{E}}{c^2 \varepsilon_0}$$





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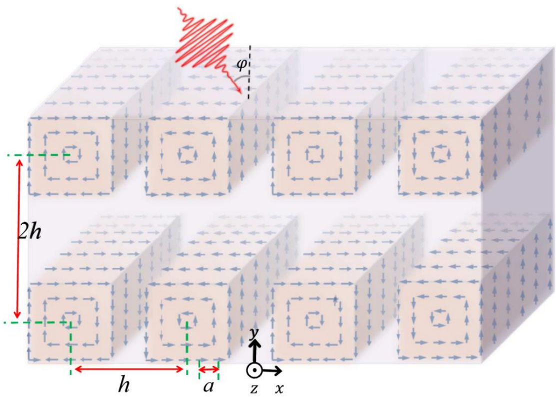
EM-Wave-FVL-Interaction – Rigorous Coupled-Wave Method [4,5]

- Fourier expansion of $\mathbf{E}$ and $\mathbf{H}$

$$\begin{pmatrix} E_x \\ E_z \\ H_x \\ H_z \end{pmatrix} = \sum_{n=-N}^{N} \begin{pmatrix} e_{xn} \\ e_{zn} \\ Y_0\, h_{xn} \\ Y_0 h_{zn} \end{pmatrix} \cdot e^{j\left(k_x + \frac{2\pi n}{h}\right)x}, \quad Y_0 = \sqrt{\frac{\varepsilon_0}{\mu_0}}$$

$$\frac{\mathrm{d}}{\mathrm{d}y} \begin{pmatrix} \boldsymbol{e}_x \\ \boldsymbol{e}_z \\ \boldsymbol{h}_x \\ \boldsymbol{h}_z \end{pmatrix} = i\frac{\omega}{c} \begin{pmatrix} \boldsymbol{U}_{11} & 0 & 0 & \boldsymbol{U}_{14} \\ 0 & 0 & \boldsymbol{I} & 0 \\ 0 & \boldsymbol{U}_{32} & 0 & 0 \\ \boldsymbol{U}_{41} & 0 & 0 & \boldsymbol{U}_{44} \end{pmatrix} \cdot \begin{pmatrix} \boldsymbol{e}_x \\ \boldsymbol{e}_z \\ \boldsymbol{h}_x \\ \boldsymbol{h}_z \end{pmatrix}$$



[2] R. Khomeriki et al., „Photonic ferroelectric vortex lattice," *Phys. Rev. B*, vol. 109, no. 4, p. 045428, Jan. 2024.

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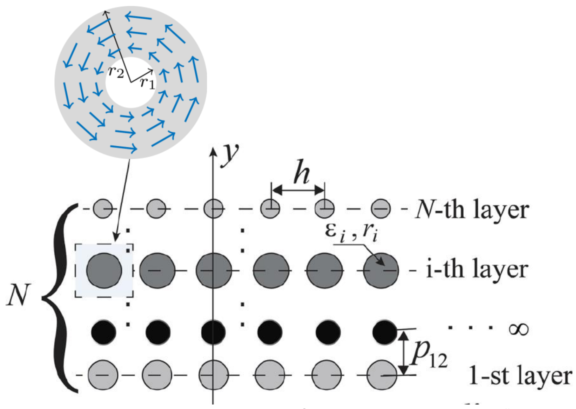
EM-Wave-FVL-Interaction – T-Matrix Method with Lattice Sums [6]

- **T**-matrix: Relating expansion coefficients of incident and scattered field

$$T_n = -\frac{B_{1n}\,J_n'(k_0 r_2) - B_{2n}\,J_n(k_0 r_2)}{B_{3n}\,H_n^{(1)'}(k_0 r_2) - B_{4n}\,H_n^{(1)}(k_0 r_2)}$$

- Accounting for the vortex texture in $B_{i\,n}$
- Lattice sums: solving the scattering problem of a periodic structure



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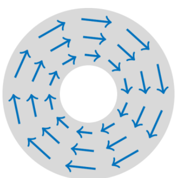
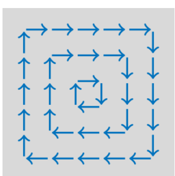
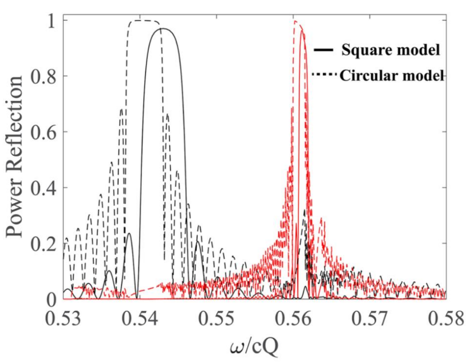
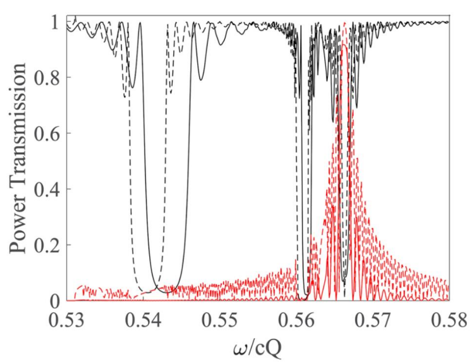
EM-Wave-FVL-Interaction – T-Matrix Method with Lattice Sums

- Comparison of the square and circular model









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Model Including Ferroelectric Dynamics – FDTD

- More sophisticated model: Ferroelectric dynamics
- Governing equations:
  - Time-dependent Landau-Ginzburg-Devonshire equation
  - (elastodynamic equation)
  - Maxwell equations
- Dependent variables (TE): P_x, P_y, E_x, E_y, H_z
- Discretization in space and time (Yee-discretization, FDTD)

$$\alpha_k \ddot{P}_i + \frac{1}{L}\dot{P} = -\frac{\delta F}{\delta P_i} \qquad (1)$$

$$\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = -\mu_0 \frac{\partial H_z}{\partial t} \qquad (2)$$

$$\varepsilon_0 \varepsilon_{11} \frac{\partial E_x}{\partial t} + \frac{\partial P_x}{\partial t} = \frac{\partial H_z}{\partial y} \qquad (3)$$

$$\varepsilon_0 \varepsilon_{33} \frac{\partial E_y}{\partial t} + \frac{\partial P_y}{\partial t} = -\frac{\partial H_z}{\partial x} \qquad (4)$$

$$F = \iiint \left(\alpha_{ij} P_i P_j + \alpha_{ijk\ell} P_i P_j P_k P_\ell + \alpha_{ijklmn} P_i P_j P_k P_\ell P_m P_n + \frac{1}{2} g_{ijkl} \frac{\partial P_i}{\partial x_j} \frac{\partial P_k}{\partial x_\ell} + \frac{1}{2} c_{ijkl} \varepsilon_{ij} \varepsilon_{kl} - q_{ijkl} \varepsilon_{ij} P_k P_\ell - \frac{1}{2} \kappa_b E_i E_i - E_i P_i \right) \mathrm{d}V$$

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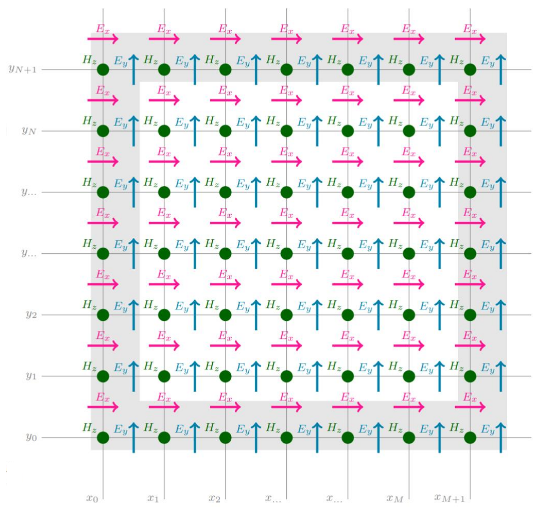
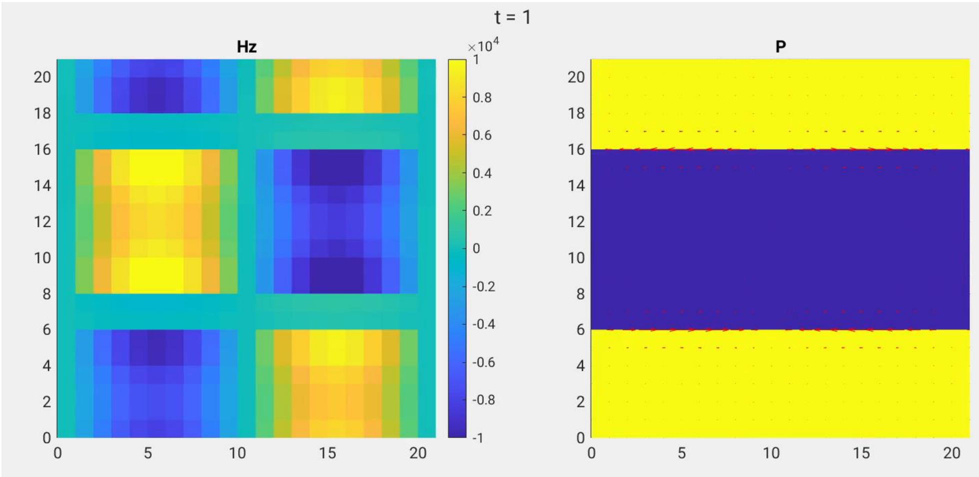


Model Including Ferroelectric Dynamics – FDTD



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Model Including Ferroelectric Dynamics – Perturbation method

$$\alpha_k \ddot{P}_i + \frac{1}{L}\dot{P} = -\frac{\delta F}{\delta P_i}$$

$$\rho \ddot{u}_i + \beta \dot{u}_i = -\frac{\delta F}{\delta u_i}$$

$$\frac{1}{c^2}\left(\varepsilon_0 \ddot{E}_i + \ddot{P}_i\right) = \varepsilon_0 \Delta E_i + \nabla_i(\nabla \cdot \mathbf{P})$$

$$\alpha_k \ddot{P}_x = g_0\left(\frac{\partial^2 P_x}{\partial x^2} + \frac{\partial^2 P_x}{\partial y^2}\right) - 2\, a_1 P_x + E_x \underbrace{-4\, a_{11} P_x^3 - 2\, a_{12} P_x P_y^2 - 6\, a_{111} P_x^5 - \dots}_{N_x(\mathbf{P})}$$

$$\frac{1}{c^2}\left(\varepsilon \ddot{E}_x + \ddot{P}_x\right) = \varepsilon\left(\frac{\partial^2 E_x}{\partial x^2} + \frac{\partial^2 E_x}{\partial y^2}\right) + \frac{\partial^2 P_x}{\partial x^2} + \frac{\partial^2 P_y}{\partial x\, \partial y}$$

- Reductive perturbation theory [7]: $\mathbf{p}(t,\mathbf{r}) = \sum_{s=1}^{\infty} \alpha^s \sum_{m=-\infty}^{\infty} \mathbf{p}_m^s(\alpha t, \alpha^{2t}, \dots, \mathbf{r})\, \mathrm{e}^{jm\omega t}$
- Linear approximation: $s = 1$, $m = 1$

$$\alpha_k \omega^2 p_{mx}^{(1)} + g_0\left(\frac{\partial^2 p_{mx}^{(1)}}{\partial x^2} + \frac{\partial^2 p_{mx}^{(1)}}{\partial y^2}\right) + \delta E_{mx}^{(1)} - V_x p_{mx}^{(1)} = 0,$$

$$\varepsilon\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\delta E_{my}^{(1)} + \frac{\partial^2 p_{my}^{(1)}}{\partial y^2} + \frac{\partial^2 p_{mx}^{(1)}}{\partial x\, \partial y} = 0$$

$V_x = 2a_1(y) + G_x(x,y)$ → periodic

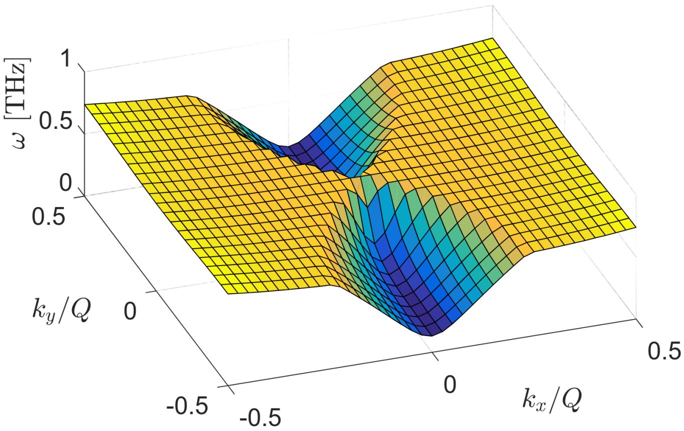
Solutions: Bloch waves

[7] T. Taniuti and N. Yajima, „Perturbation method for nonlinear wave modulation. I," *J. Math. Phys.*, vol. 10, no. 8, pp. 1369-1372, Aug. 1969.

Model Including Ferroelectric Dynamics – Perturbation method

$$\alpha_k \ddot{P}_i + \frac{1}{L}\dot{P} = -\frac{\delta F}{\delta P_i}$$
$$\rho \ddot{u}_i + \beta \dot{u}_i = -\frac{\delta F}{\delta u_i}$$
$$\frac{1}{c^2}\left(\varepsilon_0 \ddot{E}_i + \ddot{P}_i\right) = \varepsilon_0 \Delta E_i + \nabla_i(\nabla \cdot \mathbf{P})$$

- Reductive perturbation theory [7]:
- Linear approximation: $s = 1$, $m = 1$



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Conclusion and Outlook

- Interaction of EM-Waves with ferroelectric vortex lattices have been modeled using different models:
  - Rotator-model with Bloch-mode analysis
  - Rigorous coupled wave method
  - T-matrix method with lattice sums technique
- Ferroelectric dynamics are incorporated via TD-LGD equation using 2 methods:
  - Extended FDTD approach
  - Reductive perturbation method
- EM-Wave interaction including ferroelectric dynamics will be studied:
  - FDTD-approach
  - Reductive perturbation method (nonlinear) → nonlinear Schrödinger equation

Thank you for your attention!

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