

Photonic modes in colloidal / complex nematic resonators

Iztok Bajc

Frédéric Hecht

Slobodan Žumer

Univerza v Ljubljani



Fakulteta za matematiko in fiziko

Univerza v Ljubljani

Slovenija



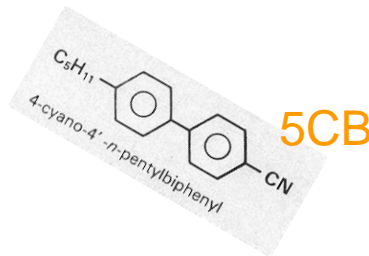
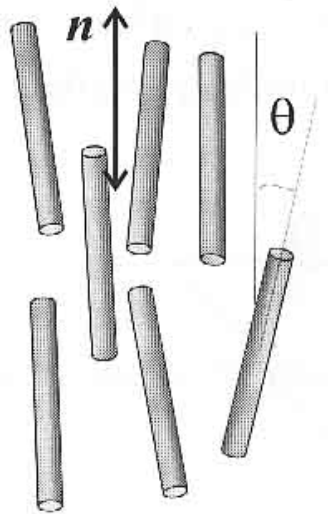
Outline

- **Nematic liquid crystals - properties**
- **Motivational nematic photonic systems**
- **Computational methods**
- **Example: EM eigen modes in a nematic system**
- **Possible further work**

Nematic liquid crystals

Liquid crystals (LC) are an oily material:

- Flow like a *liquid*
- But are also *partially ordered* - like *crystals*.
- In nematic LC molecules are *rodlike*.
- Tend to align in a *preferred direction*.

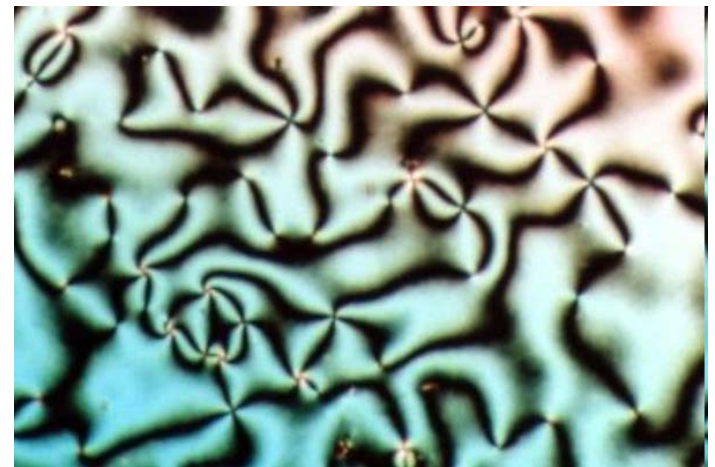


Isotropic liquid phase
(higher temperature)

Low enough
temperature



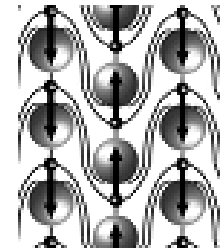
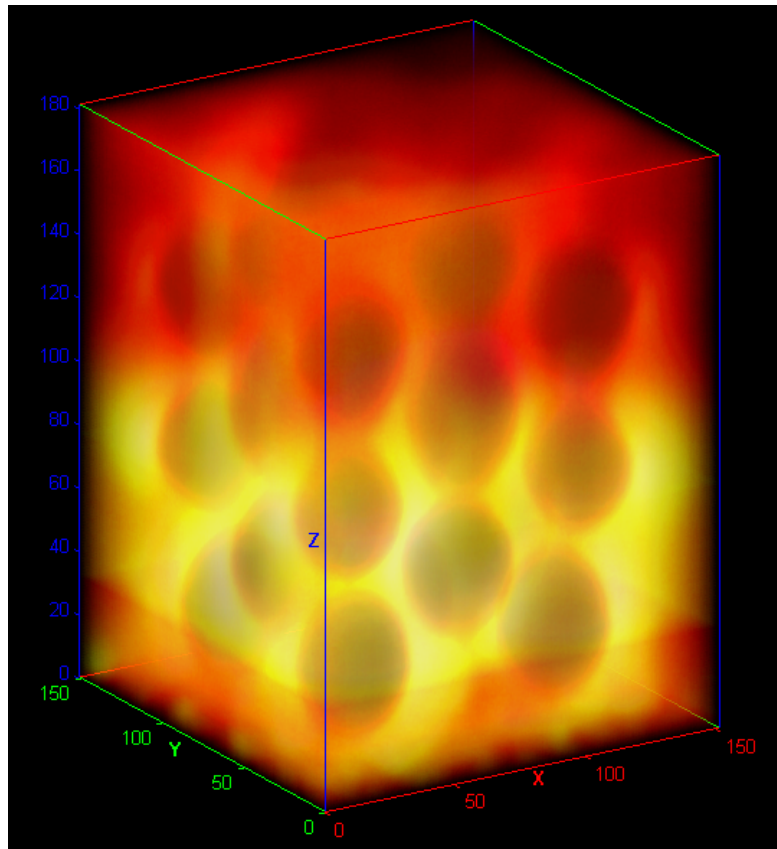
Partially ordered



Motivational system 1:

Nematic photonic crystals

Larger 3D
structures



3×3×3 dipolar crystal.

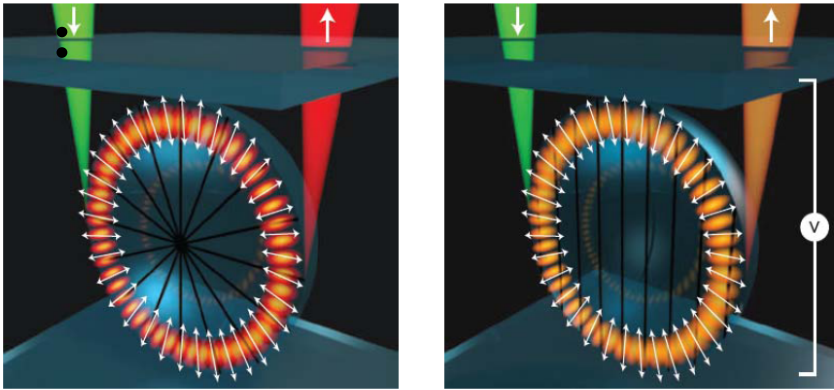
Experiment by Andriy Nych,
2012 (*submitted*).

(Recently built
also 6×6×6)

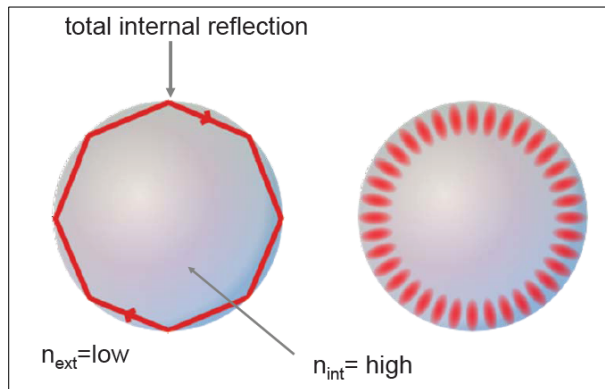
Motivational systems 2,3:

Nematic and chiral nematic droplets

2



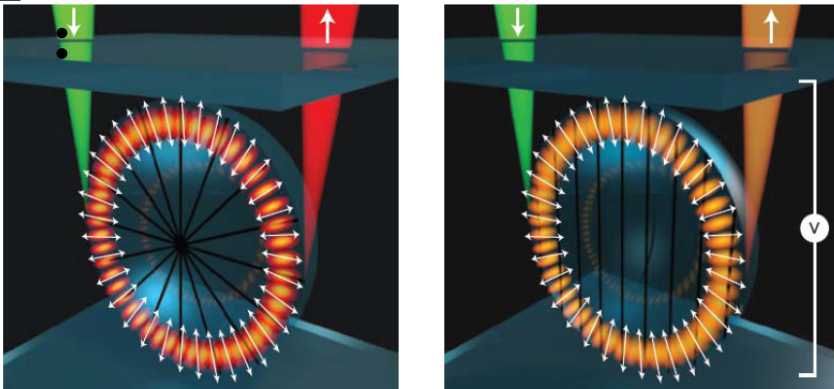
Whispering Gallery Modes (WGM) in a **microresonator**.



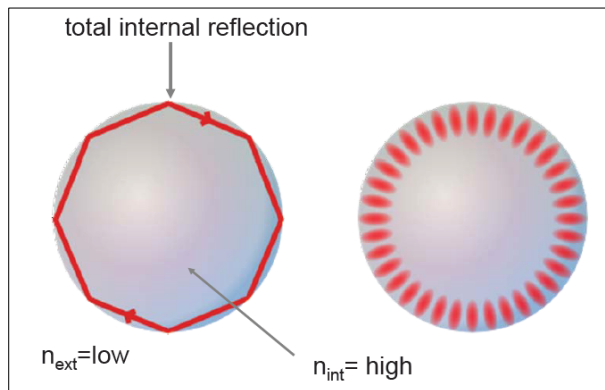
Motivational systems 2,3:

Nematic and chiral nematic droplets

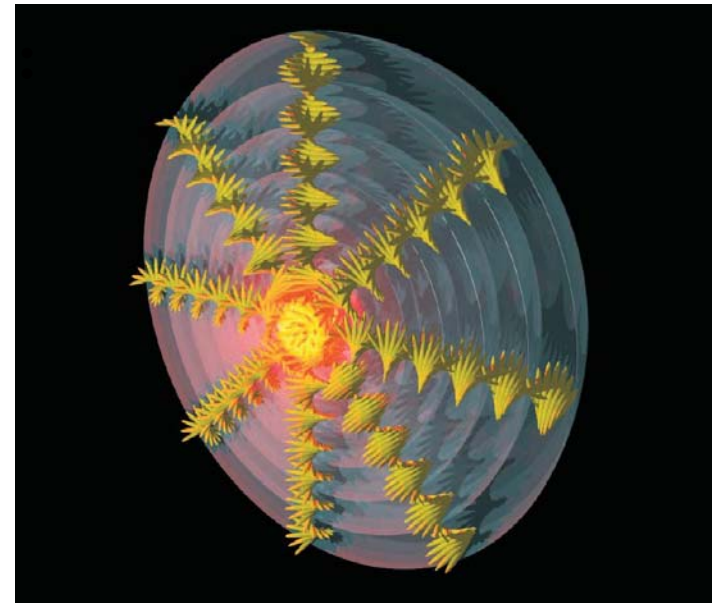
2



Whispering Gallery Modes (WGM) in a **microresonator**.



3



M. Humar, I. Muševič, *3D microlasers from self-assembled cholesteric LC*, Optics Express, 2010.

Bragg-onion optical microcavity ($R \sim 15\mu\text{m}$):
stimulated light emission (from dye molecules in the liquid crystal).

Computational photonics

- **Detail dimensions** comparable with **wavelength**.



*Numerical solution of **full** Maxwell equations*

Time-harmonic expansion

1) Time-domain **propagation**

2) Frequency-domain **response**

3) Frequency-domain **eigen problems**

Eigen problems in frequency-domain

Maxwell equations:

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\vec{\nabla} \times \vec{H} = \frac{\partial \vec{D}}{\partial t}$$

$$\vec{\nabla} \cdot \vec{H} = 0$$

$$\vec{\nabla} \cdot \vec{D} = 0$$

Eigen problems in frequency-domain

Maxwell equations:

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\vec{\nabla} \times \vec{H} = \frac{\partial \vec{D}}{\partial t}$$

$$\vec{\nabla} \cdot \vec{H} = 0$$

$$\vec{\nabla} \cdot \vec{D} = 0$$

Time-harmonic expansion

$$\vec{E}(\vec{r}, t) = \vec{E}(\vec{r})e^{i\omega t}$$

Eigen problems in frequency-domain

Maxwell equations:

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\vec{\nabla} \times \vec{H} = \frac{\partial \vec{D}}{\partial t}$$

$$\vec{\nabla} \cdot \vec{H} = 0$$

$$\vec{\nabla} \cdot \vec{D} = 0$$

Time-harmonic expansion

$$\vec{E}(\vec{r}, t) = \vec{E}(\vec{r})e^{i\omega t}$$

Constitutive relations

$$\vec{D} = \underline{\underline{\epsilon}}(\vec{r})\vec{E}$$

$$\vec{B} = \mu\vec{H} \approx \vec{H}$$

Eigen problems in frequency-domain

Maxwell equations:

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\vec{\nabla} \times \vec{H} = \frac{\partial \vec{D}}{\partial t}$$

$$\vec{\nabla} \cdot \vec{H} = 0$$

$$\vec{\nabla} \cdot \vec{D} = 0$$

Time-harmonic expansion

$$\vec{E}(\vec{r}, t) = \vec{E}(\vec{r})e^{i\omega t}$$

Constitutive relations

$$\vec{D} = \underline{\underline{\epsilon}}(\vec{r})\vec{E}$$

$$\vec{B} = \mu\vec{H} \approx \vec{H}$$

$$\vec{\nabla} \times \vec{E} = i\omega\vec{B}$$

$$\vec{\nabla} \times \vec{H} = -i\omega\underline{\underline{\epsilon}}(\vec{r})\vec{E}$$

$$\vec{\nabla} \cdot \vec{H} = 0$$

$$\vec{\nabla} \cdot [\underline{\underline{\epsilon}}(\vec{r})\vec{E}] = 0$$

Eigen problems in frequency-domain

Maxwell equations:

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\vec{\nabla} \times \vec{H} = \frac{\partial \vec{D}}{\partial t}$$

$$\vec{\nabla} \cdot \vec{H} = 0$$

$$\vec{\nabla} \cdot \vec{D} = 0$$

Time-harmonic expansion

$$\vec{E}(\vec{r}, t) = \vec{E}(\vec{r})e^{i\omega t}$$

Constitutive relations

$$\vec{D} = \underline{\underline{\epsilon}}(\vec{r})\vec{E}$$

$$\vec{B} = \mu\vec{H} \approx \vec{H}$$

$$\vec{\nabla} \times \vec{E} = i\omega\vec{B}$$

$$\vec{\nabla} \times \vec{H} = -i\omega\underline{\underline{\epsilon}}(\vec{r})\vec{E}$$

$$\vec{\nabla} \cdot \vec{H} = 0$$

$$\vec{\nabla} \cdot [\underline{\underline{\epsilon}}(\vec{r})\vec{E}] = 0$$

$$\vec{\nabla} \times \underline{\underline{\epsilon}}(\vec{r})^{-1} \vec{\nabla} \times \vec{H} = \omega^2 \vec{H}$$

$$\vec{\nabla} \cdot \vec{H} = 0$$

+ Boundary conditions

(For ideal conductor:

$$\vec{H} \cdot \vec{\nu} = 0)$$

Eigen problems in frequency-domain

Maxwell equations:

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\vec{\nabla} \times \vec{H} = \frac{\partial \vec{D}}{\partial t}$$

$$\vec{\nabla} \cdot \vec{H} = 0$$

$$\vec{\nabla} \cdot \vec{D} = 0$$

Time-harmonic expansion

$$\vec{E}(\vec{r}, t) = \vec{E}(\vec{r})e^{i\omega t}$$

Constitutive relations

$$\vec{D} = \underline{\underline{\epsilon}}(\vec{r})\vec{E}$$

$$\vec{B} = \mu\vec{H} \approx \vec{H}$$

$$\vec{\nabla} \times \vec{E} = i\omega\vec{B}$$

$$\vec{\nabla} \times \vec{H} = -i\omega\underline{\underline{\epsilon}}(\vec{r})\vec{E}$$

$$\vec{\nabla} \cdot \vec{H} = 0$$

$$\vec{\nabla} \cdot [\underline{\underline{\epsilon}}(\vec{r})\vec{E}] = 0$$

**Vector Helmholtz
eigen equation**
(the *curl-curl eqn*)

$$\vec{\nabla} \times \underline{\underline{\epsilon}}(\vec{r})^{-1} \vec{\nabla} \times \vec{H} = \omega^2 \vec{H}$$

$$\vec{\nabla} \cdot \vec{H} = 0$$

+ Boundary conditions

(For ideal conductor:

$$\vec{H} \cdot \vec{\nu} = 0)$$

Eigen problems in frequency-domain

Maxwell equations:

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\vec{\nabla} \times \vec{H} = \frac{\partial \vec{D}}{\partial t}$$

$$\vec{\nabla} \cdot \vec{H} = 0$$

$$\vec{\nabla} \cdot \vec{D} = 0$$

Time-harmonic expansion

$$\vec{E}(\vec{r}, t) = \vec{E}(\vec{r})e^{i\omega t}$$

Constitutive relations

$$\vec{D} = \underline{\underline{\varepsilon}}(\vec{r})\vec{E}$$

$$\vec{B} = \mu\vec{H} \approx \vec{H}$$

$$\vec{\nabla} \times \vec{E} = i\omega\vec{B}$$

$$\vec{\nabla} \times \vec{H} = -i\omega\underline{\underline{\varepsilon}}(\vec{r})\vec{E}$$

$$\vec{\nabla} \cdot \vec{H} = 0$$

$$\vec{\nabla} \cdot [\underline{\underline{\varepsilon}}(\vec{r})\vec{E}] = 0$$

Fully anisotropic permittivity

**Vector Helmholtz
eigen equation**
(the *curl-curl* eqn)

$$\vec{\nabla} \times \underline{\underline{\varepsilon}}(\vec{r})^{-1} \vec{\nabla} \times \vec{H} = \omega^2 \vec{H}$$

$$\vec{\nabla} \cdot \vec{H} = 0$$

+ Boundary conditions

(For ideal conductor:

$$\vec{H} \cdot \vec{\nu} = 0)$$

Helmholtz and Schroedinger eqns

Helmholtz and Schroedinger eqns

Vector Helmholtz equation

$$\vec{\nabla} \times \underline{\underline{\epsilon}}(\vec{r})^{-1} \vec{\nabla} \times \vec{H} = \omega^2 \vec{H}$$

+ **condition** $\vec{\nabla} \cdot \vec{H} = 0$

Schroedinger equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(\vec{r})\psi = E\psi$$

Helmholtz and Schroedinger eqns

Vector Helmholtz equation

$$\vec{\nabla} \times \underline{\underline{\epsilon}}(\vec{r})^{-1} \vec{\nabla} \times \vec{H} = \omega^2 \vec{H}$$

+ condition $\vec{\nabla} \cdot \vec{H} = 0$

Schroedinger equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(\vec{r})\psi = E\psi$$

- **Helmholtz eigen problem** shares some similarities with **Schroedinger eigen problem** for noninteracting electrons (mathematical, and to some extent also numerical).

Helmholtz and Schroedinger eqns

Vector Helmholtz equation

$$\vec{\nabla} \times \underline{\underline{\epsilon}}(\vec{r})^{-1} \vec{\nabla} \times \vec{H} = \omega^2 \vec{H}$$

+ condition $\vec{\nabla} \cdot \vec{H} = 0$

Schroedinger equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(\vec{r})\psi = E\psi$$

- **Helmholtz eigen problem** shares some similarities with **Schroedinger eigen problem** for noninteracting electrons (mathematical, and to some extent also numerical).
- *One of the differences:* Helmholtz scale independent (radio-, micro-, optical waves,...), while in Schroedinger scale set by Planck constant.

Helmholtz and Schroedinger eqns

Vector Helmholtz equation

$$\vec{\nabla} \times \underline{\underline{\epsilon}}(\vec{r})^{-1} \vec{\nabla} \times \vec{H} = \omega^2 \vec{H}$$

+ condition $\vec{\nabla} \cdot \vec{H} = 0$

Schroedinger equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(\vec{r})\psi = E\psi$$

- **Helmholtz eigen problem** shares some similarities with **Schroedinger eigen problem** for **noninteracting electrons** (mathematical, and to some extent also numerical).
- *One of the differences:* Helmholtz scale independent (radio-, micro-, optical waves,...), while in Schroedinger scale set by Planck constant.
- But the underlying physics is different. → The quantum world quite tricky.

Helmholtz and Schroedinger eqns

Vector Helmholtz equation

$$\vec{\nabla} \times \underline{\underline{\varepsilon}}(\vec{r})^{-1} \vec{\nabla} \times \vec{H} = \omega^2 \vec{H}$$

+ condition $\vec{\nabla} \cdot \vec{H} = 0$

Schroedinger equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(\vec{r})\psi = E\psi$$

- **Helmholtz eigen problem** shares some similarities with **Schroedinger eigen problem** for noninteracting electrons (mathematical, and to some extent also numerical).
- *One of the differences:* Helmholtz scale independent (radio-, micro-, optical waves,...), while in Schroedinger scale set by Planck constant.
- But the underlying physics is different. → The quantum world quite tricky.
- Example of Schroedinger eqn with periodic b.c. and localized defects: [1].

Formulation and numerics for Helmholtz

Formulation and numerics for Helmholtz

$$\int_{\Omega} \varepsilon(\vec{r})^{-1} (\vec{\nabla} \times \vec{H}) \cdot (\vec{\nabla} \times \vec{V}) d\Omega = \omega^2 \int_{\Omega} \vec{H} \cdot \vec{V} d\Omega$$

*Basic variational
formulation of
Helmholtz eqn*

[1] A. Bossavit, *Computational Electromagnetism*, Academic Press, 1998.

[2] J.C. Nédélec, *Mixed Finite Elements in R^3* , Numer. Math. 35, 315 - 341 (1980).

Formulation and numerics for Helmholtz

$$\int_{\Omega} \varepsilon(\vec{r})^{-1} (\vec{\nabla} \times \vec{H}) \cdot (\vec{\nabla} \times \vec{V}) d\Omega = \omega^2 \int_{\Omega} \vec{H} \cdot \vec{V} d\Omega$$

+ variational terms [1] to impose $\operatorname{div} H = 0$

(to avoid “spurious modes”)

*Basic variational
formulation of
Helmholtz eqn*

[1] A. Bossavit, *Computational Electromagnetism*, Academic Press, 1998.

[2] J.C. Nédélec, *Mixed Finite Elements in R^3* , Numer. Math. 35, 315 - 341 (1980).

Formulation and numerics for Helmholtz

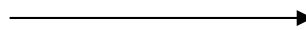
$$\int_{\Omega} \varepsilon(\vec{r})^{-1} (\vec{\nabla} \times \vec{H}) \cdot (\vec{\nabla} \times \vec{V}) d\Omega = \omega^2 \int_{\Omega} \vec{H} \cdot \vec{V} d\Omega$$

+ variational terms [1] to impose $\text{div } H = 0$

(to avoid “spurious modes”)

Rewritten into a code in
FreeFem++, it reduces to a
sparse matrix eigen problem:

$$Ax = \omega^2 Bx$$



Solved with C++ module
Arpack++ for large eigen
systems.

*Basic variational
formulation of
Helmholtz eqn*

[1] A. Bossavit, *Computational Electromagnetism*, Academic Press, 1998.

[2] J.C. Nédélec, *Mixed Finite Elements in R^3* , Numer. Math. 35, 315 - 341 (1980).

Formulation and numerics for Helmholtz

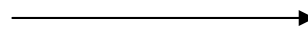
$$\int_{\Omega} \varepsilon(\vec{r})^{-1} (\vec{\nabla} \times \vec{H}) \cdot (\vec{\nabla} \times \vec{V}) d\Omega = \omega^2 \int_{\Omega} \vec{H} \cdot \vec{V} d\Omega$$

+ variational terms [1] to impose $\text{div } H = 0$

(to avoid “spurious modes”)

Rewritten into a code in
FreeFem++, it reduces to a
sparse matrix eigen problem:

$$Ax = \omega^2 Bx$$



Solved with C++ module
Arpack++ for large eigen
systems.

*Basic variational
formulation of
Helmholtz eqn*

Edge (Nedelec) vector elements [1,2] used.

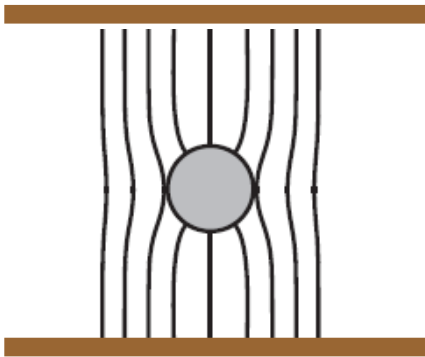
[1] A. Bossavit, *Computational Electromagnetism*, Academic Press, 1998.

[2] J.C. Nedelec, *Mixed Finite Elements in R^3* , Numer. Math. 35, 315 - 341 (1980).

Example:

EM modes of the **nematic quadrupole** (2D)

System geometry:

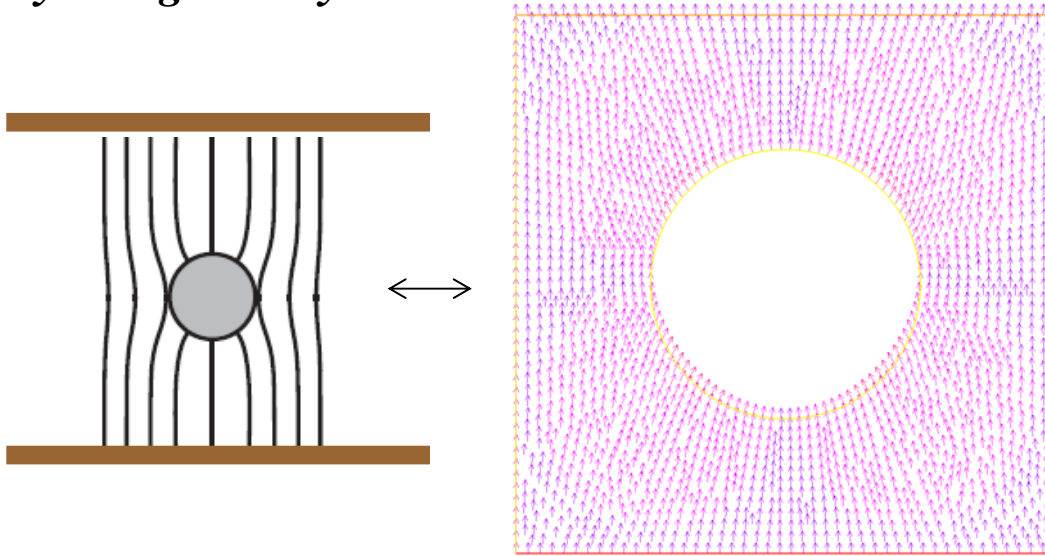


Nematic quadrupolar
configuration

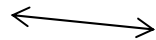
Example:

EM modes of the **nematic quadrupole** (2D)

System geometry:



Nematic quadrupolar
configuration



Nematic structure
by analytical ansatz

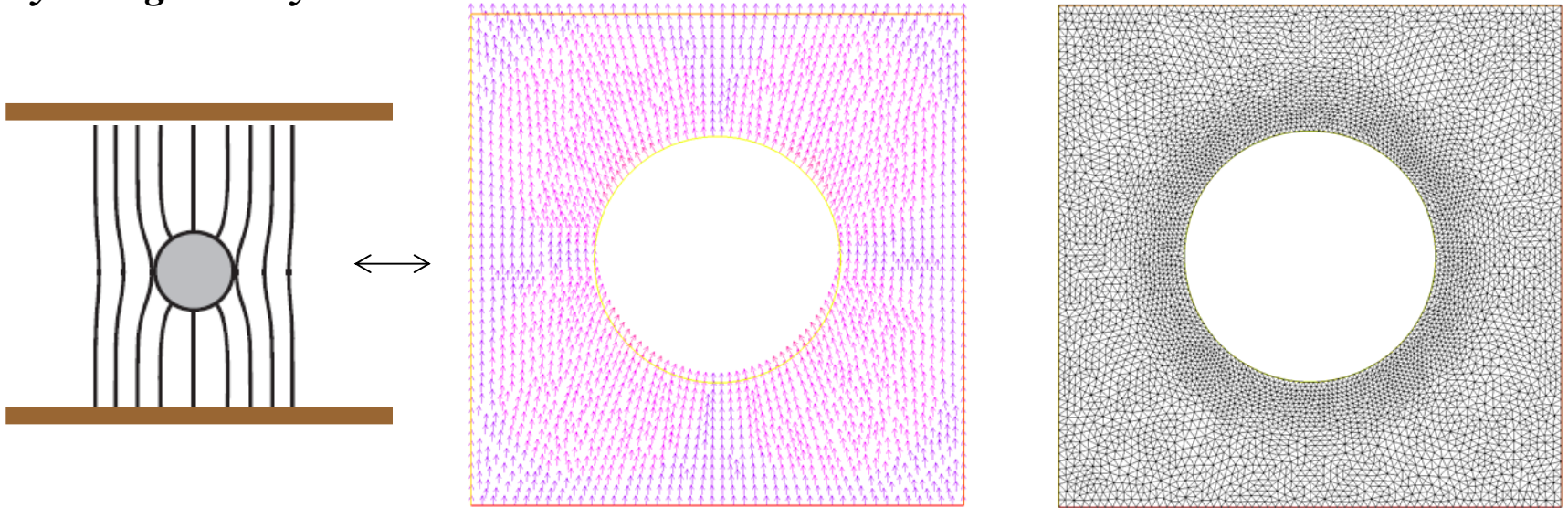


Induces *anisotropic dielectric tensor*.

Example:

EM modes of the **nematic quadrupole** (2D)

System geometry:



Nematic quadrupolar
configuration



Nematic structure
by analytical ansatz



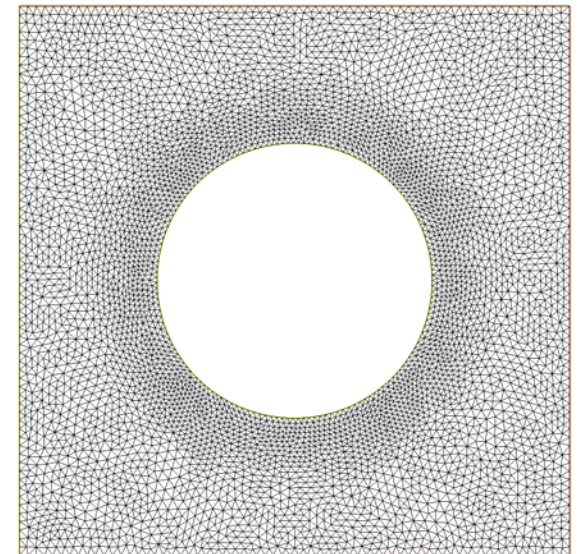
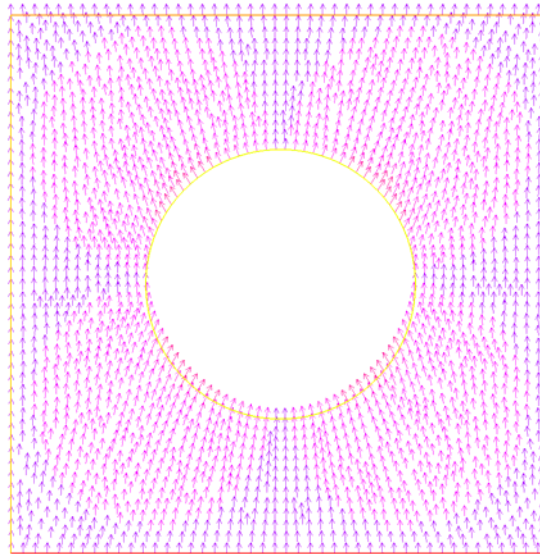
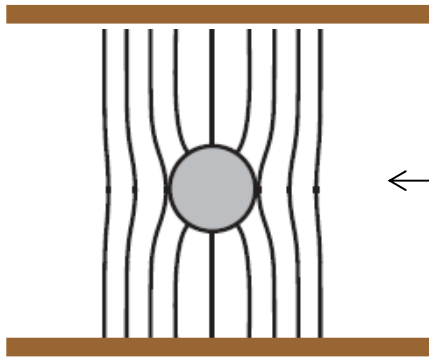
Induces *anisotropic
dielectric tensor*.

2D mesh: ~5000 vertices

Example:

EM modes of the **nematic quadrupole** (2D)

System geometry:



Nematic quadrupolar
configuration



Nematic structure
by analytical ansatz



Induces *anisotropic
dielectric tensor*.

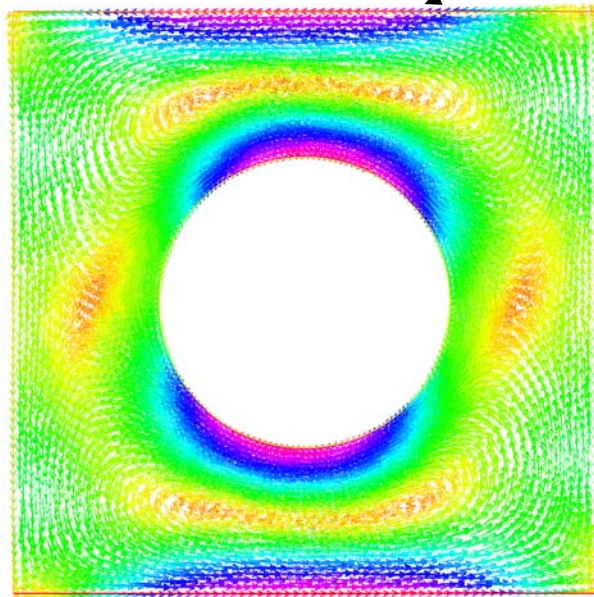
2D mesh: ~5000 vertices

We compute EM modes
on this nematic structure

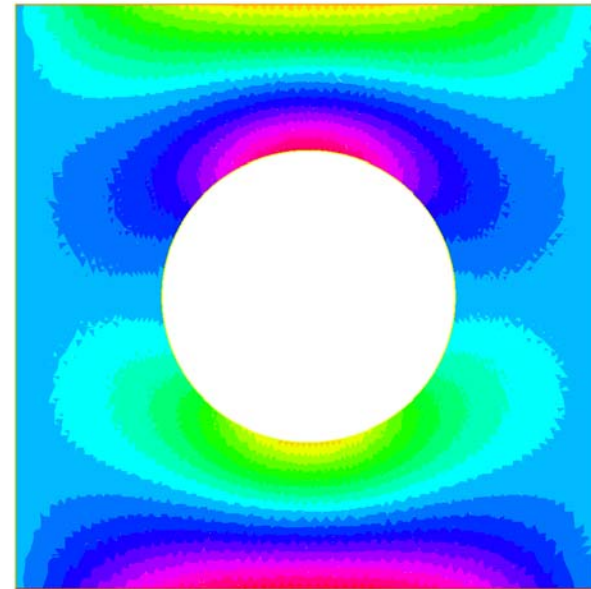
EM modes of the **nematic quadrupole** (2D)

1st mode:

metal on surface, i.e, ideal conductor boundary conditions



Vec Value
0
0.0180073
0.0360146
0.0540219
0.0720292
0.0900365
0.108044
0.126051
0.144058
0.162066
0.180073
0.19808
0.216088
0.234095
0.252102
0.27011
0.288117
0.306124
0.324132
0.342139

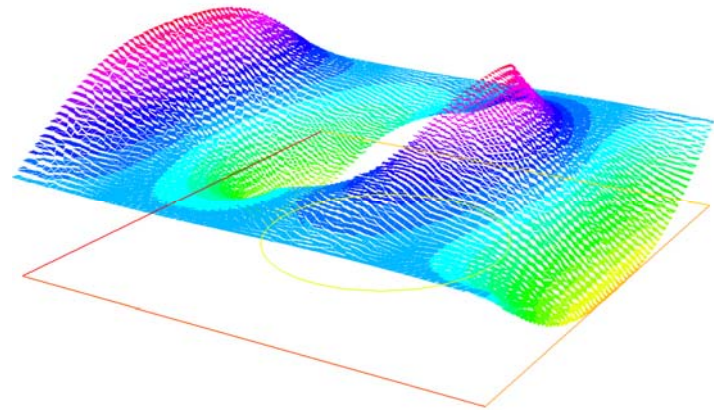


IsoValue
-0.359052
-0.32126
-0.283468
-0.245675
-0.207883
-0.17009
-0.132298
-0.0945055
-0.0567131
-0.0189206
0.0188718
0.0566642
0.0944566
0.132249
0.170041
0.207834
0.245626
0.283419
0.321211
0.359004

(H_x, H_y)

$$\omega^2 = 0.42$$

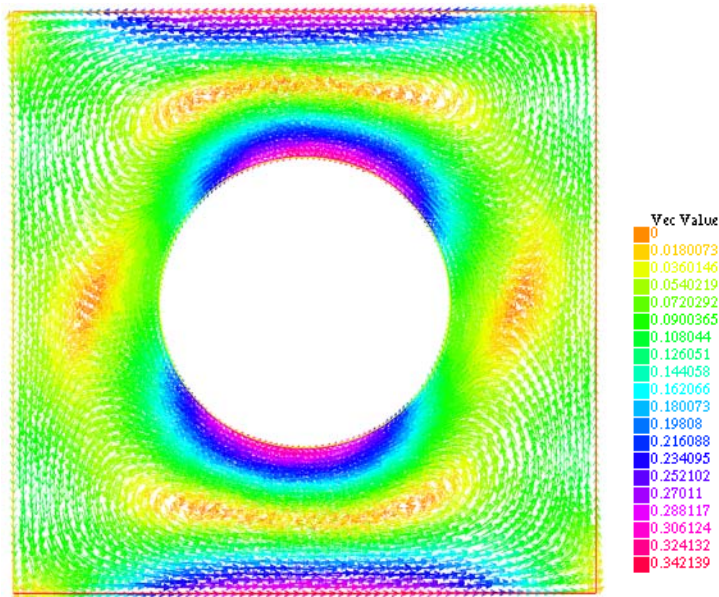
multiplicity = 1



H_x

EM modes of the **nematic quadrupole** (2D)

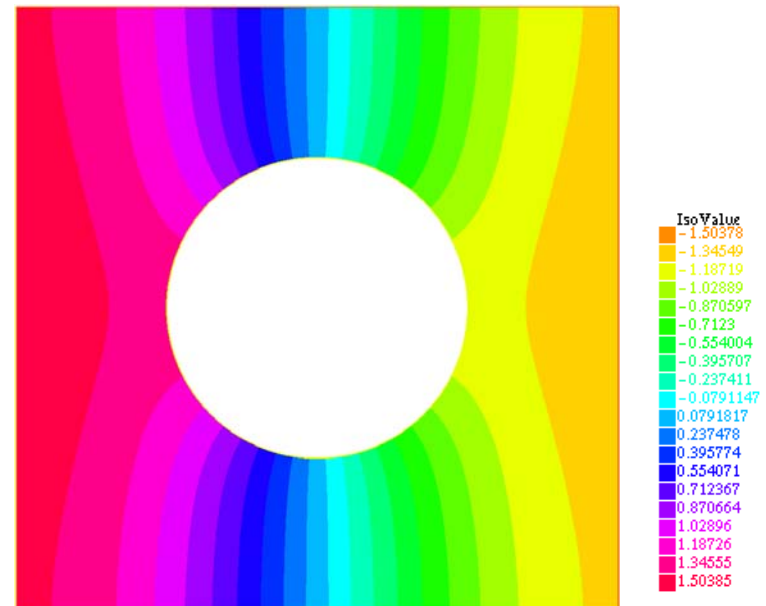
1st mode:



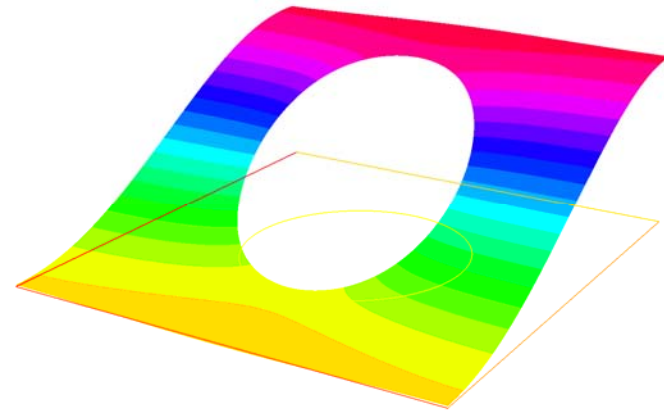
(H_x, H_y)

$$\omega^2 = 0.42$$

multiplicity = 1

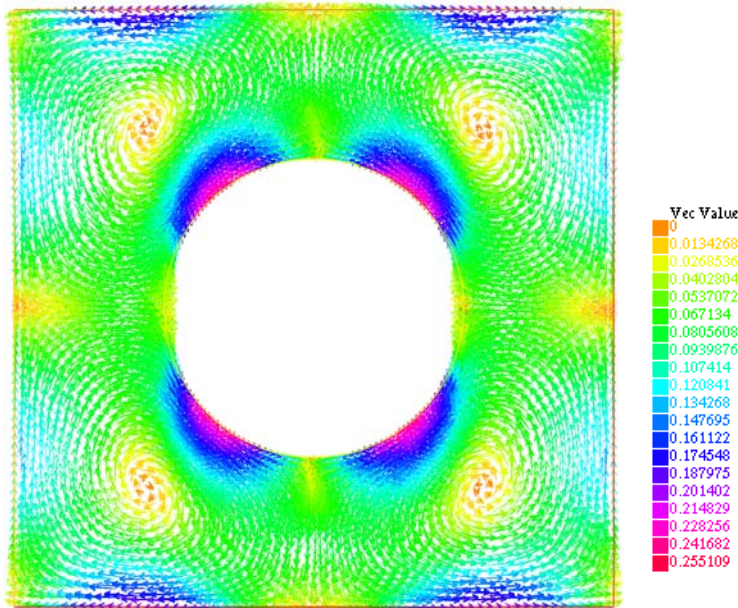


H_z



EM modes of the **nematic quadrupole** (2D)

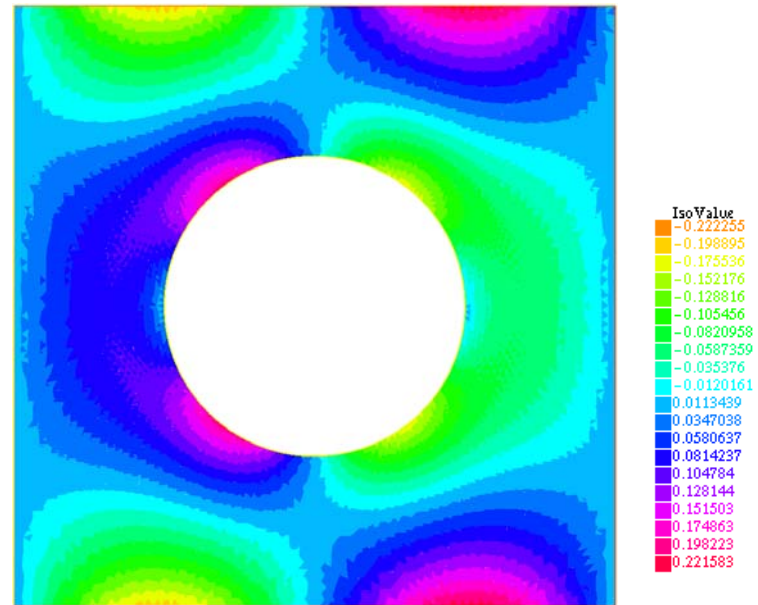
2nd mode:



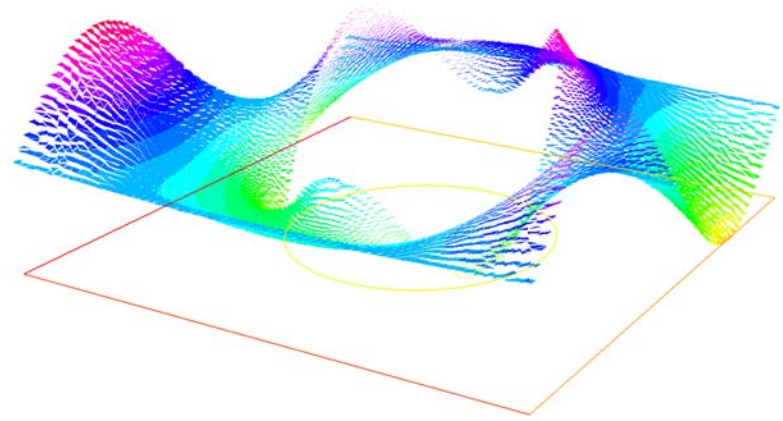
(H_x, H_y)

$$\omega^2 = 0.73$$

multiplicity = 1

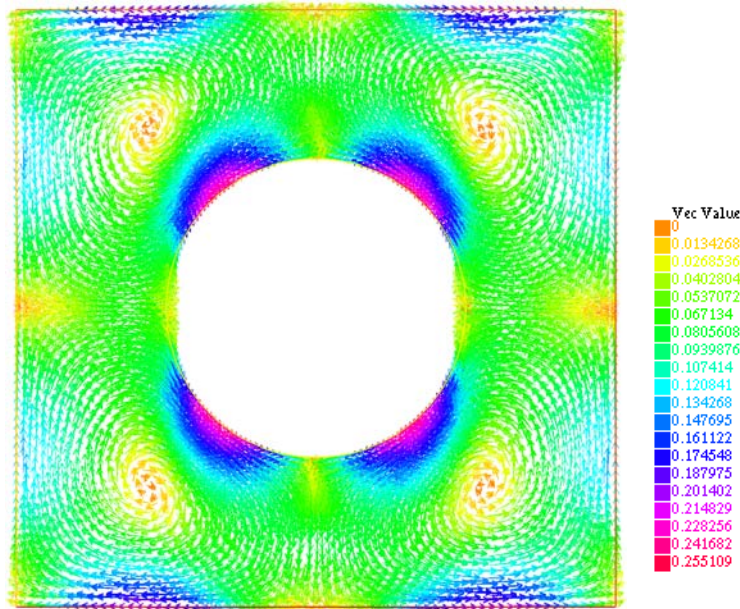


H_x



EM modes of the **nematic quadrupole** (2D)

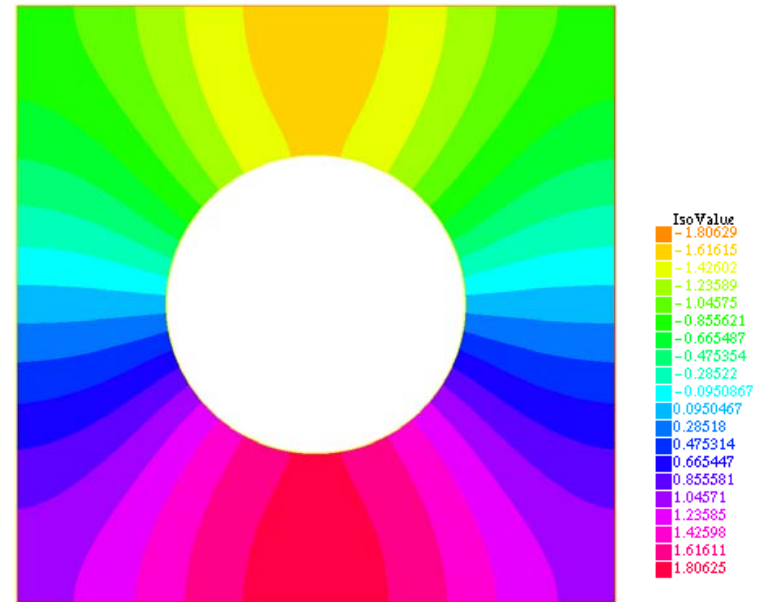
2nd mode:



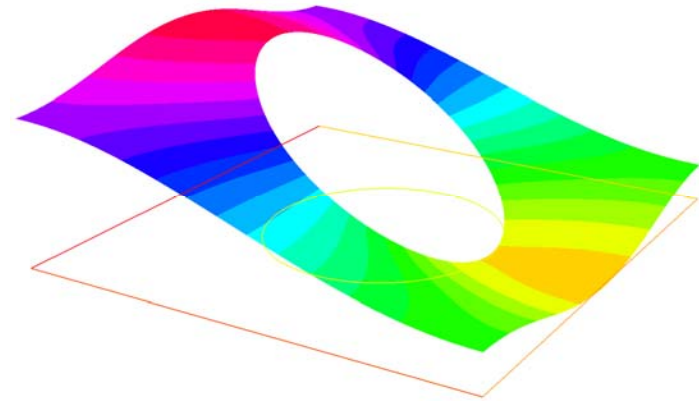
(H_x, H_y)

$$\omega^2 = 0.73$$

multiplicity = 1

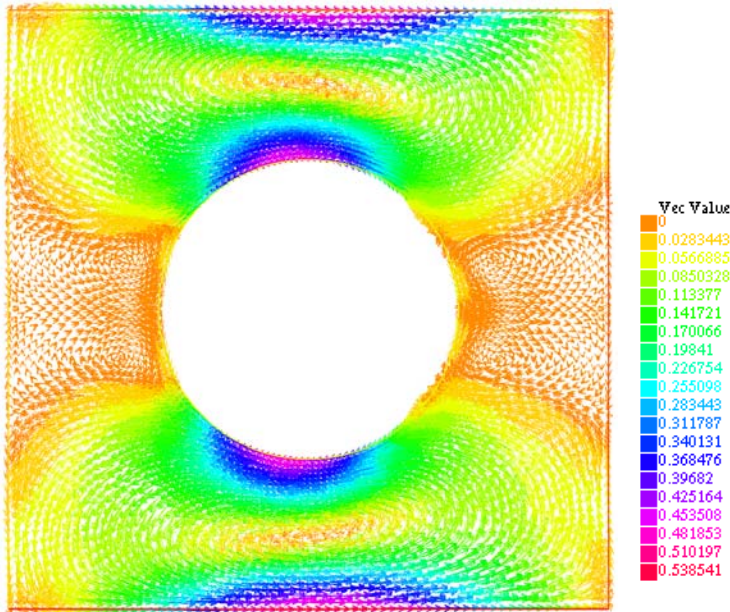


H_z



EM modes of the **nematic quadrupole** (2D)

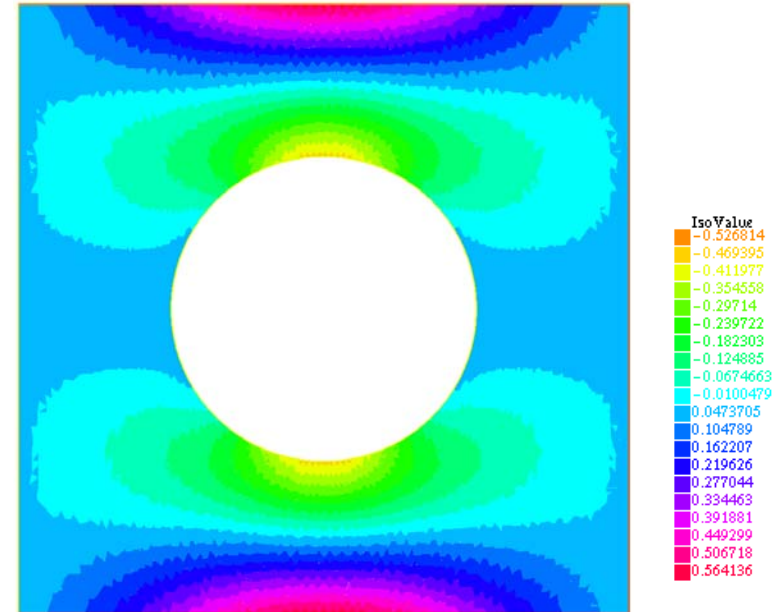
3rd mode:



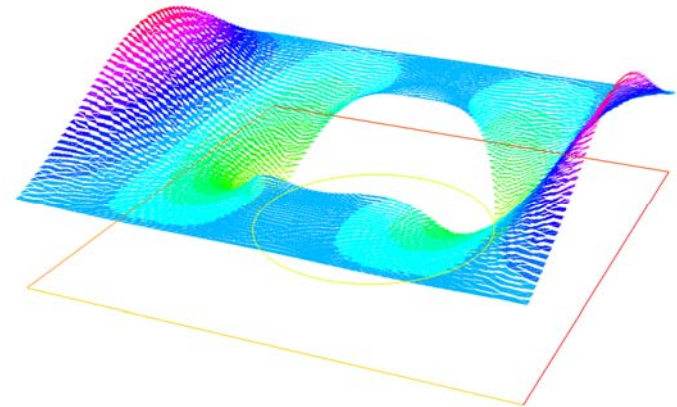
(H_x, H_y)

$$\omega^2 = 1.79$$

multiplicity = 1

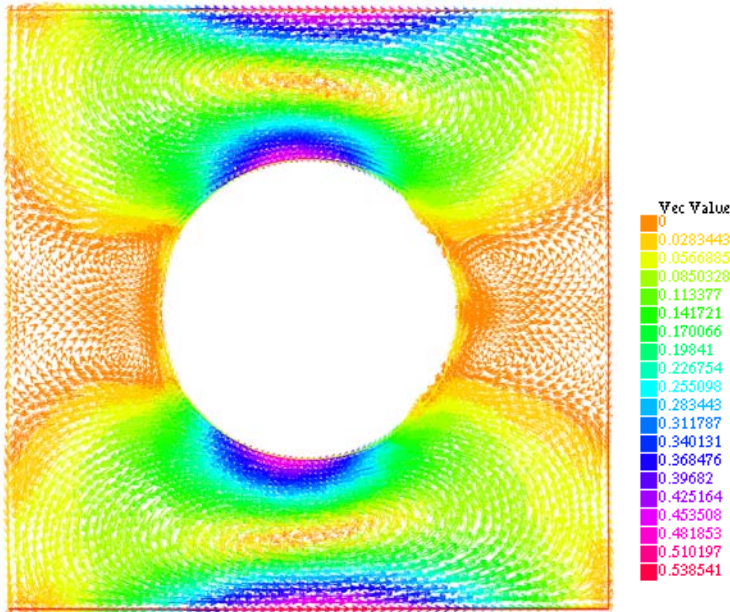


H_x



EM modes of the **nematic quadrupole** (2D)

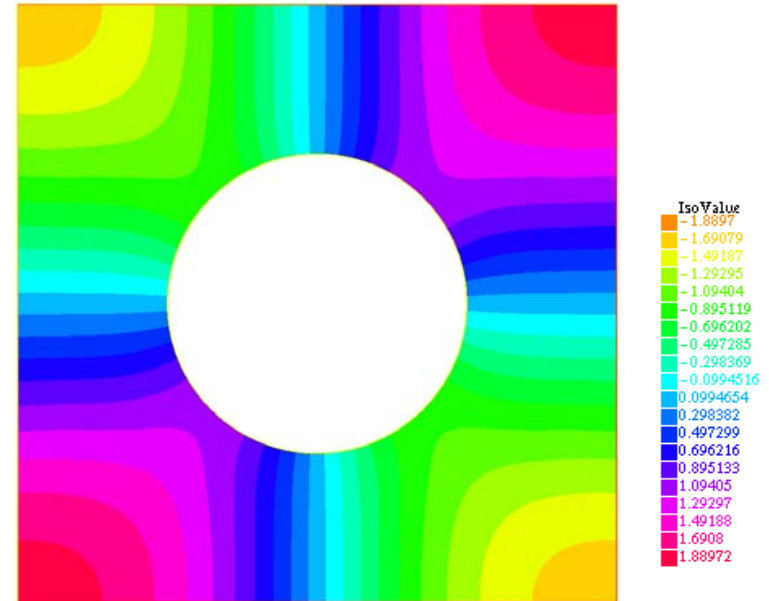
3rd mode:



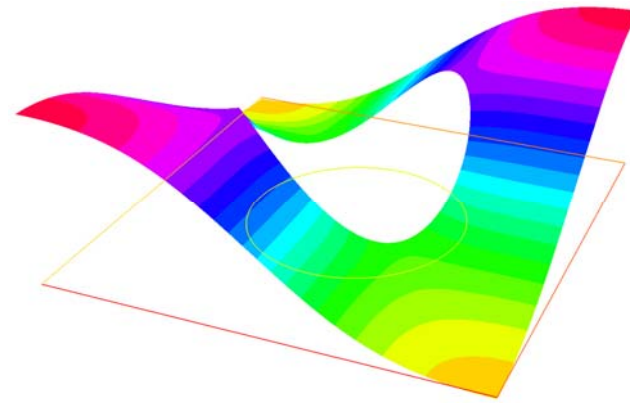
(H_x, H_y)

$$\omega^2 = 1.79$$

multiplicity = 1

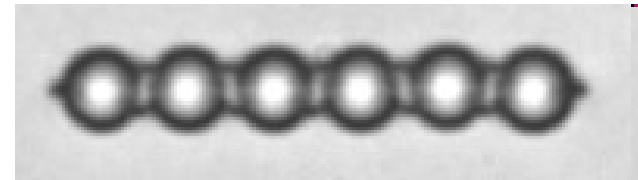
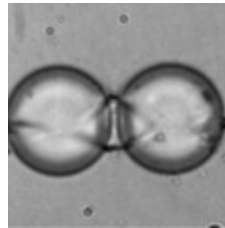


H_z

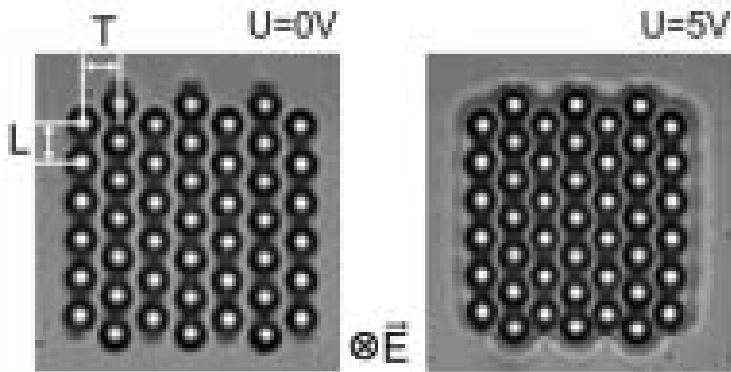


EM modes for more complex colloidal nematic structures?

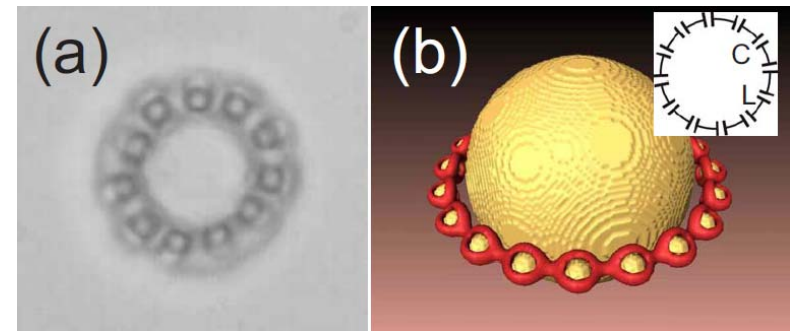
For **1D** structures?



EM waveguide?



For **2D** structures – crystals?



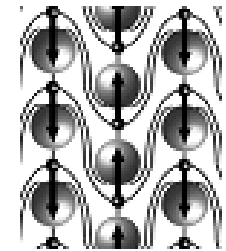
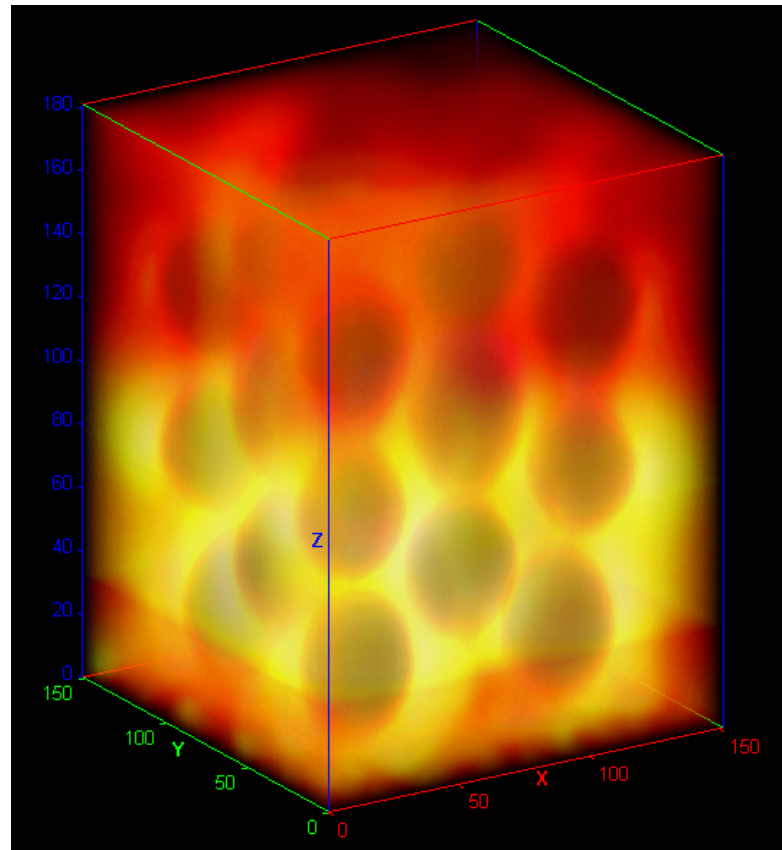
Large and small particles? →

Ring-split resonator?

(Škarabot, Ravnik et al., PRE, 2008.)

Nematic photonic crystals?

Large 3D
structures



3×3×3 dipolar crystal.

Experiment by Andriy Nych,
2010 (*to be published*).



Recently built
also 6×6×6

Future work

Computational:

- Computation of 3D modes in a **chiral nematic droplet** with at least 5-6 layers, on one processor.

Theoretical / mathematical:

- **Statistical** behaviour and **coherence** phenomena of EM resonant modes in chiral nematic droplet.

Further:

- Going to Schroedinger equation and computation of a (periodical) **quantum system**?

