Computational Photonics

Scattering theory: extensions

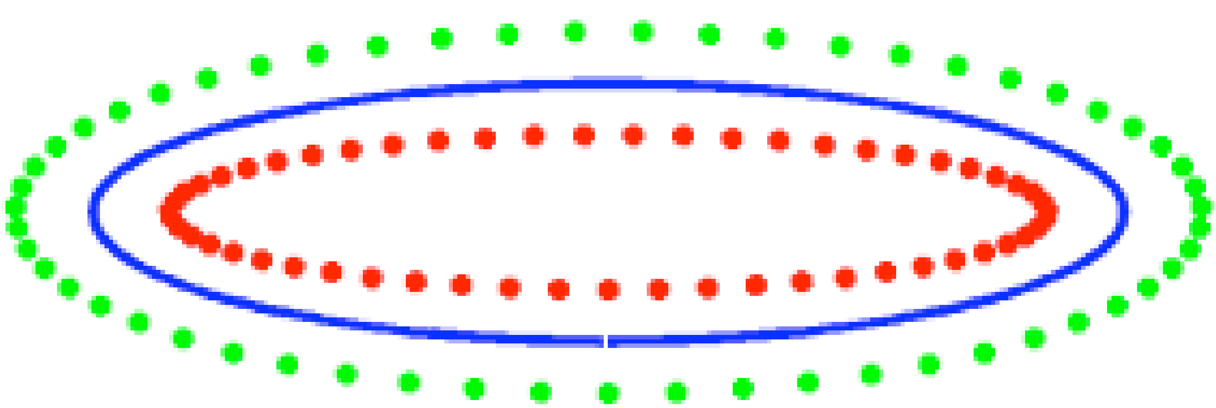
Multiple Multipole Method

For arbitrary shaped particles

"basically" exactly the same; but more multipoles are necessary for fulfilling the boundary conditions

(multipoles = points around which the fields are expanded in spherical waves)

fields in homogenous domains are written as superposition of multipoles
fulfilment of the boundary conditions gives the amplitudes of each mode



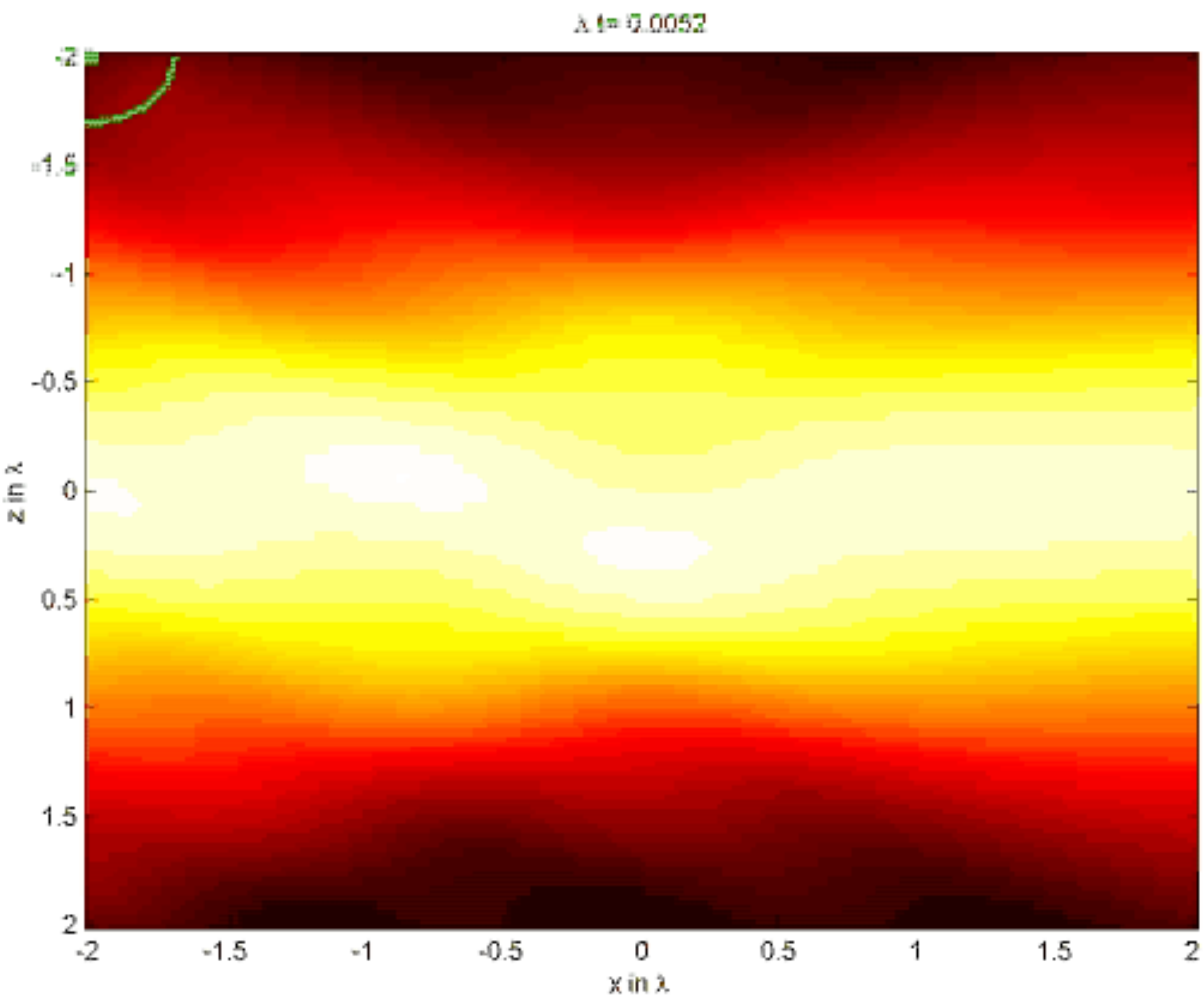
multipoles outside describe the field inside

multipoles inside describe the field outside

problems in finding appropriate position for multipoles and the number of expansion orders

Multiple Multipole Method

useful for the simulation of a larger number of diffraction events on the same structure
time consuming finding appropriate position of the multipoles



investigation of the force on nano particles

particle in a Gaussian beam

(r=0.3λ, n=1.2, ω=λ, TE)

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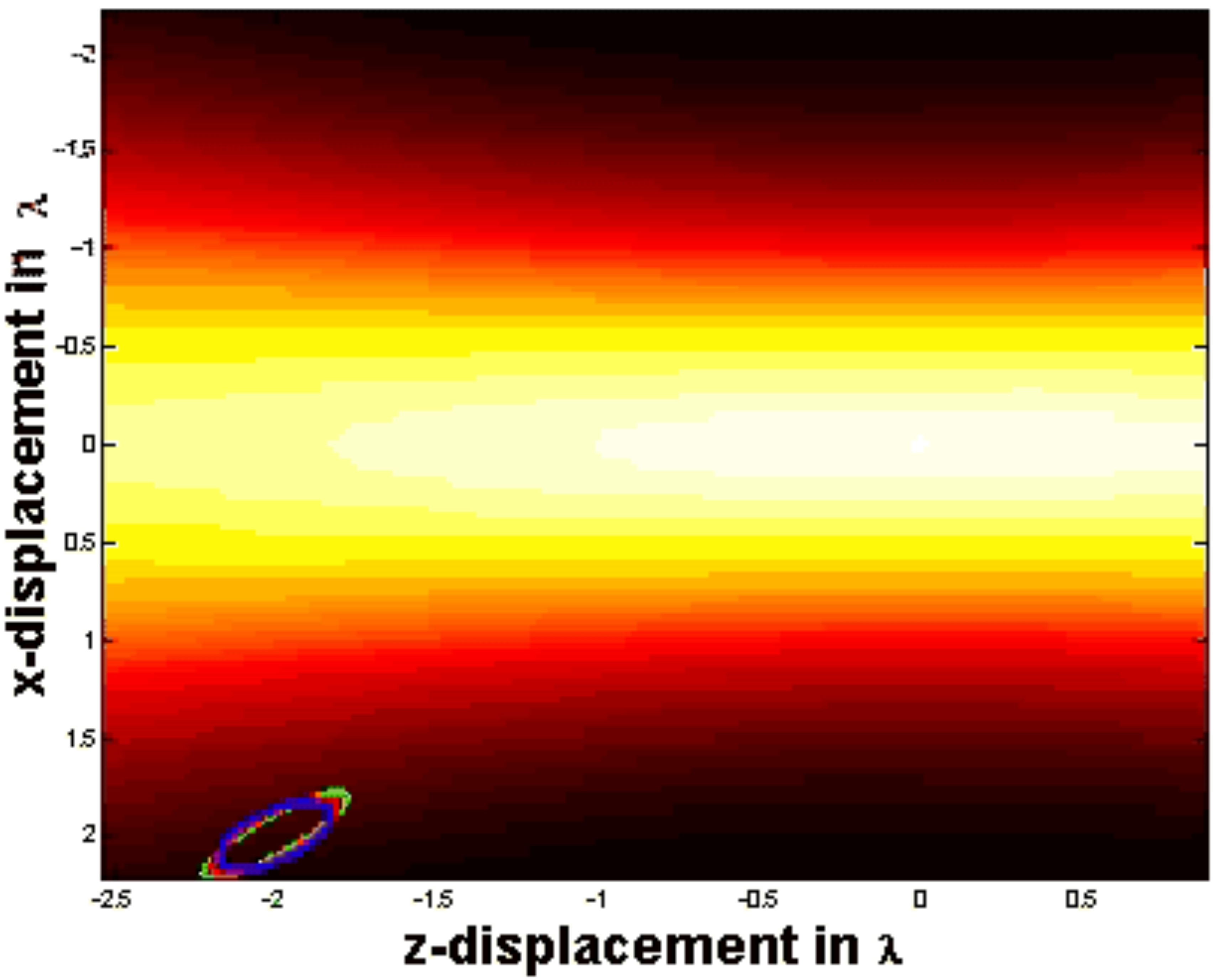
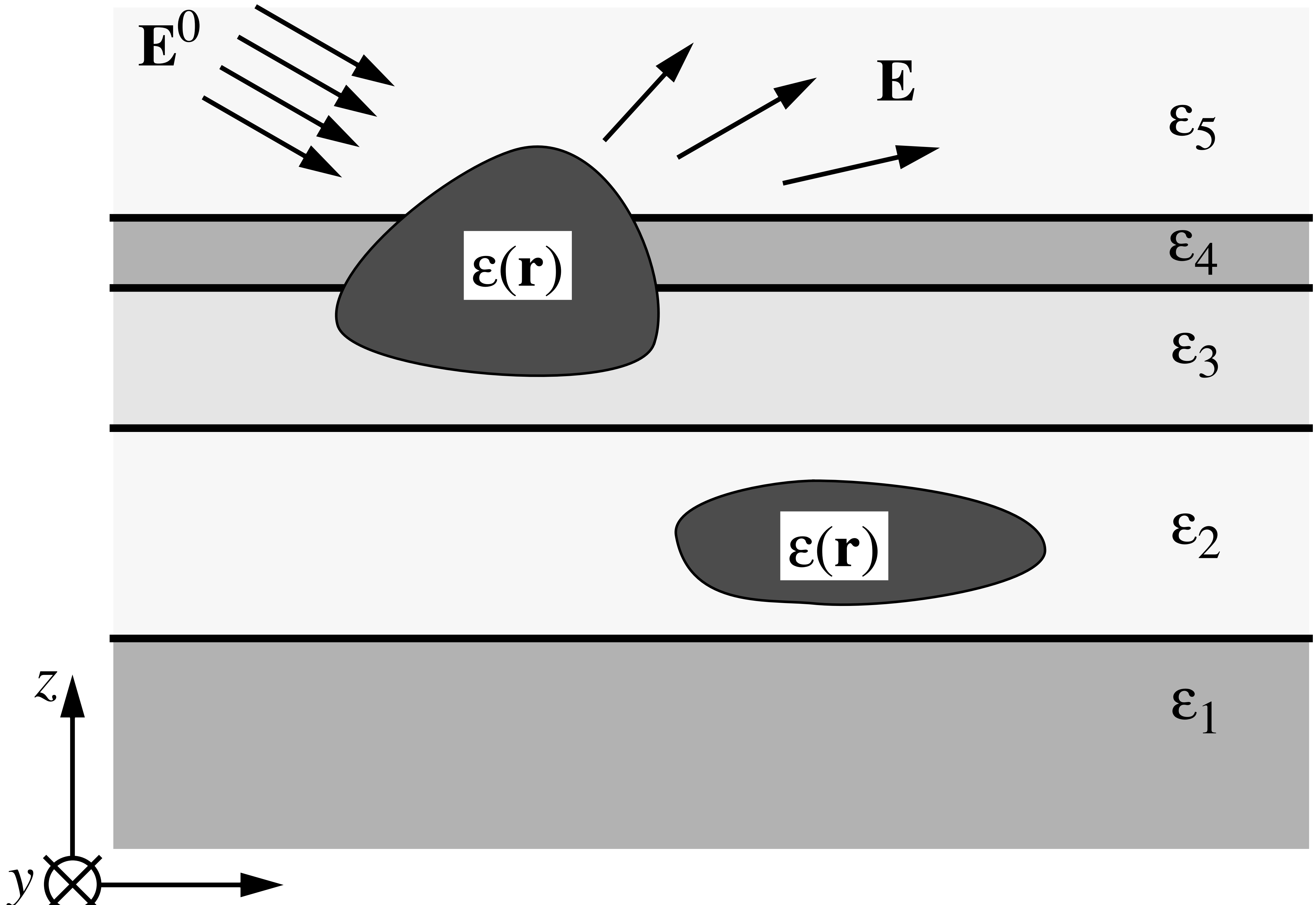


investigation of the force on nano particles

particle in a Gaussian beam

(r_{Ref}=0.01λ, n=1.5, ω=λ, TE)

Scattering problem solved by the Greens function



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Formulation of the scattering problem

- time harmonic oscillating field with a fixed frequency $e^{-i\omega t}$
- electric field is a solution to the vectorial wave equation

$$\nabla \times \nabla \times \mathbf{E}(\mathbf{r}) - k_0^2 \epsilon(\mathbf{r}) \mathbf{E}(\mathbf{r}) = 0$$

$$\nabla \cdot \epsilon(\mathbf{r}) \mathbf{E}(\mathbf{r}) = 0$$

- medium decomposed into background and scatterer

$$\epsilon(\mathbf{r}) = \epsilon_{\mathrm{B}}(\mathbf{r}) + \Delta\epsilon(\mathbf{r})$$

$$\nabla \times \nabla \times \mathbf{E}(\mathbf{r}) - k_0^2 \epsilon_{\mathbf{B}}(\mathbf{r}) \mathbf{E}(\mathbf{r}) = k_0^2 \left[\epsilon(\mathbf{r}) - \epsilon_{\mathbf{B}}(\mathbf{r})\right] \mathbf{E}(\mathbf{r})$$

$$\nabla \times \nabla \times \mathbf{E}(\mathbf{r}) - k_0^2 \epsilon_{\mathbf{B}}(\mathbf{r}) \mathbf{E}(\mathbf{r}) = k_0^2 \Delta\epsilon(\mathbf{r}) \mathbf{E}(\mathbf{r})$$

Lippmann-Schwinger equation

Basic idea of a Greens functions

- solution to inhomogenous differential equation is given by the sum of the homogenous and partial solution:

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_0(\mathbf{r}) + \mathbf{E}_S(\mathbf{r})$$

⇨ incident field

$$\nabla \times \nabla \times \mathbf{E}_0(\mathbf{r}) - k_0^2 \epsilon_{\mathbf{B}}(\mathbf{r})\mathbf{E}_0(\mathbf{r}) = 0$$

⇨ partial solution
(scattered field)

$$\mathbf{E}_S(\mathbf{r}) = k_0^2 \int \Delta\epsilon(\mathbf{r})\mathbf{G}(\mathbf{r},\mathbf{r}') \cdot \mathbf{E}(\mathbf{r}')d\mathbf{r}'$$

Green's function of the system

$$\mathbf{G}(\mathbf{r},\mathbf{r}')$$

for inhomogenous background

$$\mathbf{G}(\mathbf{r},\mathbf{r}') \neq \mathbf{G}(\mathbf{r}-\mathbf{r}')$$

Properties of the Greens functions

- solution to a wave equation with a point source term
- point source is represented by three orthogonal dipoles

$$\nabla \times \nabla \times \mathbf{G}(\mathbf{r},\mathbf{r}') - k_0^2 \epsilon(\mathbf{r}) \mathbf{G}(\mathbf{r},\mathbf{r}') = \mathbf{1}\delta(\mathbf{r}-\mathbf{r}')$$

with: $k_0^2 = \frac{\omega^2}{c^2}$ and $\mathbf{1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

$$\nabla \cdot \epsilon(\mathbf{r}) \mathbf{G}(\mathbf{r},\mathbf{r}') = -\nabla \cdot \delta(\mathbf{r}-\mathbf{r}')\mathbf{1}$$

$$\mathbf{G}(\mathbf{r},\mathbf{r}') = \begin{bmatrix} G_{xx} & G_{xy} & G_{xz} \\ G_{yx} & G_{yy} & G_{yz} \\ G_{zx} & G_{zy} & G_{zz} \end{bmatrix}$$

Basic idea of a Greens functions

- point like excitation of a field in space

⇒ Greens function describes the response of an environment to this singular excitation

⇒ e.g. the field value in every point $\mathbf{r}$ upon excitation at $\mathbf{r}'$

2D Greens function free space

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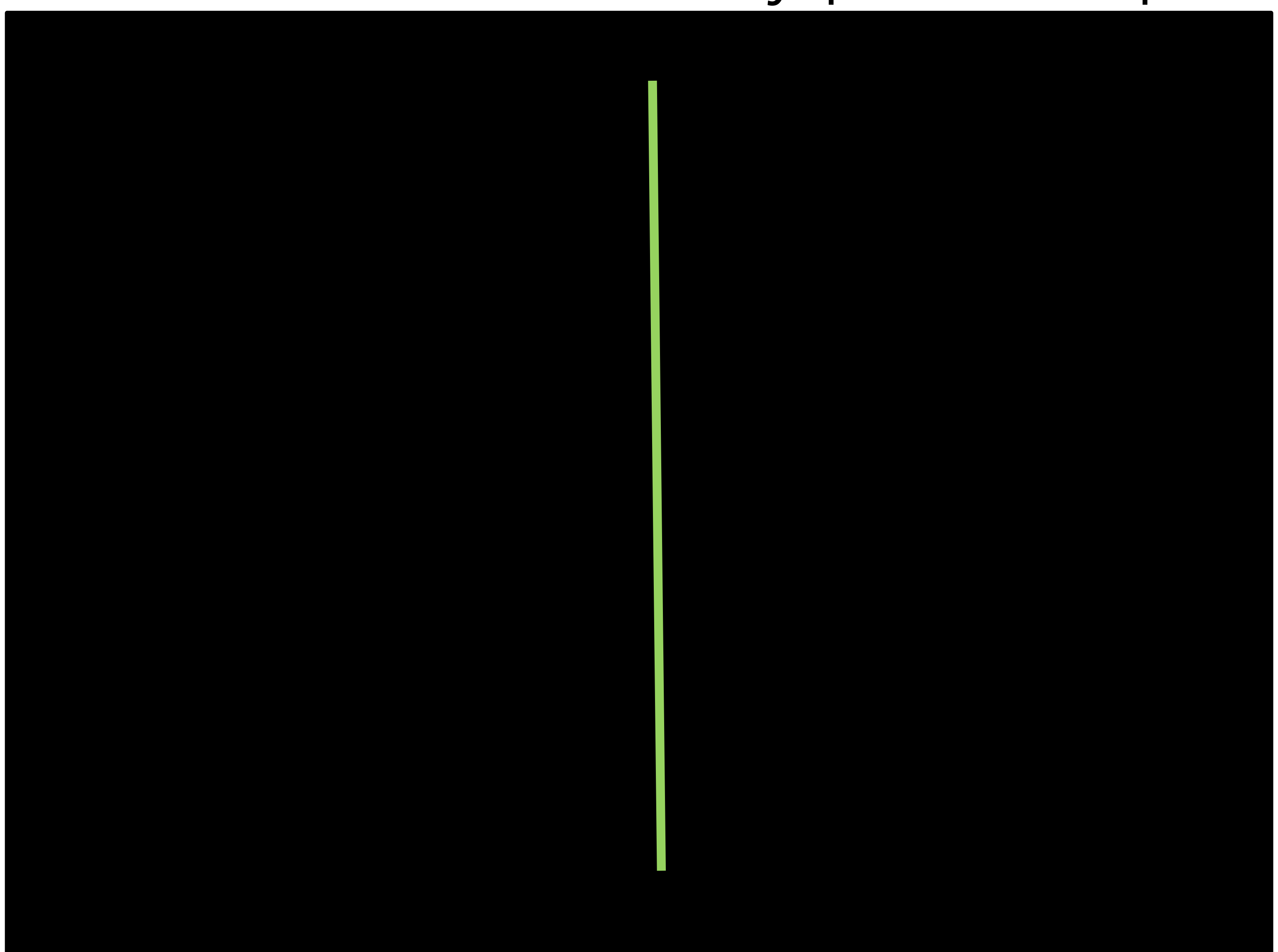

2D Greens function half space (position dependent!)

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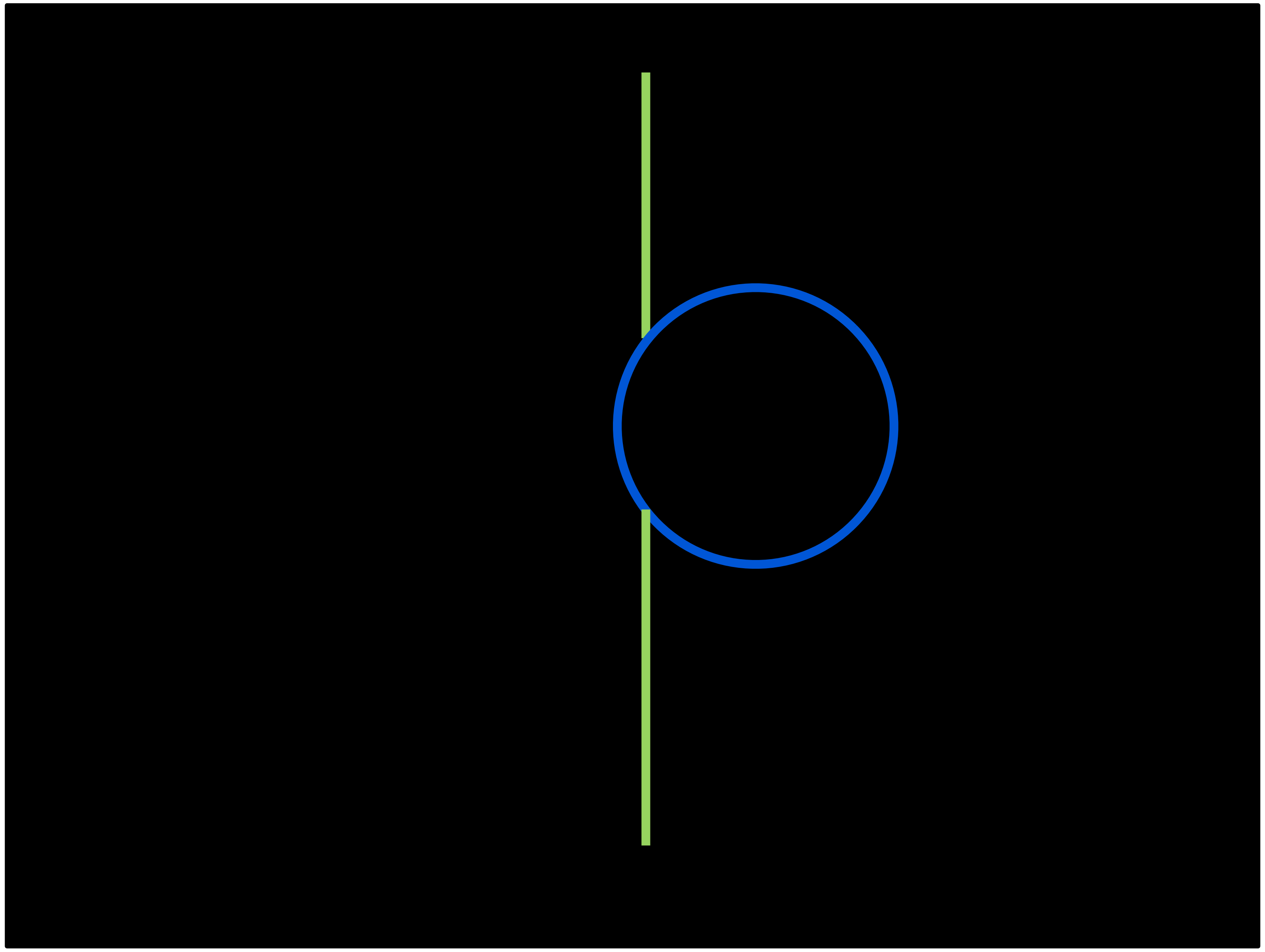


2D Greens function half space + cylinder (position dependent!)

Greens function of the homogenous (free) space

⟹ solution to the wave vector equation with a point source

$$\mathbf{G}_H(\mathbf{r},\mathbf{r}') = \left(\mathbf{1} + \frac{\nabla\nabla}{k_B^2}\right)\frac{e^{ik_BR}}{4\pi R}$$

P. M. Morse and H. Feshbach, Methods of Theoretical Physics (McGraw–Hill, New York, 1953)

$$R = |\,\mathbf{R}\,| = |\,\mathbf{r} - \mathbf{r}'\,| \qquad k_B^2 = \frac{\omega^2}{c^2}\epsilon_B$$

⟹ last term is called the free space scalar Greens function

$$G_0(R) = \frac{e^{ik_BR}}{4\pi R}$$

Greens function of the homogenous (free) space

$$\mathbf{G}_H(\mathbf{r},\mathbf{r}') = \mathbf{G}_H^{(0)}(\mathbf{r},\mathbf{r}') + \mathbf{G}_H^{(1)}(\mathbf{r},\mathbf{r}') + \mathbf{G}_H^{(2)}(\mathbf{r},\mathbf{r}')$$

far-field term

$$\mathbf{G}_H^{(0)}(\mathbf{r},\mathbf{r}') = \left(\mathbf{1} - \frac{\mathbf{RR}}{\mid \mathbf{R} \mid^2}\right) G_0(\mathbf{r},\mathbf{r}')$$

near-field terms

$$\mathbf{G}_H^{(1)}(\mathbf{r},\mathbf{r}') = \left(\mathbf{1}\frac{ik_B \mid \mathbf{R} \mid}{k_B^2 \mid \mathbf{R} \mid^2} - \mathbf{RR}\frac{3ik_B \mid \mathbf{R} \mid}{k_B^2 \mid \mathbf{R} \mid^4}\right) G_0(\mathbf{r},\mathbf{r}')$$

$$\mathbf{G}_H^{(2)}(\mathbf{r},\mathbf{r}') = \left(\mathbf{1}\frac{-1}{k_B^2 \mid \mathbf{R} \mid^2} + \mathbf{RR}\frac{3}{k_B^2 \mid \mathbf{R} \mid^4}\right) G_0(\mathbf{r},\mathbf{r}')$$

Lippmann-Schwinger equation

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_0(\mathbf{r}) + k_0^2 \int \Delta\epsilon(\mathbf{r})\mathbf{G}(\mathbf{r},\mathbf{r}')\cdot\mathbf{E}(\mathbf{r}')d\mathbf{r}'$$

- in general challenging to solve because $\mathbf{E}(\mathbf{r})$ appears on both sides

- simplifications are possible, e.g. first order Born series

$$\mathbf{E}(\mathbf{r}) \approx \mathbf{E}_0(\mathbf{r})$$

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_0(\mathbf{r}) + k_0^2 \int \Delta\epsilon(\mathbf{r})\mathbf{G}(\mathbf{r},\mathbf{r}')\cdot\mathbf{E}_0(\mathbf{r}')d\mathbf{r}'$$

- directly solvable, integral expresses the scattering from a polarisable medium where the magnitude of polarisation depends on permittivity contrast and incident field amplitude

Solving the scattering problem

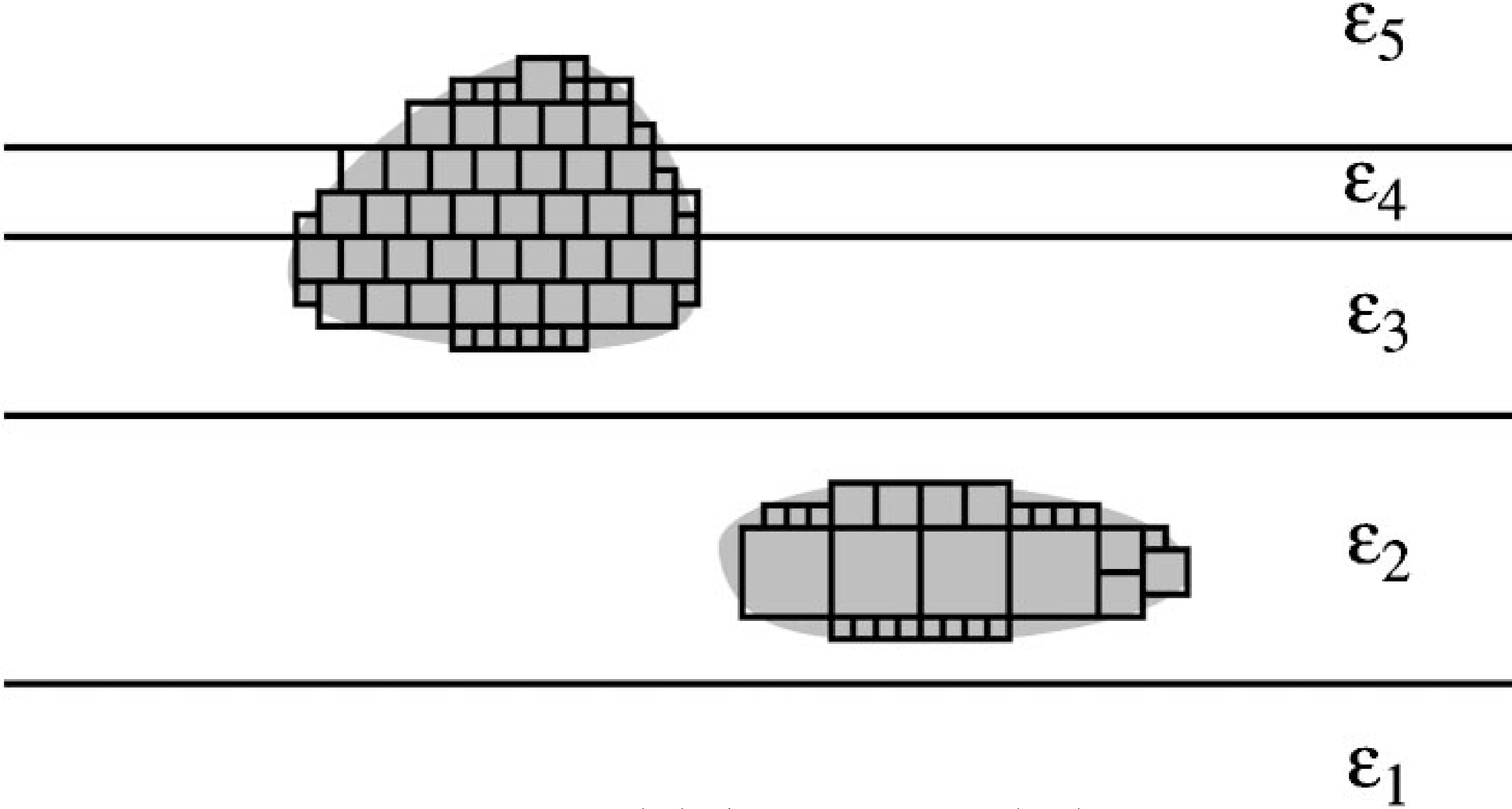
$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_0(\mathbf{r}) + k_0^2 \int \Delta\epsilon(\mathbf{r})\mathbf{G}(\mathbf{r},\mathbf{r}') \cdot \mathbf{E}(\mathbf{r}')d\mathbf{r}'$$

- numerical solution necessary beyond lowest order perturbation theory
- numerical problem is the singularity of the Green's function at $\mathbf{G}(\mathbf{r},\mathbf{r})$
- source (self-term) dyadic has to be taken explicitly into account

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_0(\mathbf{r}) + \lim_{\delta V \to 0} \int_{V-\delta V} k_0^2 \Delta\epsilon(\mathbf{r})\mathbf{G}(\mathbf{r},\mathbf{r}') \cdot \mathbf{E}(\mathbf{r}')d\mathbf{r}' - \mathbf{L} \cdot \frac{\Delta\epsilon(\mathbf{r})}{\epsilon_B}\mathbf{E}(\mathbf{r})$$

⟹ equation has to be discretized and solved

Discretising the scatterer



$$\Delta\epsilon_i = \Delta\epsilon_i(\mathbf{r}) \mid_{\mathbf{r}\in V_i} \approx \Delta\epsilon(\mathbf{r}_i)$$

$$\mathbf{E}_i = \mathbf{E}_i(\mathbf{r}) \mid_{\mathbf{r}\in V_i} \approx \mathbf{E}(\mathbf{r}_i)$$

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Discretizing the equation

$$
\begin{aligned}
\mathbf{E}_i \quad = \quad & \mathbf{E}_i^0 \\
& + \sum_{j=1,\ j\neq i}^{N} \mathbf{G}_{i,j} \cdot k_0^2 \Delta\epsilon_j \mathbf{E}_j V_j \\
& + \mathbf{M}_i \cdot k_0^2 \Delta\epsilon_i \mathbf{E_i} \\
& - \mathbf{L} \cdot \frac{\Delta\epsilon_i}{\epsilon_B} \mathbf{E}_i
\end{aligned}
$$

Computer Physics Communication, 144, 111 (2002)

Calculating the self action terms

- finiteness of the exclusion volume requires to solve in principle for

$$\mathbf{M}_i = \lim \int_{V_i - \delta V} d\mathbf{r}' \mathbf{G}(\mathbf{r}_i, \mathbf{r}')$$

- difficult to evaluate but detrimental for numerical precision
- analytical expressions are available for certain shapes of volumes

A. D. Yaghjian, "Electric dyadic Green's functions in the source region", Proc. IEEE **68**, *248* (1980)

- for example assuming a sphere

$$\mathbf{M}_i = \frac{2}{3k_f^2} \left[\left(1 - ik_f R_i^{\text{eff}}\right) e^{ik_f R_i^{\text{eff}}} - 1 \right] \mathbf{1}$$

$$R_i^{\text{eff}} = \left(\frac{3}{4\pi} V_i \right)^{1/3}$$

Calculating the self action terms

- one has to solve in principle for

$$\mathbf{M}_i = \lim \int_{V_i - \delta V} d\mathbf{r}' \mathbf{G}(\mathbf{r}_i, \mathbf{r}')$$

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- for example assuming a sphere

$$\mathbf{L} = \frac{1}{3}\mathbf{1}$$

Solving the equation

$$\mathbf{A} \begin{pmatrix} E_1^x \\ E_1^y \\ E_1^z \\ E_2^x \\ E_2^y \\ E_2^z \end{pmatrix} = \begin{pmatrix} E_1^{0x} \\ E_1^{0y} \\ E_1^{0z} \\ E_2^{0x} \\ E_2^{0y} \\ E_2^{0z} \end{pmatrix}$$

⇨ system of linear equations can be solved by standard matrix inversion techniques

Solving the equation

- a fraction of the matrix is

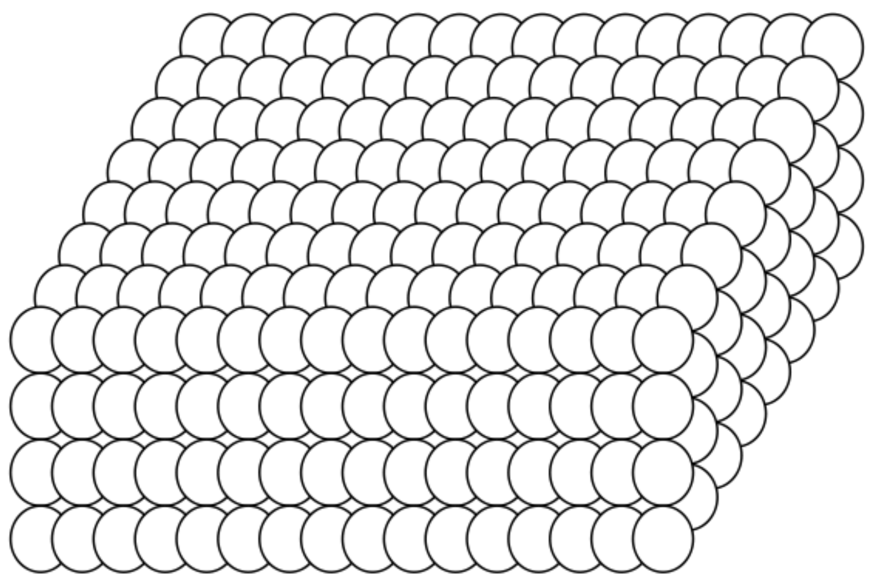
$$\mathbf{A} =$$

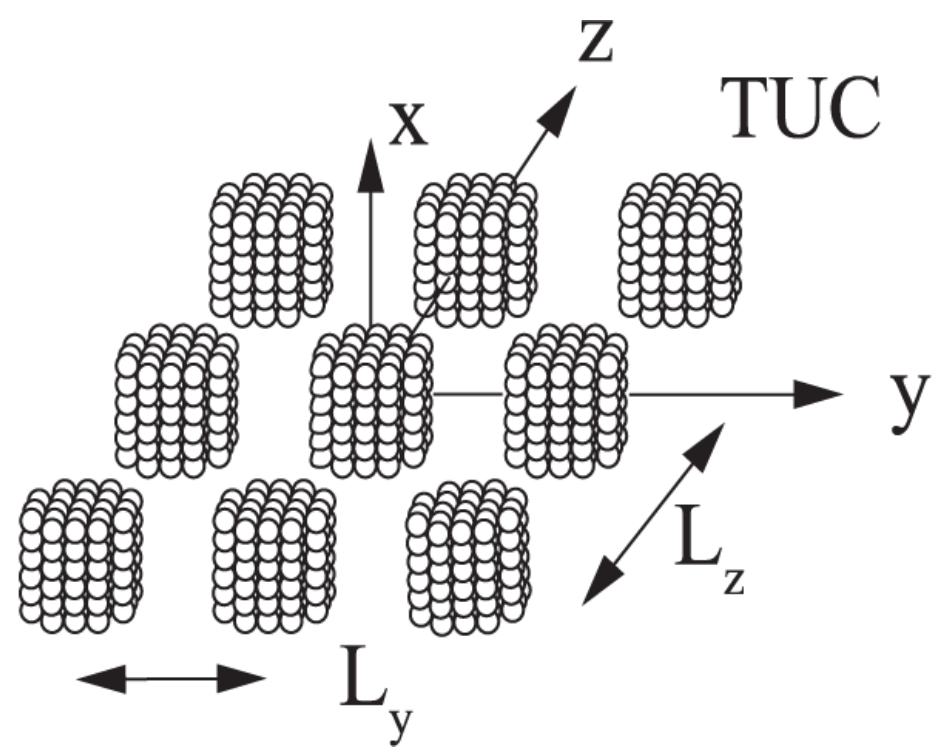
$$\left[\begin{array}{cccc}
1 - M_1^{xx} k_0^2 \delta\epsilon_1 + L_1^{xx} \frac{\delta\epsilon_1}{\epsilon_B} & 0 & 0 & -G_{12}^{xx} k_0^2 \delta\epsilon_2 V_2 \\
0 & 1 - M_1^{yy} k_0^2 \delta\epsilon_1 + L_1^{yy} \frac{\delta\epsilon_1}{\epsilon_B} & 0 & -G_{12}^{yx} k_0^2 \delta\epsilon_2 V_2 \\
0 & 0 & 1 - M_1^{zz} k_0^2 \delta\epsilon_1 + L_1^{zz} \frac{\delta\epsilon_1}{\epsilon_B} & -G_{12}^{zx} k_0^2 \delta\epsilon_2 V_2 \\
-G_{21}^{xx} k_0^2 \delta\epsilon_1 V_1 & -G_{21}^{xy} k_0^2 \delta\epsilon_1 V_1 & -G_{21}^{xz} k_0^2 \delta\epsilon_1 V_1 & 1 - M_2^{xx} k_0^2 \delta\epsilon_2 + L_2^{xx} \frac{\delta\epsilon_2}{\epsilon_B} \\
-G_{21}^{yx} k_0^2 \delta\epsilon_1 V_1 & -G_{21}^{yy} k_0^2 \delta\epsilon_1 V_1 & -G_{21}^{yz} k_0^2 \delta\epsilon_1 V_1 & 0 \\
-G_{21}^{zx} k_0^2 \delta\epsilon_1 V_1 & -G_{21}^{zy} k_0^2 \delta\epsilon_1 V_1 & -G_{21}^{zz} k_0^2 \delta\epsilon_1 V_1 & 0
\end{array} \right.$$

Weak vs. strong formulation

- neglecting the source terms simplifies the implementation: weak formulation

- approximating the object in terms of small spheres





- treating the spheres in the dipole limit and solve self-consistently the scattering

- numerical strategy called discrete dipole approximation

Weak vs. strong formulation

individual polarisability

$$\mathbf{P}_j = \alpha_j \mathbf{E}_j$$

simplified scattering equation

$$\mathbf{E}_j = \mathbf{E}_{\mathrm{inc},j} - \sum_{k \neq j} \mathbf{A}_{jk} \mathbf{P}_k$$

quantities of interest

$$C_{\mathrm{ext}} = \frac{4\pi k}{|\mathbf{E}_0|^2} \sum_{j=1}^{N} \mathrm{Im}(\mathbf{E}_{\mathrm{inc},j}{}^{*} \cdot \mathbf{P}_j)$$

$$C_{\mathrm{abs}} = \frac{4\pi k}{|\mathbf{E}_0|^2} \sum_{j=1}^{N} \left\{ \mathrm{Im}[\mathbf{P}_j \cdot (\alpha_j{}^{-1})^{*} \mathbf{P}_j{}^{*}] - \frac{2}{3} k^3 |\mathbf{P}_j|^2 \right\}$$

far-field expression

$$\mathbf{E}_{\mathrm{sca}} = \frac{k^2 \exp(ikr)}{r} \sum_{j=1}^{N} \exp(-ik\hat{r} \cdot \mathbf{r}_j)(\hat{r}\hat{r} - \mathbf{1}_3)\mathbf{P}_j$$

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