THE T MATRIX

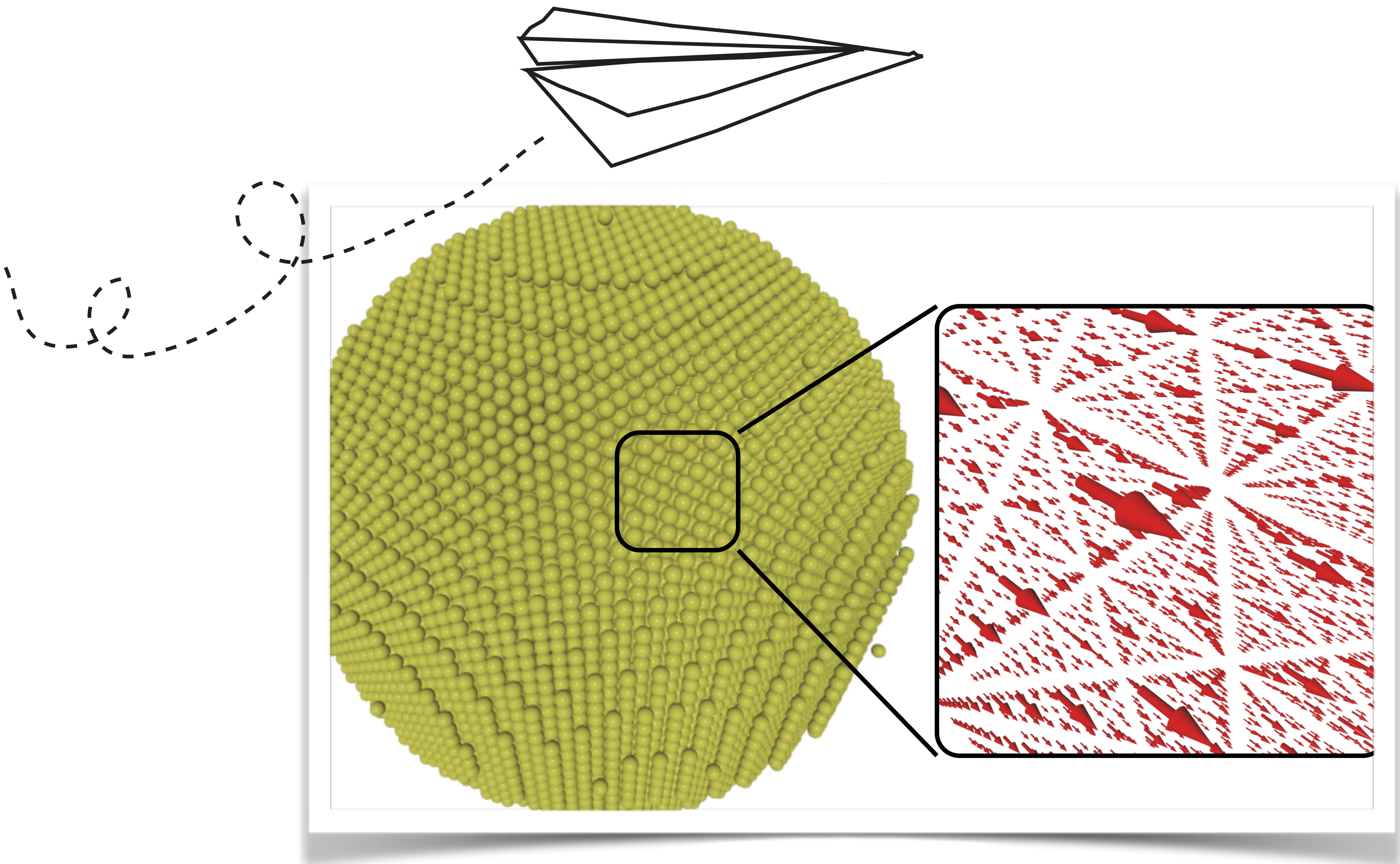
baptiste auguié

30/09/2016

“ [...] arguably the most efficient and elegant approach when it is applicable

– Anonymous

The Scattering Problem



Computational Light Scattering

- Finite differences (time domain)
- Finite elements
- Boundary elements
- **T-matrix**
- Mie theory
- Periodic structures, ...
- Approximations, ...

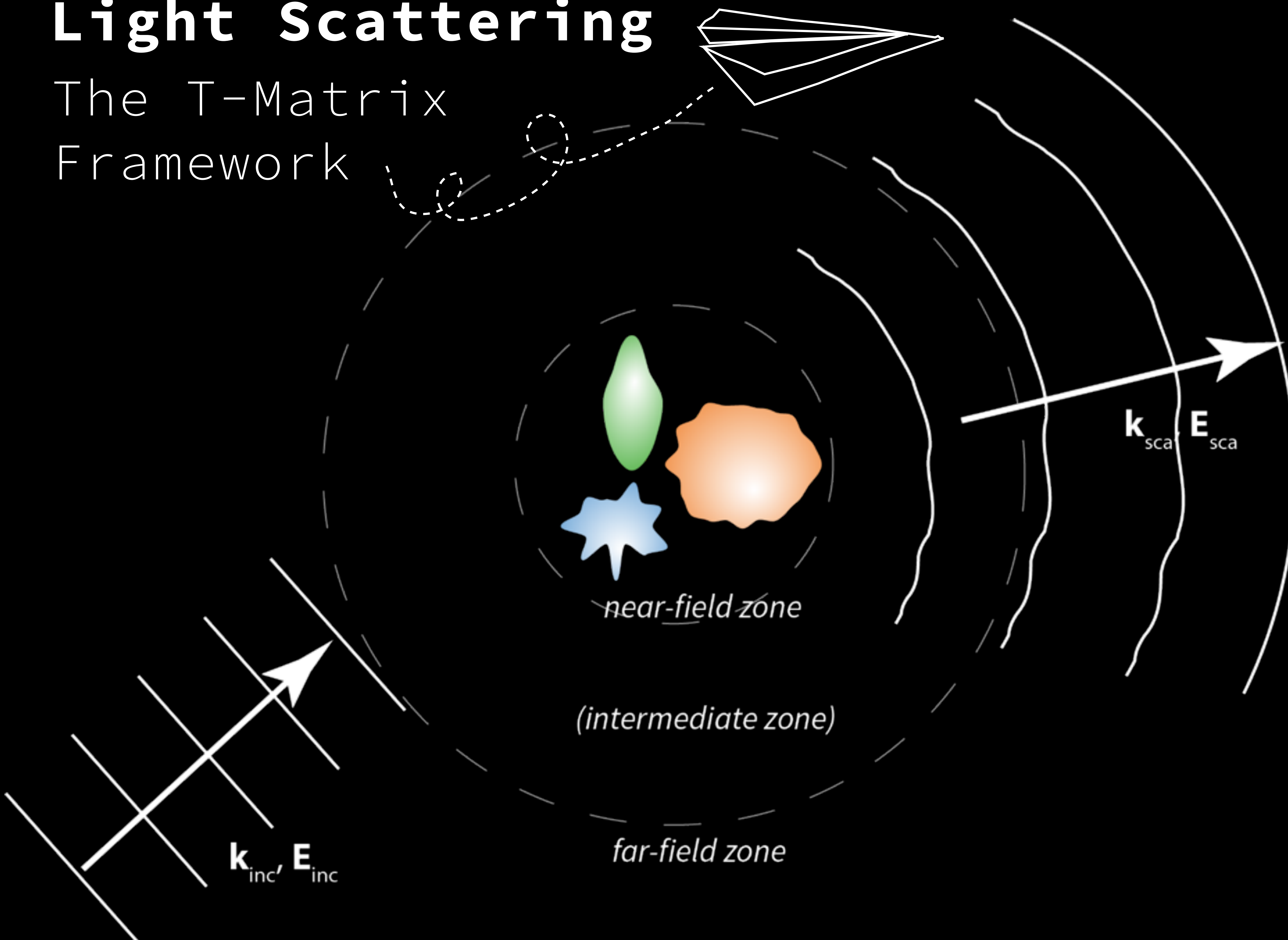
Numerical

Analytical

M. Mishchenko, *Scattering, Absorption, and Emission of Light by Small Particles,* Cambridge (2002)
M. Kahnert, *Numerical methods in electromagnetic scattering theory*, JQSRT **79** (2003)

Light Scattering

The T-Matrix Framework



Transition Matrix

$$\mathbf{E}_{\text{inc}} = E_0 \sum_{n,m} a_{nm}\mathbf{M}^{(1)}_{nm}(k_1\mathbf{r}) + b_{nm}\mathbf{N}^{(1)}_{nm}(k_1\mathbf{r})$$

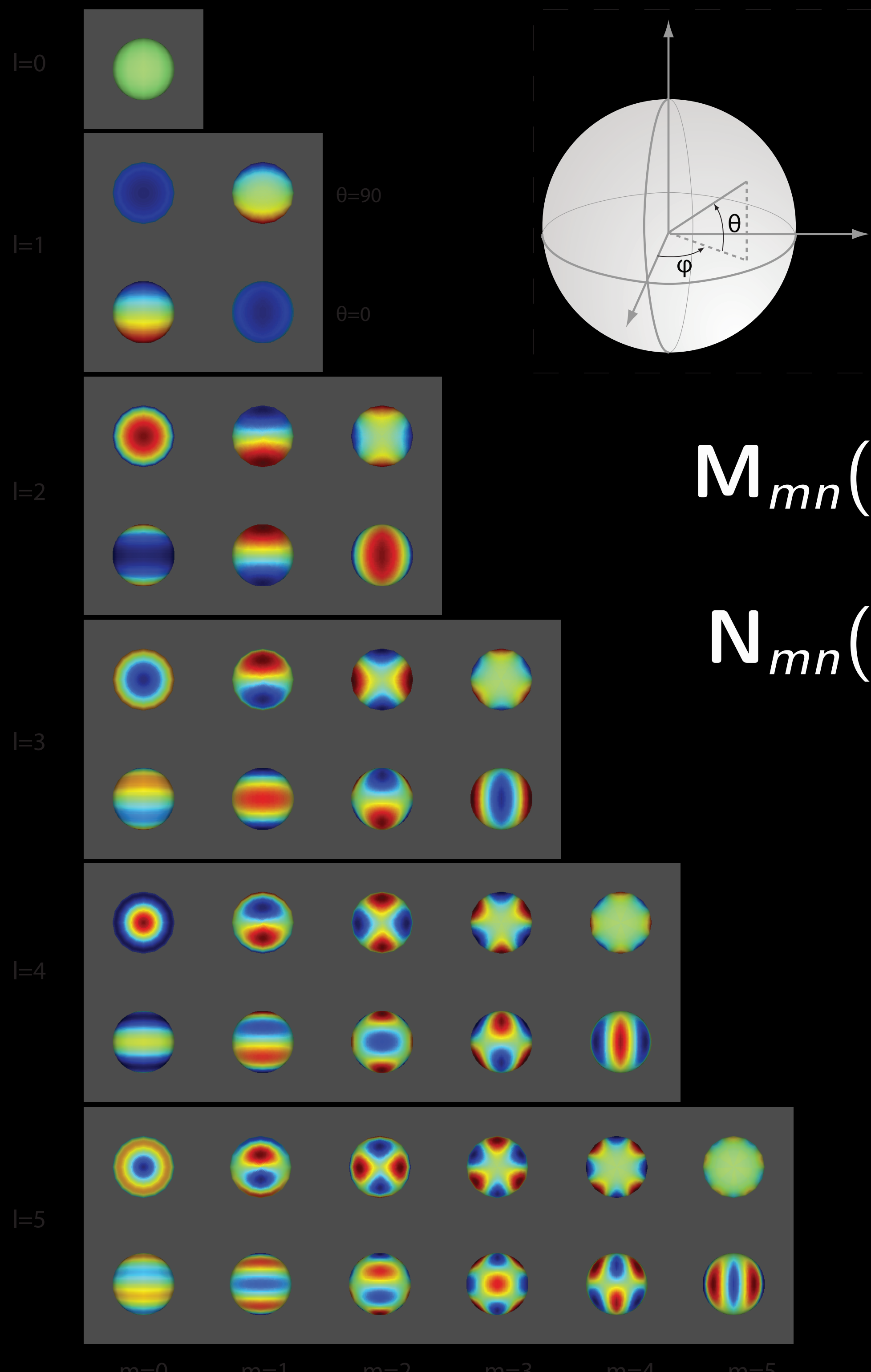
$$\mathbf{E}_{\text{sca}} = E_0 \sum_{n,m} p_{nm}\mathbf{M}^{(3)}_{nm}(k_1\mathbf{r}) + q_{nm}\mathbf{N}^{(3)}_{nm}(k_1\mathbf{r})$$

$$\begin{pmatrix}\mathbf{p}\\ \mathbf{q}\end{pmatrix} = \mathbf{T}\begin{pmatrix}\mathbf{a}\\ \mathbf{b}\end{pmatrix}$$

$$\mathbf{T} = \begin{pmatrix}\mathbf{T}^{11} & \mathbf{T}^{12}\\ \mathbf{T}^{21} & \mathbf{T}^{22}\end{pmatrix}$$

electric–electric
magnetic–electric
electric–magnetic
magnetic–magnetic

Scattering & VSWFs



Vector Spherical Wave Functions

$$\mathbf{M}_{mn}(k\mathbf{r}) = N_n h_n(k\mathbf{r}) \nabla \times (\mathbf{r} Y_n^m(\theta, \phi))$$

$$\mathbf{N}_{mn}(k\mathbf{r}) = \frac{h_n(k\mathbf{r})}{kr N_n} \hat{\mathbf{r}} Y_n^m(\theta, \phi) + N_n \left[h_{n-1}(k\mathbf{r}) - \frac{n h_n(k\mathbf{r})}{kr} \right] \mathbf{r} \nabla Y_n^m(\theta, \phi)$$

kind of like

spherical harmonics

Incident Field $\begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix} = \cdots$

$$\mathbf{E} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} a_{mn} \mathbf{M}^{(1)}(k_1, \mathbf{r}) + b_{mn} \mathbf{N}^{(1)}(k_1, \mathbf{r})$$

- "simple" angular functions for a plane wave (family of Legendre functions) "easy"
- **point-matching** for an arbitrary beam harder

Calculating T

— painful —

5 *T*-matrix method and Lorenz–Mie theory 145

The boundary conditions require continuity of the tangential components of the electric and magnetic fields, i.e.,

$$\left.\begin{array}{l}\hat{\mathbf{n}}\times\mathbf{E}_{+}(\mathbf{r})=\hat{\mathbf{n}}\times\mathbf{E}_{-}(\mathbf{r})\\ \hat{\mathbf{n}}\times\mathbf{H}_{+}(\mathbf{r})=\hat{\mathbf{n}}\times\mathbf{H}_{-}(\mathbf{r})\end{array}\right\},\qquad \mathbf{r}\in S, \tag{5.178}$$

where the subscript minus labels the fields on the *interior* side of the particle surface (cf. Eqs. (1.13) and (1.15)). Substituting Eqs. (5.176)–(5.178) into Eq. (5.173) and using Eq. (5.169), we have

$$\begin{bmatrix}\mathbf{a}\\ \mathbf{b}\end{bmatrix}=\mathbf{Q}\begin{bmatrix}\mathbf{c}\\ \mathbf{d}\end{bmatrix}=\begin{bmatrix}\mathbf{Q}^{11} & \mathbf{Q}^{12}\\ \mathbf{Q}^{21} & \mathbf{Q}^{22}\end{bmatrix}\begin{bmatrix}\mathbf{c}\\ \mathbf{d}\end{bmatrix}, \tag{5.179}$$

where

$$Q^{11}_{mnm'n'}=-\mathrm{i}k_1k_2J^{21}_{mnm'n'}-\mathrm{i}k_1^2J^{12}_{mnm'n'}, \tag{5.180}$$

$$Q^{12}_{mnm'n'}=-\mathrm{i}k_1k_2J^{11}_{mnm'n'}-\mathrm{i}k_1^2J^{22}_{mnm'n'}, \tag{5.181}$$

$$Q^{21}_{mnm'n'}=-\mathrm{i}k_1k_2J^{22}_{mnm'n'}-\mathrm{i}k_1^2J^{11}_{mnm'n'}, \tag{5.182}$$

$$Q^{22}_{mnm'n'}=-\mathrm{i}k_1k_2J^{12}_{mnm'n'}-\mathrm{i}k_1^2J^{21}_{mnm'n'}, \tag{5.183}$$

and

$$\begin{bmatrix}J^{11}_{mnm'n'}\\ J^{12}_{mnm'n'}\\ J^{21}_{mnm'n'}\\ J^{22}_{mnm'n'}\end{bmatrix}=(-1)^m\int_S \mathrm{d}S\,\hat{\mathbf{n}}\cdot\begin{bmatrix}\mathrm{Rg}\mathbf{M}_{m'n'}(k_2r,\vartheta,\varphi)\times\mathbf{M}_{-mn}(k_1r,\vartheta,\varphi)\\ \mathrm{Rg}\mathbf{M}_{m'n'}(k_2r,\vartheta,\varphi)\times\mathbf{N}_{-mn}(k_1r,\vartheta,\varphi)\\ \mathrm{Rg}\mathbf{N}_{m'n'}(k_2r,\vartheta,\varphi)\times\mathbf{M}_{-mn}(k_1r,\vartheta,\varphi)\\ \mathrm{Rg}\mathbf{N}_{m'n'}(k_2r,\vartheta,\varphi)\times\mathbf{N}_{-mn}(k_1r,\vartheta,\varphi)\end{bmatrix} \tag{5.184}$$

Similarly, substituting Eqs. (5.176)–(5.178) into Eq. (5.175) yields

$$\begin{bmatrix}\mathbf{p}\\ \mathbf{q}\end{bmatrix}=-\mathrm{Rg}\mathbf{Q}\begin{bmatrix}\mathbf{c}\\ \mathbf{d}\end{bmatrix}=-\begin{bmatrix}\mathrm{Rg}\mathbf{Q}^{11} & \mathrm{Rg}\mathbf{Q}^{12}\\ \mathrm{Rg}\mathbf{Q}^{21} & \mathrm{Rg}\mathbf{Q}^{22}\end{bmatrix}\begin{bmatrix}\mathbf{c}\\ \mathbf{d}\end{bmatrix}, \tag{5.185}$$

where

$$\mathrm{Rg}Q^{11}_{mnm'n'}=-\mathrm{i}k_1k_2\mathrm{Rg}J^{21}_{mnm'n'}-\mathrm{i}k_1^2\,\mathrm{Rg}J^{12}_{mnm'n'}, \tag{5.186}$$

$$\mathrm{Rg}Q^{12}_{mnm'n'}=-\mathrm{i}k_1k_2\mathrm{Rg}J^{11}_{mnm'n'}-\mathrm{i}k_1^2\,\mathrm{Rg}J^{22}_{mnm'n'}, \tag{5.187}$$

$$\mathrm{Rg}Q^{21}_{mnm'n'}=-\mathrm{i}k_1k_2\mathrm{Rg}J^{22}_{mnm'n'}-\mathrm{i}k_1^2\,\mathrm{Rg}J^{11}_{mnm'n'}, \tag{5.188}$$

$$\mathrm{Rg}Q^{22}_{mnm'n'}=-\mathrm{i}k_1k_2\mathrm{Rg}J^{12}_{mnm'n'}-\mathrm{i}k_1^2\,\mathrm{Rg}J^{21}_{mnm'n'}, \tag{5.189}$$

and

$$\begin{bmatrix}\mathrm{Rg}J^{11}_{mnm'n'}\\ \mathrm{Rg}J^{12}_{mnm'n'}\\ \mathrm{Rg}J^{21}_{mnm'n'}\\ \mathrm{Rg}J^{22}_{mnm'n'}\end{bmatrix}=(-1)^m\int_S \mathrm{d}S\,\hat{\mathbf{n}}\cdot\begin{bmatrix}\mathrm{Rg}\mathbf{M}_{m'n'}(k_2r,\vartheta,\varphi)\times\mathrm{Rg}\mathbf{M}_{-mn}(k_1r,\vartheta,\varphi)\\ \mathrm{Rg}\mathbf{M}_{m'n'}(k_2r,\vartheta,\varphi)\times\mathrm{Rg}\mathbf{N}_{-mn}(k_1r,\vartheta,\varphi)\\ \mathrm{Rg}\mathbf{N}_{m'n'}(k_2r,\vartheta,\varphi)\times\mathrm{Rg}\mathbf{M}_{-mn}(k_1r,\vartheta,\varphi)\\ \mathrm{Rg}\mathbf{N}_{m'n'}(k_2r,\vartheta,\varphi)\times\mathrm{Rg}\mathbf{N}_{-mn}(k_1r,\vartheta,\varphi)\end{bmatrix} \tag{5.190}$$

- $\iint$ {products of VSWFs}
- Simplifications for axial symmetry
- **Simple for spheres**
- Requires regular shapes

  “Rayleigh hypothesis”
- Codes available :)

Rotations

Translation-Addition Theorems Etc.

... more horrible formulas
(but they exist)

Strengths

- Analytical properties, e.g. **angular averaging**

$$\langle C_{\text{ext}} \rangle = -\frac{2\pi}{k_1^2} \sum_{n,m} \text{Re}\left(T^{11}_{nn|m} + T^{22}_{nn|m} \right)$$

- Independent of incident beam
- **Multiple scattering**
- Fast, accurate, **physical meaning**

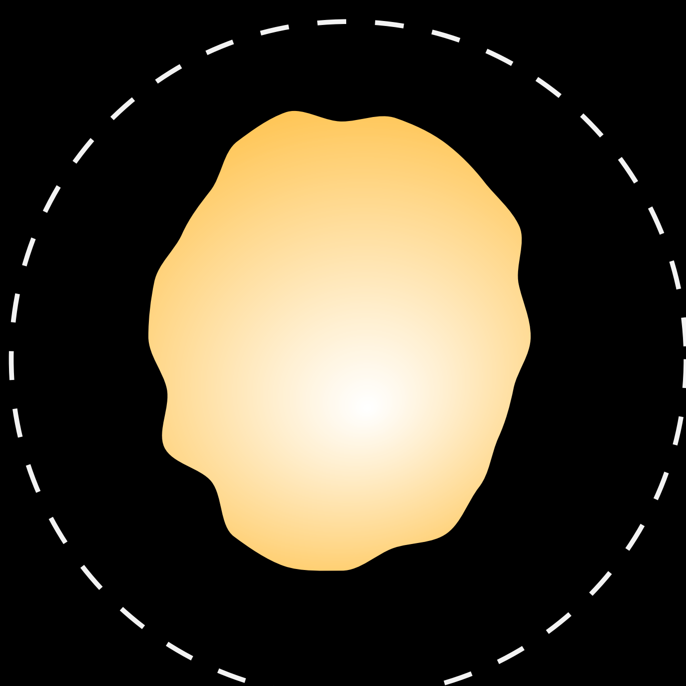
The Force
a.k.a Stress Tensor

Lorentz force $\mathbf{f} = q\left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right)$

∇xxx magic

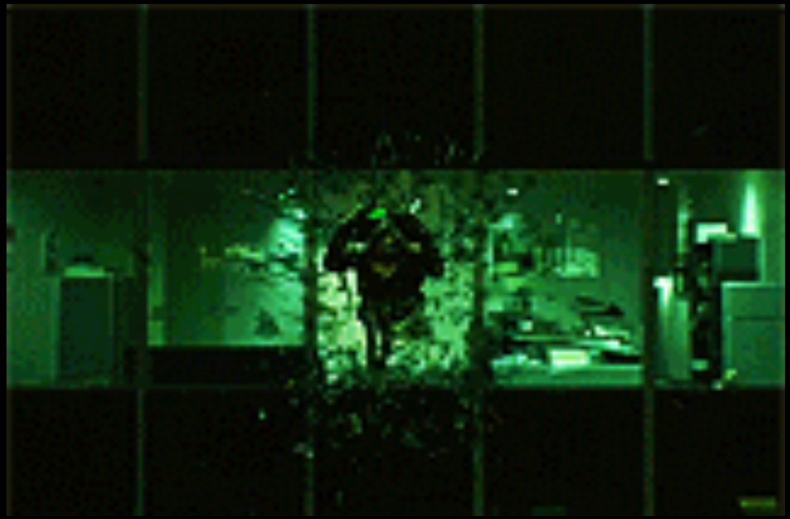
$$\mathbf{f} = \int_S \overleftrightarrow{\mathbb{T}} \cdot \mathbf{n}\, \mathrm{d}S$$

$$\overleftrightarrow{\mathbb{T}} = \varepsilon\mathbf{E}\mathbf{E} - \mu\mathbf{H}\mathbf{H} - \frac{1}{2}\left(\varepsilon E^2 + \mu H^2\right)\overleftrightarrow{\mathbb{I}}$$



arbitrary *S*

Forces (Continued)



inc. – scat.

$$F_z = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \frac{m}{n(n+1)} \Re\left(a^*_{nm} b_{nm} - p^*_{nm} q_{nm}\right) -$$

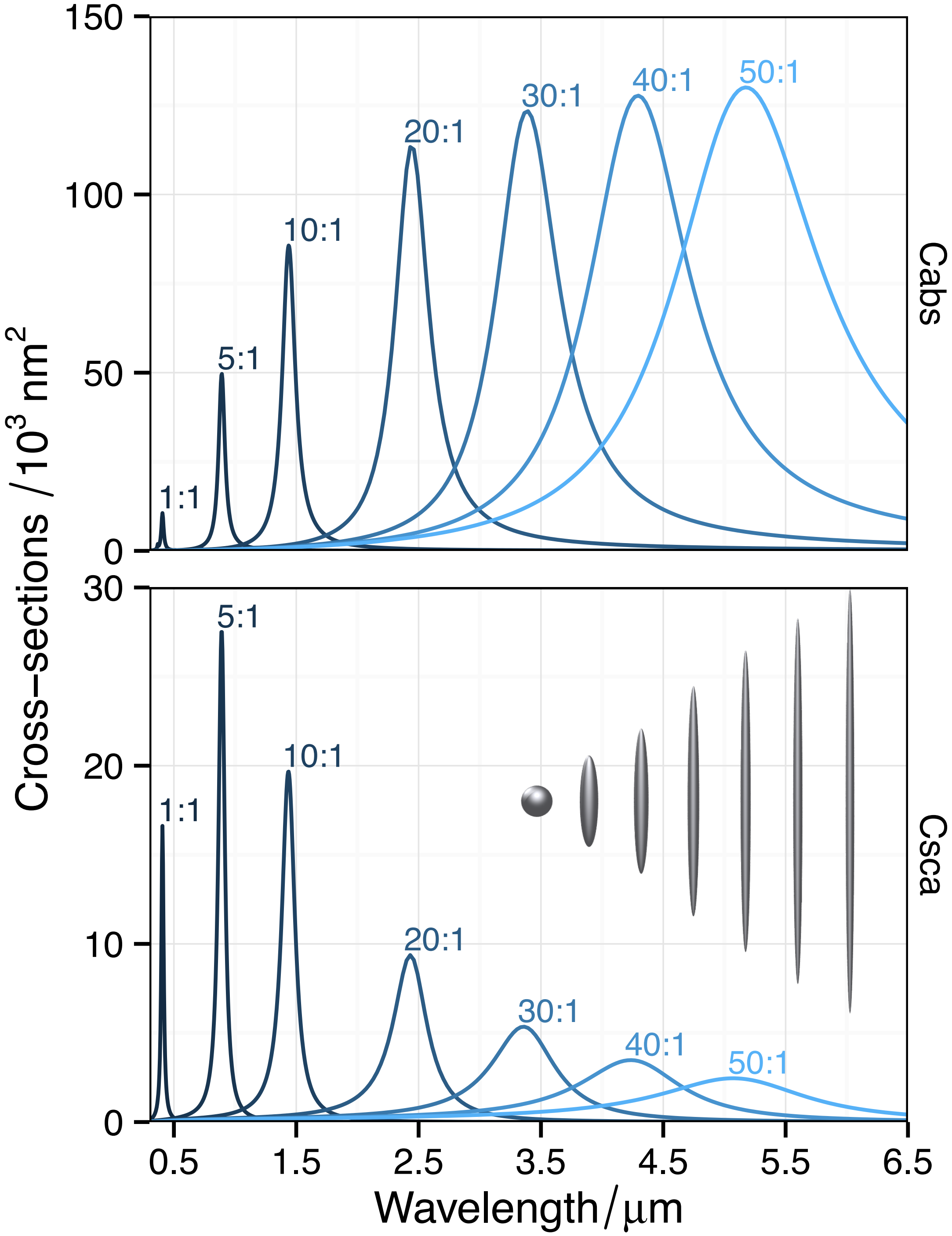
$$\frac{1}{n+1}\left[\frac{n(n+2)(n-m+1)(n+m+1)}{(2n+1)(2n+3)}\right]^{\frac{1}{2}}$$

$$\times \Re\left(a_{nm} a^*_{n+1,m} + b_{nm} b^*_{n+1,m} - p_{nm} p^*_{n+1,m} - q_{nm} q^*_{n+1,m}\right)$$

"Easy"

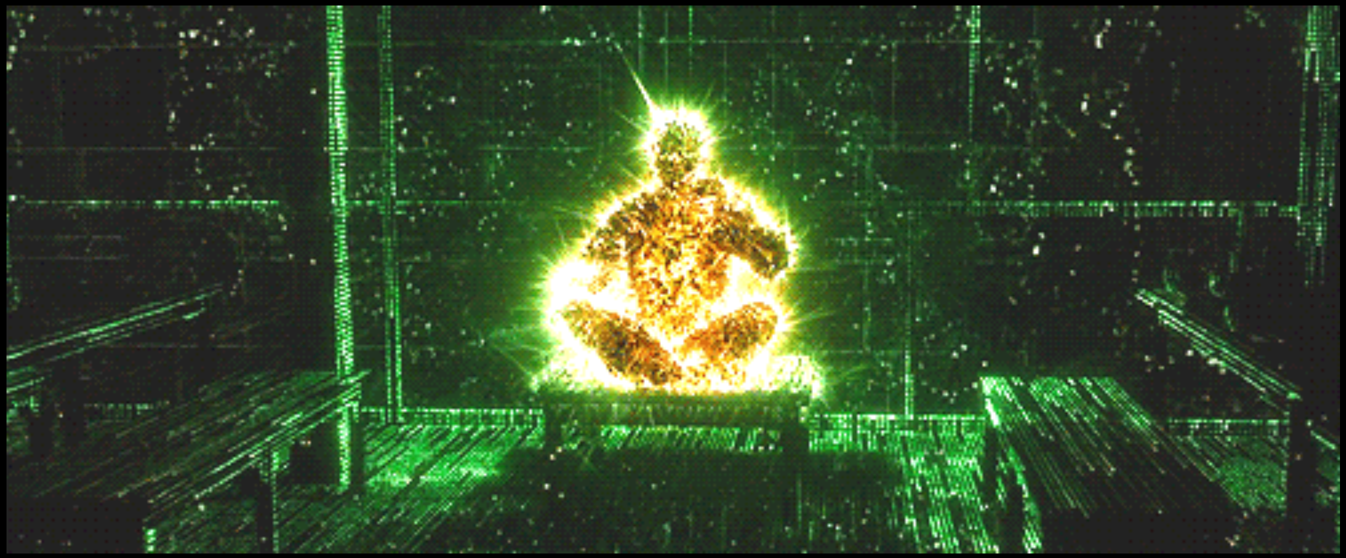
(once a,b,p,q-s are known)

Computer Requirements

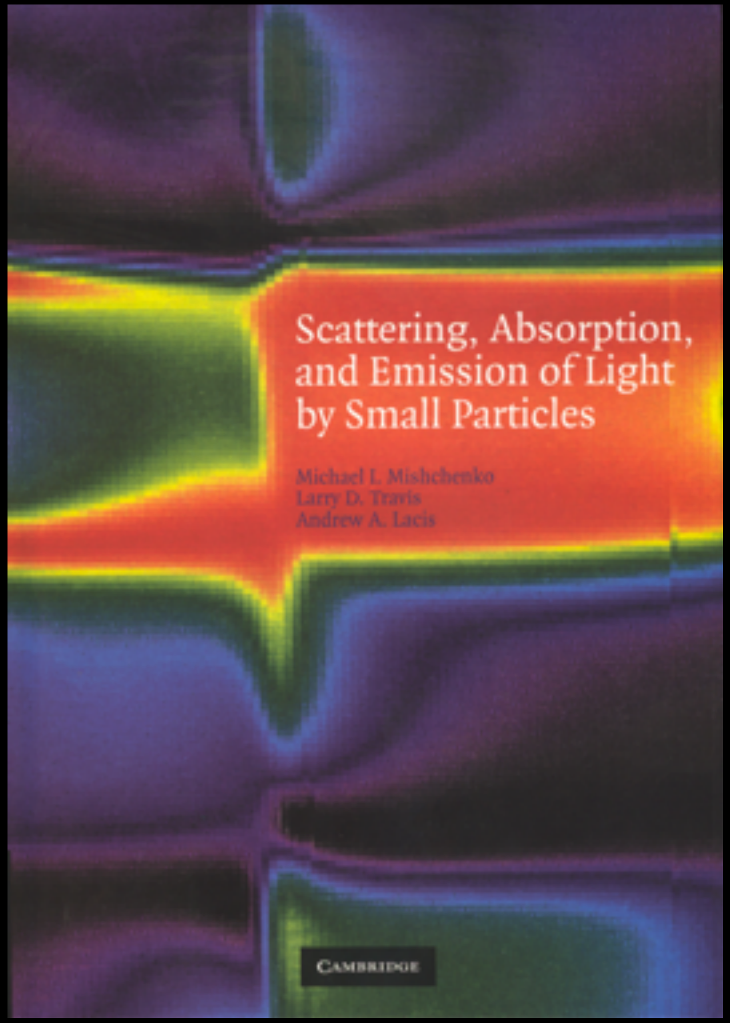


- Very fast (< 1 ″)
  for **axi-symmetric** particles
- OK for arbitrary shape
  BUT convergence + complexity
- Tweezers:
  also need incident beam

References & Open Source



M. Mishchenko



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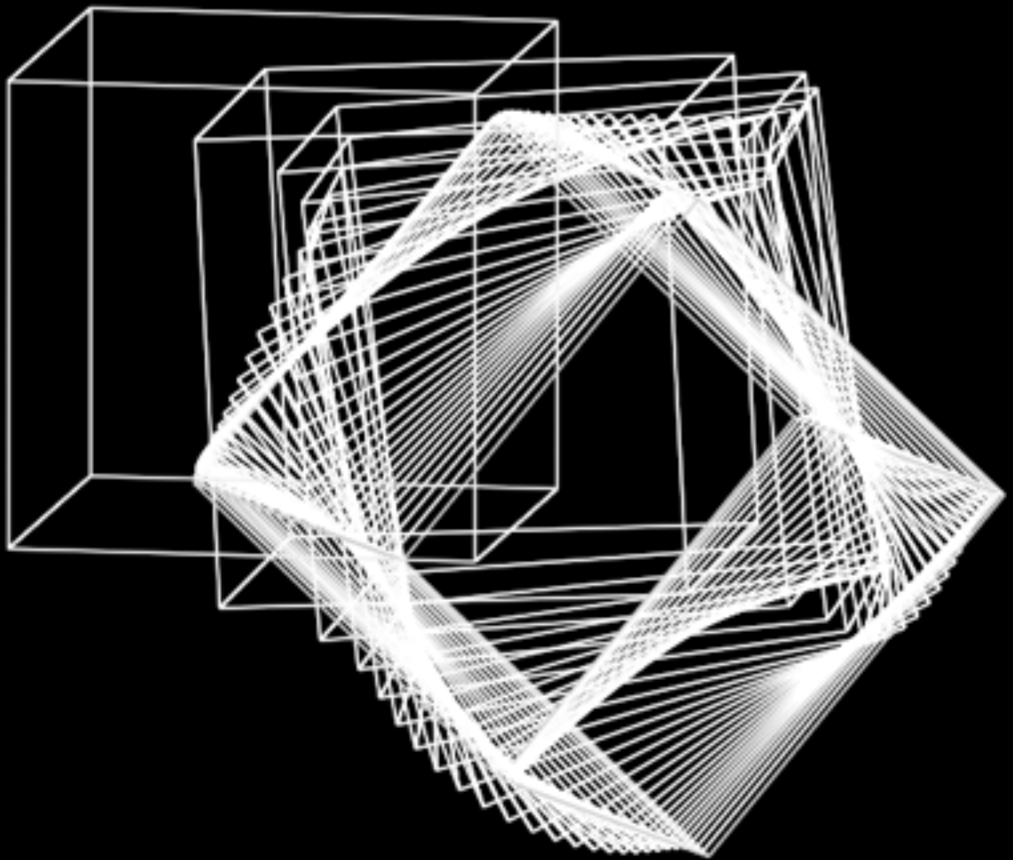
T. Nieminen
H. Rubinsztein-Dunlop



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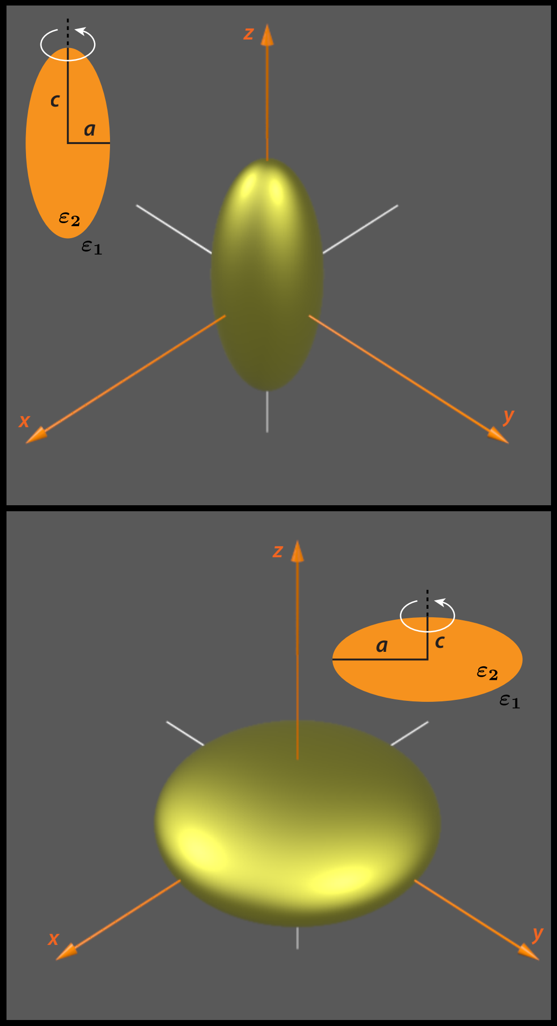
SMARTIES



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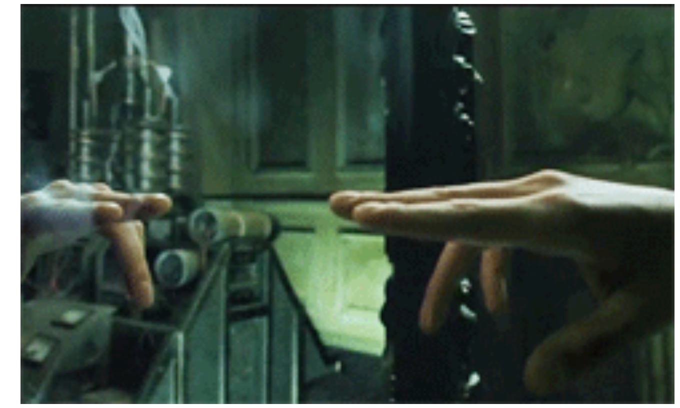
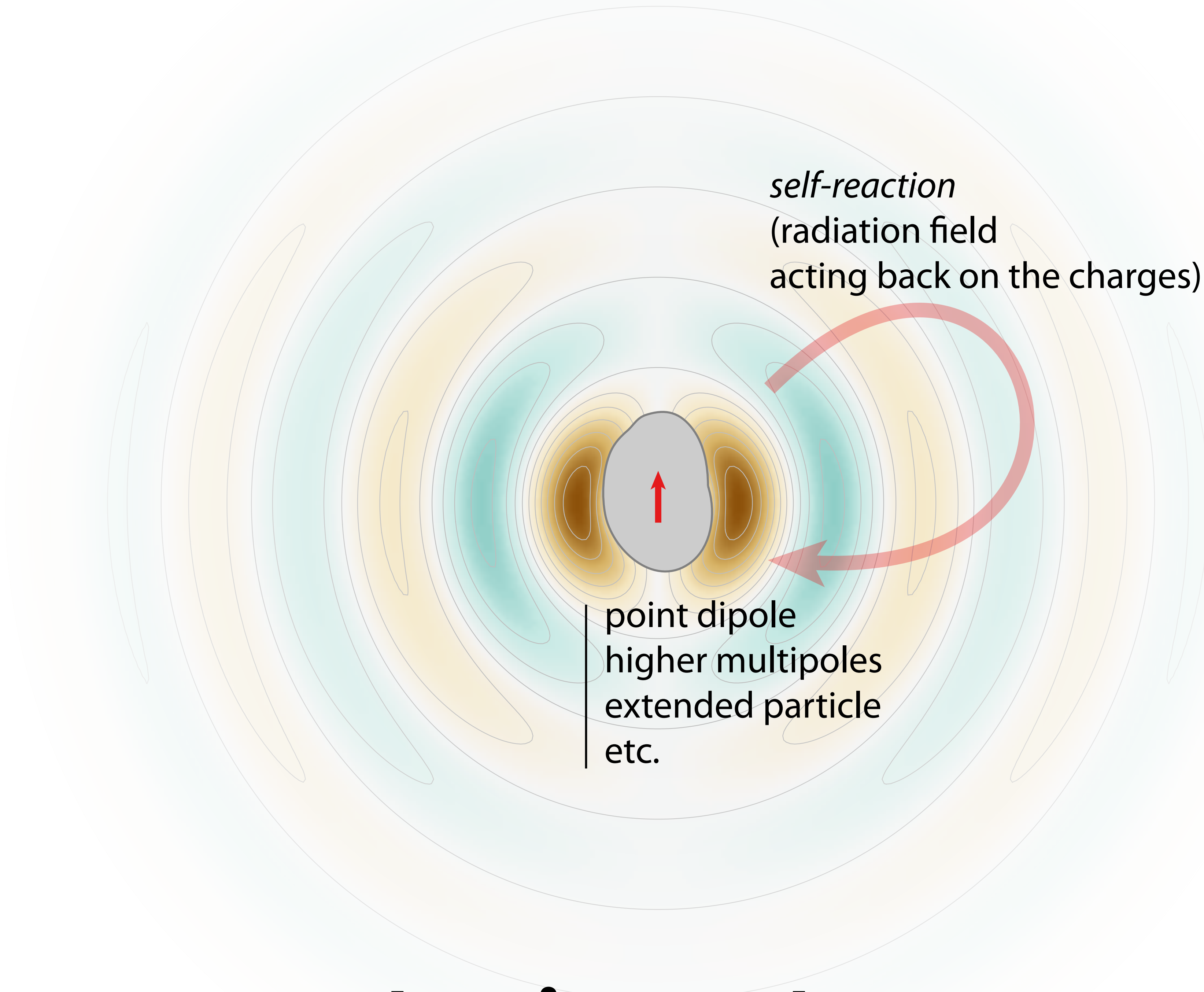
Parting Thought

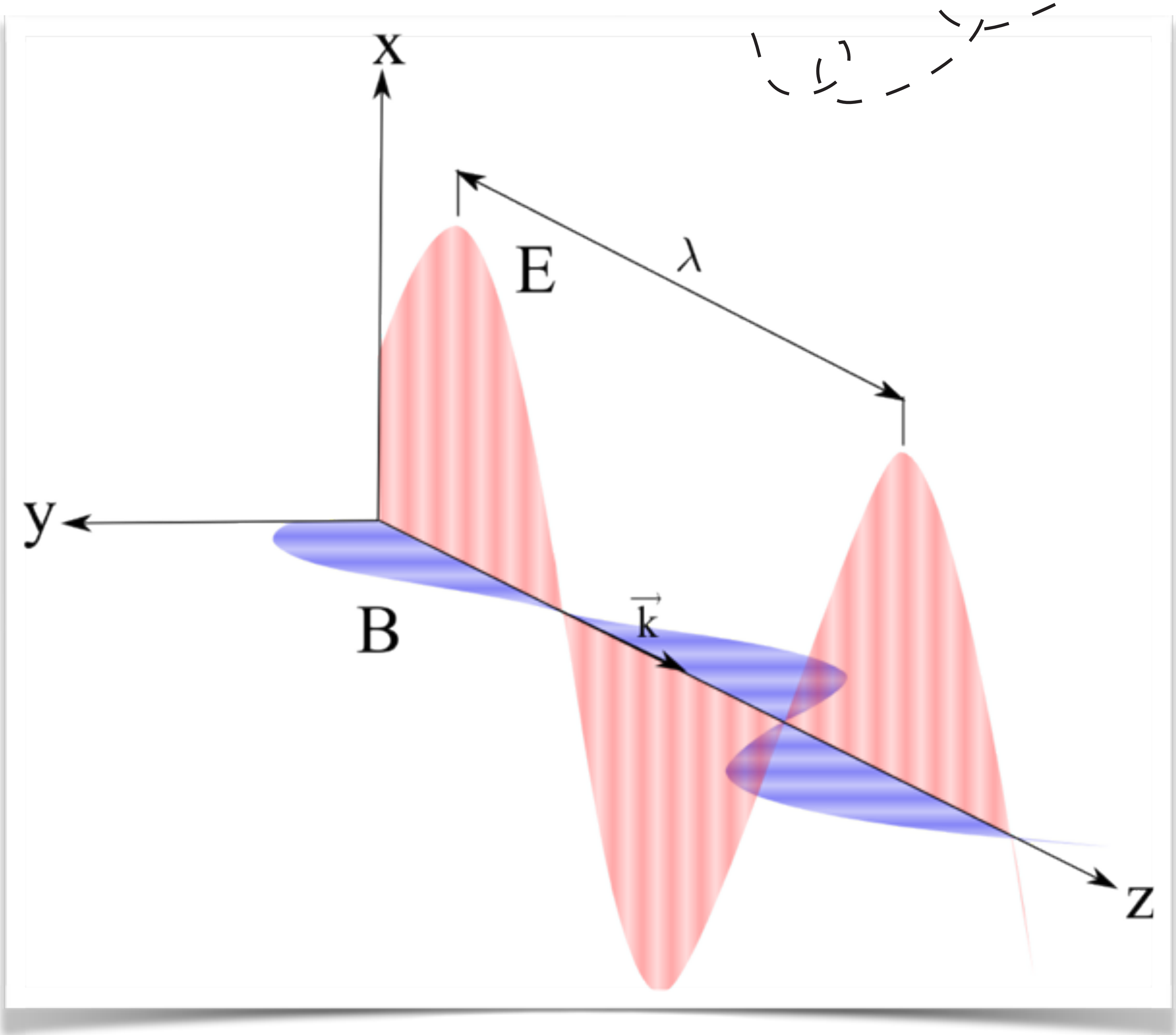
Interlude:
Radiation & Self-Reaction



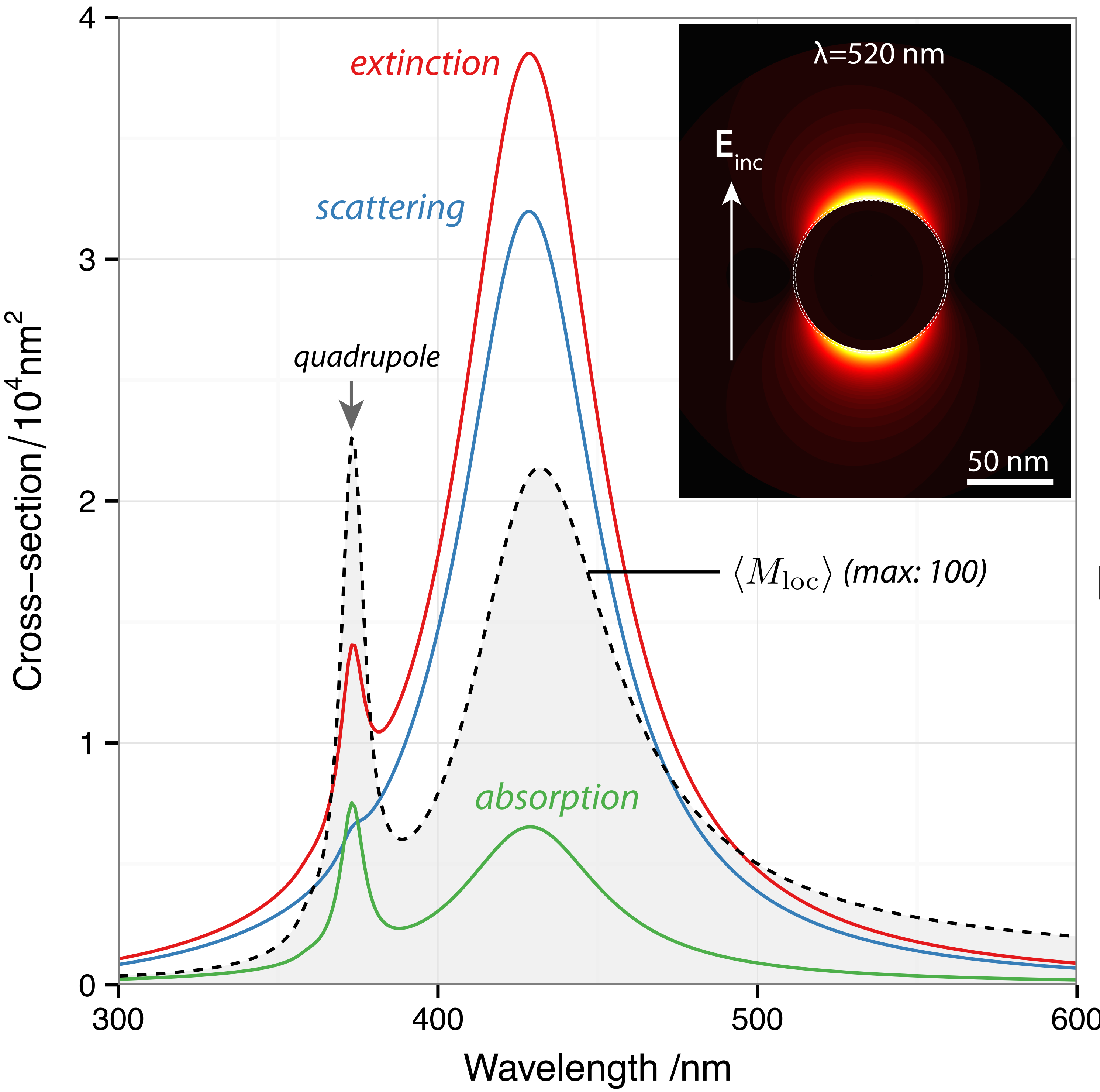


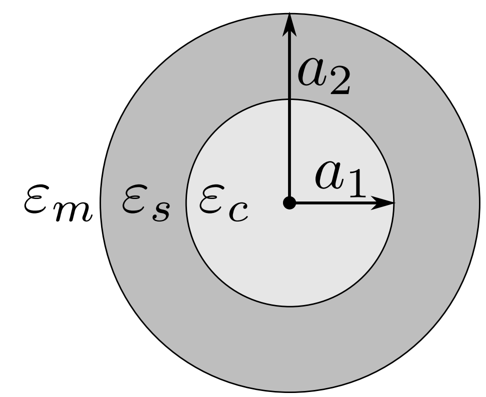
Introducing The K-Matrix

A Plane Wave



Mie Theory





$$\mathbf{E}_{\text{Inc}} = E_0 \sum_{l,m} a_{lm} \mathbf{M}^{(1)}_{lm}(k\mathbf{r}) + b_{lm} \mathbf{N}^{(1)}_{lm}(k\mathbf{r})$$

$$\mathbf{E}_{\text{Sca}} = E_0 \sum_{l,m} c_{lm} \mathbf{M}^{(3)}_{lm}(k\mathbf{r}) + d_{lm} \mathbf{N}^{(3)}_{lm}(k\mathbf{r})$$

$$c_l = \frac{s\psi_l(x)\psi_l'(sx) - \psi_l(sx)\psi_l'(x)}{\psi_l(sx)\xi_l'(x) - s\psi_l'(sx)\xi_l'(x)} a_l$$

$$d_l = \frac{\psi_l(x)\psi_l'(sx) - s\psi_l(sx)\psi_l'(x)}{s\psi_l(sx)\xi_l'(x) - \psi_l'(sx)\xi_l'(x)} b_l$$