Master's Thesis: Electromagnetic Scattering in Micro- and Nanostructured Materials

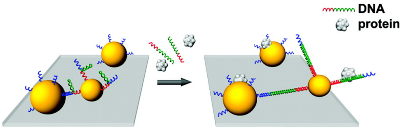
Supervisors: Jesper Mørk and Philip Trøst Kristensen

Jakob Rosenkrantz de Lasson

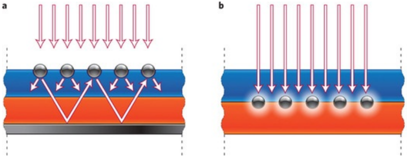
DTU Fotonik
Department of Photonics Engineering

21 August 2012

Motivation



Nanoscale plasmonic sensing
(J. I. L. Chen *et al.*, J. Am. Chem. Soc. **132** (2010))



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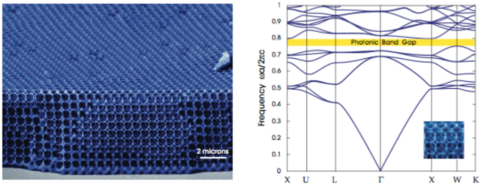

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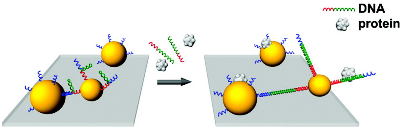

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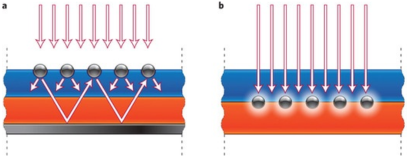

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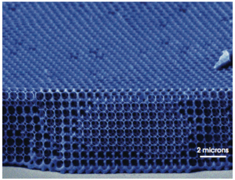

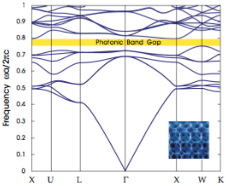

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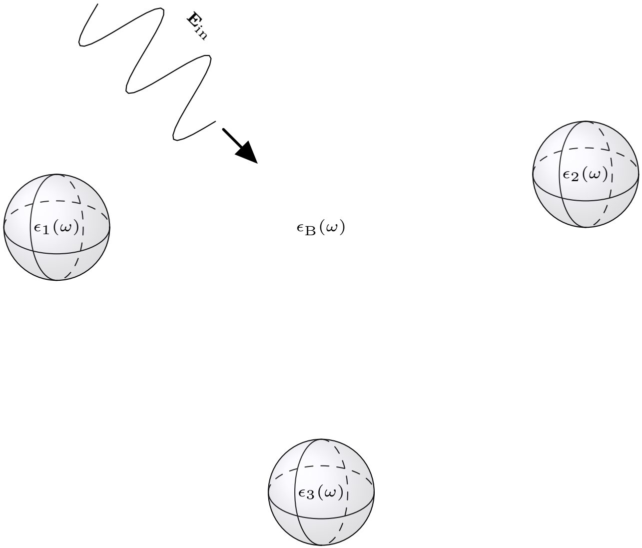
Scope of project:

Tool for simulating interaction between spherical scatterers and electromagnetic radiation in homogeneous background medium.

Outline

Geometry: N Scatterers in Homogeneous 3D Background



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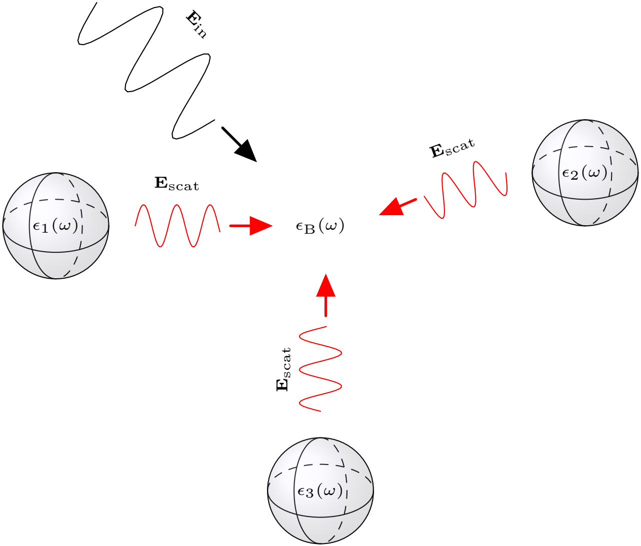

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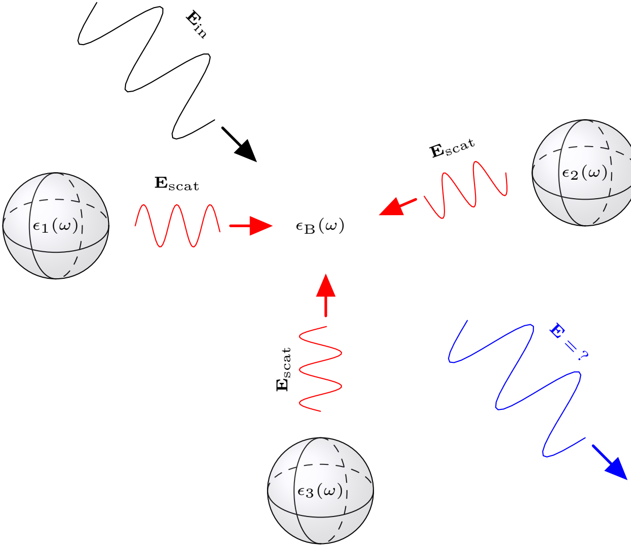

Lippmann-Schwinger Equation

- Frequency-space wave equation for electric field

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

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- Inhomogeneous PDE with formal solution

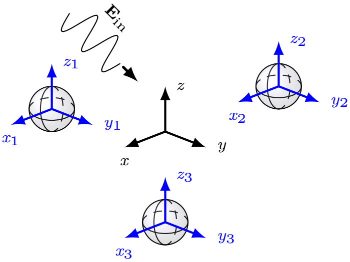
$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_{\mathrm{B}}(\mathbf{r}) + \underbrace{k_0^2 \int \mathbf{G}_{\mathrm{B}}(\mathbf{r},\mathbf{r}')\Delta\epsilon(\mathbf{r}')\mathbf{E}(\mathbf{r}')\,\mathrm{d}\mathbf{r}'}_{\equiv \mathbf{E}_{\mathrm{scat}}(\mathbf{r})}.$$

Lippmann-Schwinger equation; Implicit equation for field inside scatterers.

Field Expansion and Matrix Equation

- Local expansion of field

$$\mathbf{E}(\mathbf{r}_j) = \sum_{\alpha\,\nu} e_{j\,\alpha\,\nu}\psi_\nu^j(\mathbf{r}_j)\,\mathbf{e}_\alpha.$$



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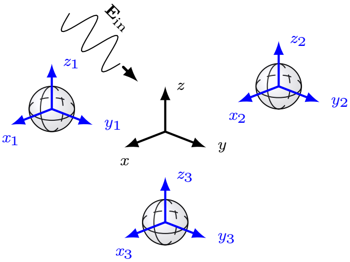
- Matrix equation for expansion coefficients

$$\mathbf{e} = \left(\mathbf{I} + \mathbf{L} - k_0^2\mathbf{G}\boldsymbol{\Delta\epsilon}\right)^{-1}\mathbf{M}_\mathrm{B}\mathbf{e}_\mathrm{B}.$$



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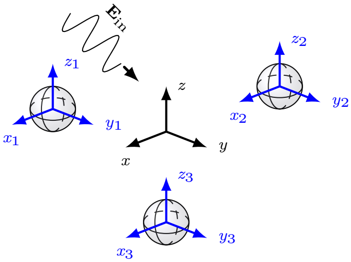

All matrices expressed analytically.
Only approximation: Truncation of set of basis functions.

Length Scales

Dipole approximation: Constant field inside scatterers.

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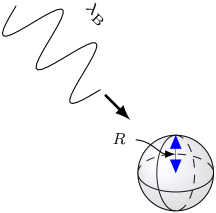

- When $R \ll \lambda_{\mathrm{B}}$, field variation across scatterer is negligible: $\mathbf{E}(\mathbf{r}_j) \simeq \mathbf{E}(\mathbf{r}_j^0)$.
- Simpler, analytic solutions, e.g. for cross sections.

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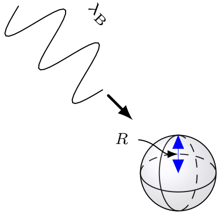
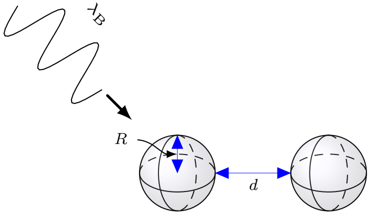
Dipole approximation: Constant field inside scatterers.





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- New length scale: d.
- With $R \ll \lambda_{\mathrm{B}}$, is dipole approximation valid if

$$d/R \gg 1?$$
$$d/R \sim 1?$$
$$d/R \ll 1?$$

Algebraic Lippmann-Schwinger Equation

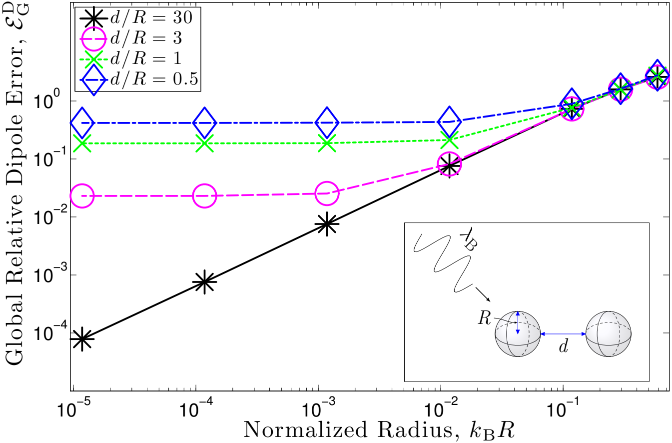
- Constant field yields algebraic Lippmann-Schwinger equation

$$\mathbf{E}^{\mathrm{D}}(\mathbf{r}_j^0) = \mathbf{E}_{\mathrm{B}}(\mathbf{r}_j^0) + k_0^2 \sum_{j'=1}^{N} \mathbf{G}_{jj'}^{\mathrm{D}} \Delta\epsilon_{j'} \mathbf{E}^{\mathrm{D}}(\mathbf{r}_{j'}^0) - \frac{\Delta\epsilon_j}{\epsilon_{\mathrm{B}}} \mathbf{L}\mathbf{E}^{\mathrm{D}}(\mathbf{r}_j^0).$$

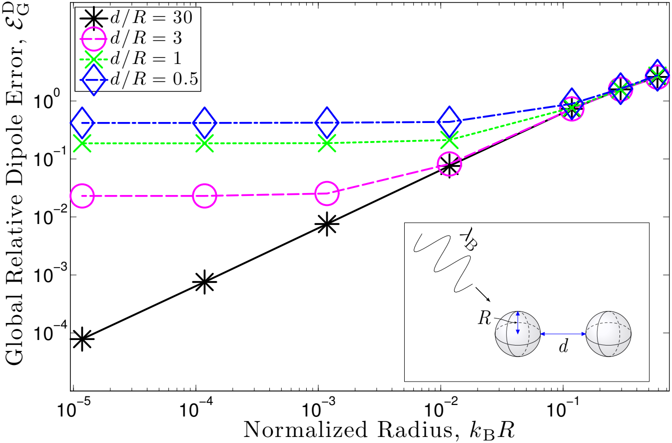
- Global relative error of dipole approximation

$$\mathcal{E}_{\mathrm{G}}^{\mathrm{D}} \equiv \sum_{j\alpha} \frac{\int_{V_j} \left| \mathbf{E}(\mathbf{r}_j') - \mathbf{E}^{\mathrm{D}}(\mathbf{r}_j^0) \right| \, \mathrm{d}\mathbf{r}_j'}{\int_{V_j} \left| \mathbf{E}(\mathbf{r}_j') \right| \, \mathrm{d}\mathbf{r}_j'}.$$

Global Relative Error of Dipole Approximation



Global Relative Error of Dipole Approximation

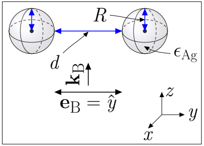


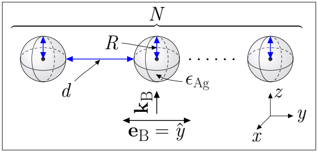
Dipole approximation is only valid when $d/R \gtrsim 3$.

Geometries and Cross Sections

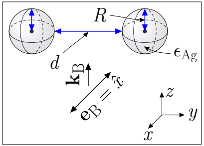
Dimer, vary d: Chain, vary N:

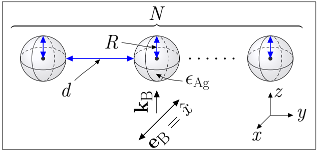
Longitudinal:





Transverse:





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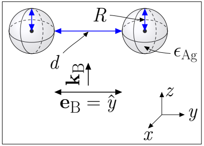

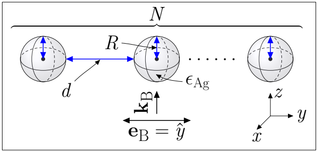

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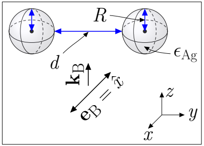
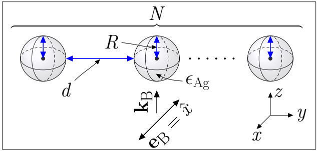
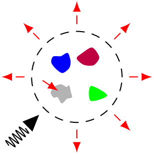


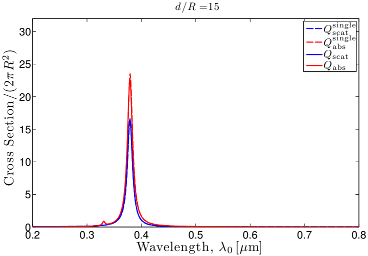


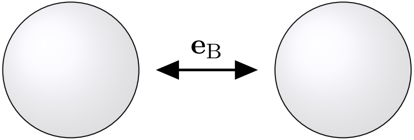
Cross sections: $C_{\mathrm{scat}} = \dfrac{P_{\mathrm{scat}}}{|\mathbf{S}_{\mathrm{B}}|}$ $\qquad C_{\mathrm{abs}} = \dfrac{P_{\mathrm{abs}}}{|\mathbf{S}_{\mathrm{B}}|}$

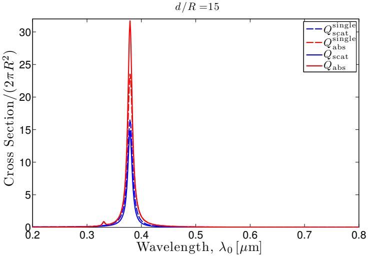
Efficiencies: $Q_{\mathrm{scat}} = \dfrac{C_{\mathrm{scat}}}{N\pi R^2}$ $\qquad Q_{\mathrm{abs}} = \dfrac{C_{\mathrm{abs}}}{N\pi R^2}$

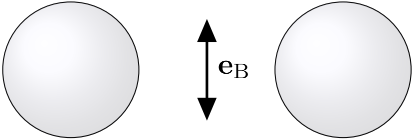


Dimer Spectra: $R = 10$ nm, Varying d









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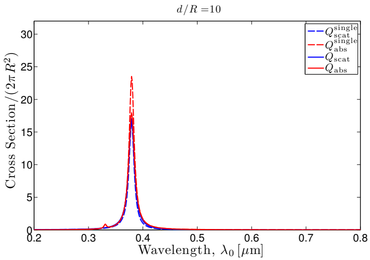

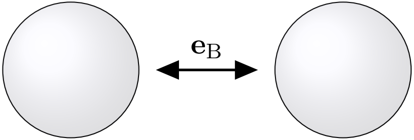

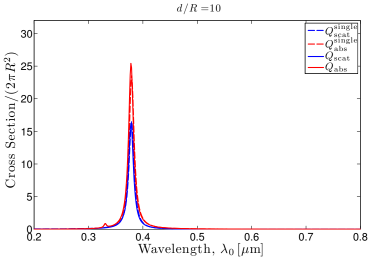

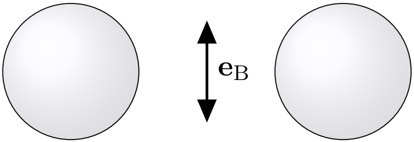

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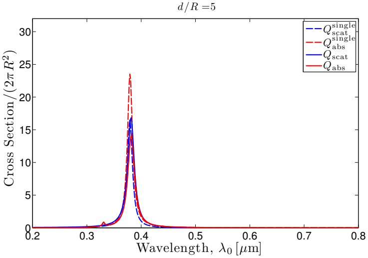

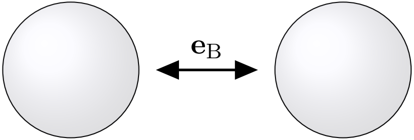

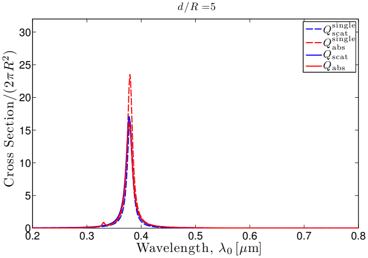

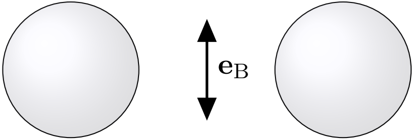

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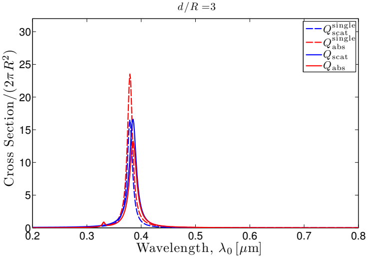

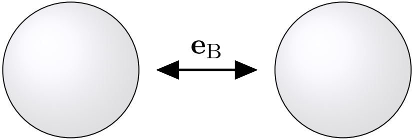

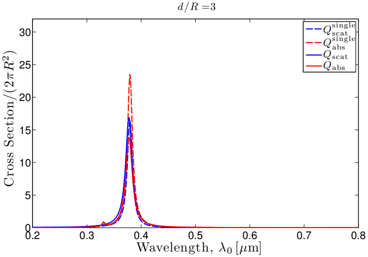

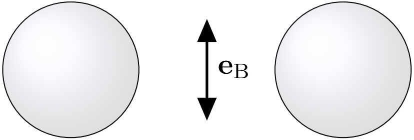

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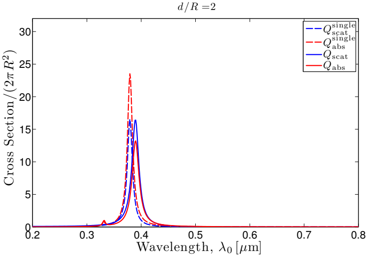

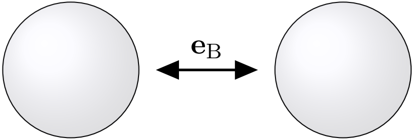

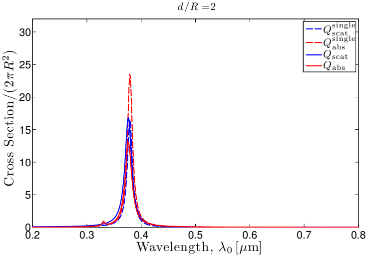

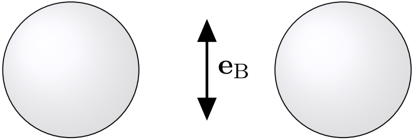

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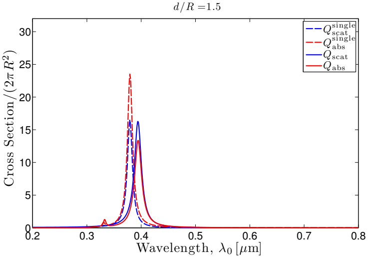

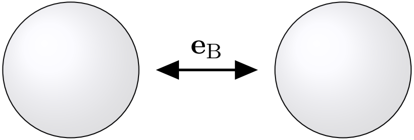

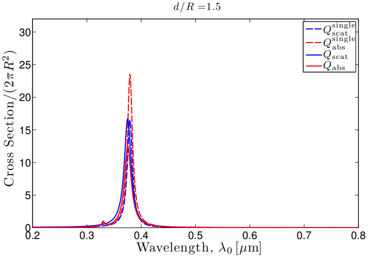

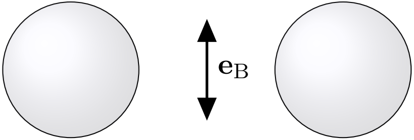

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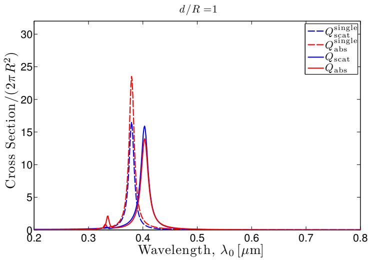

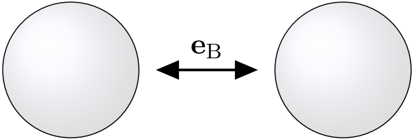

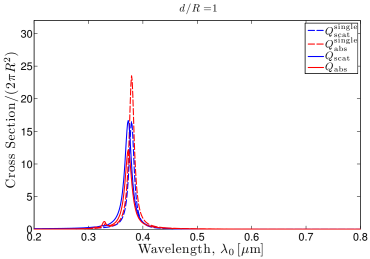

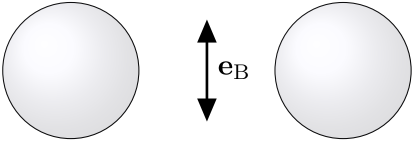

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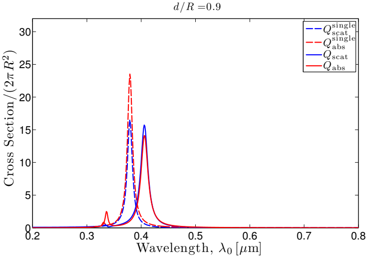

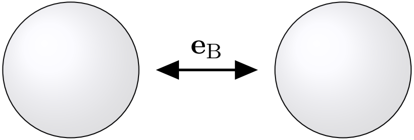

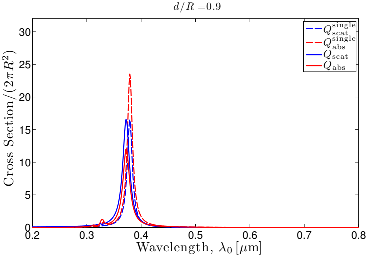

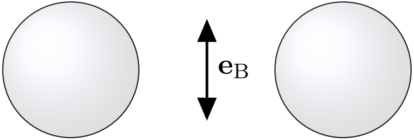

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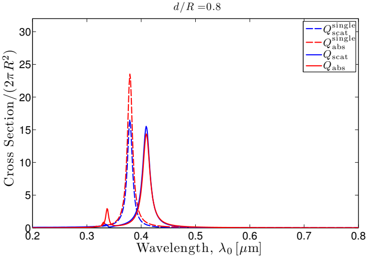

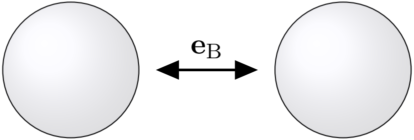

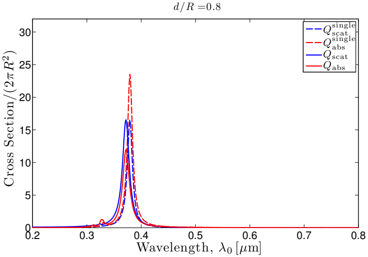

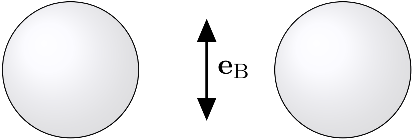

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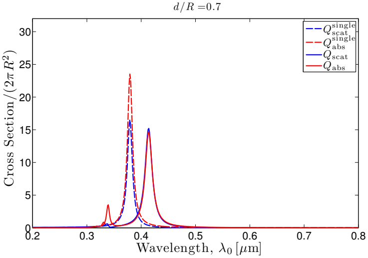

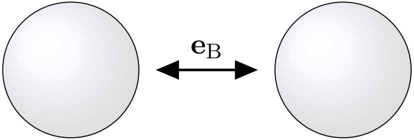

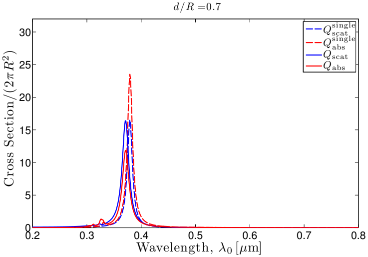

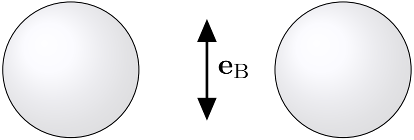

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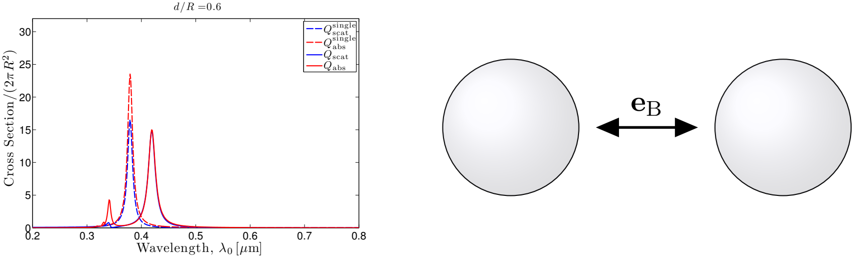

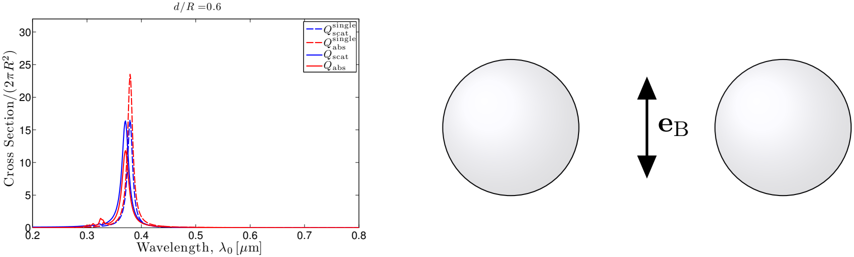

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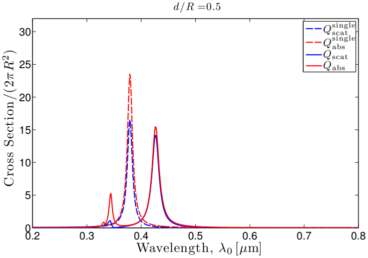

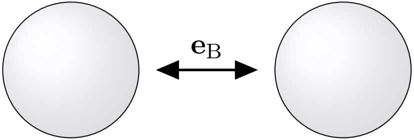

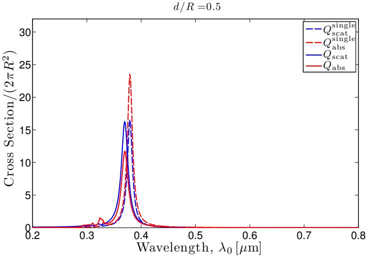

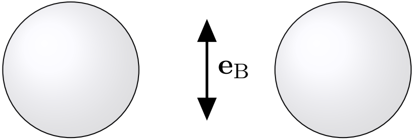

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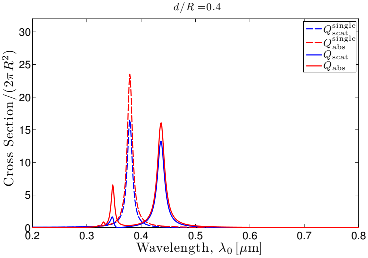

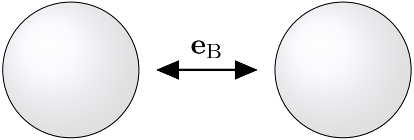

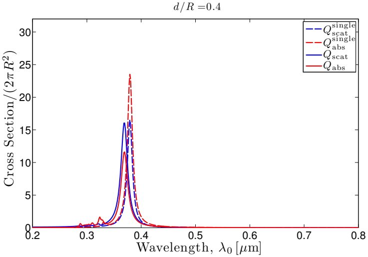

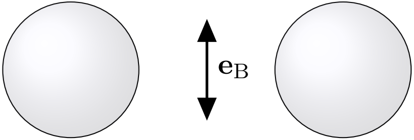

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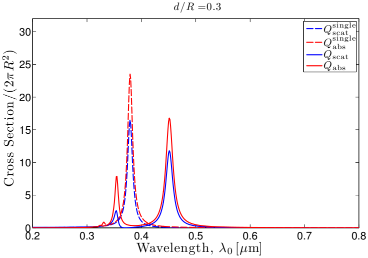

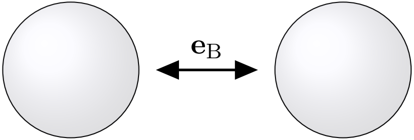

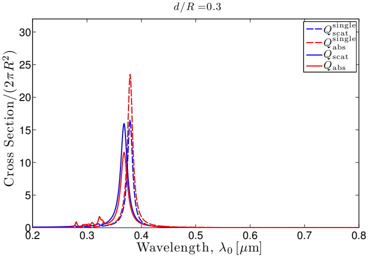

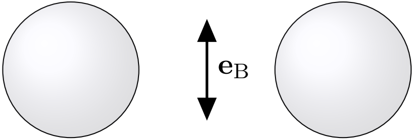

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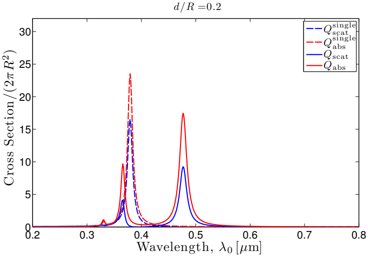

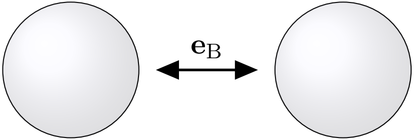

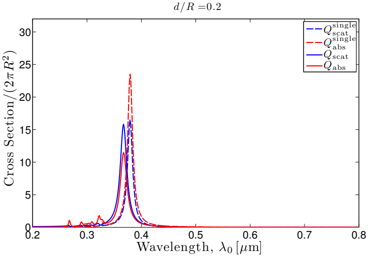

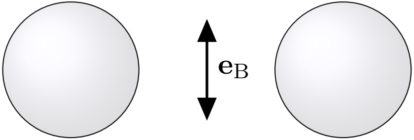

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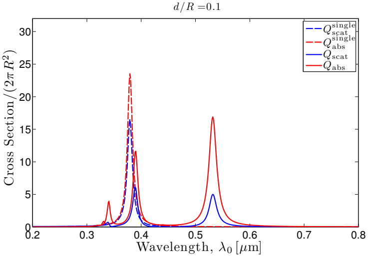

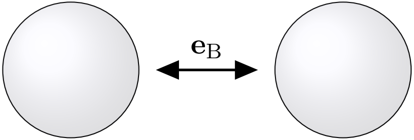

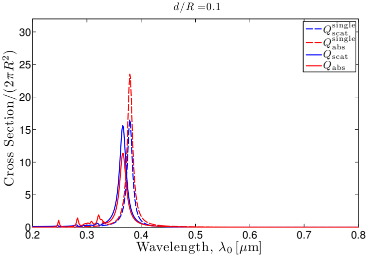

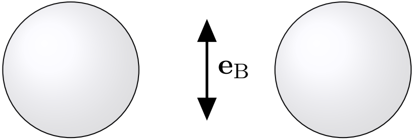

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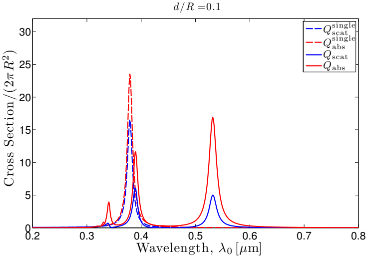

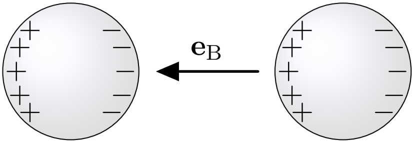

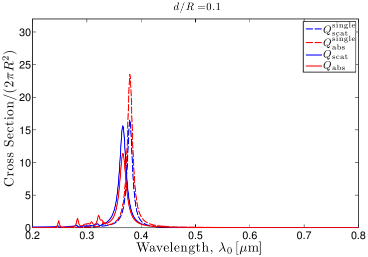

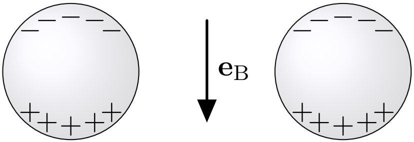

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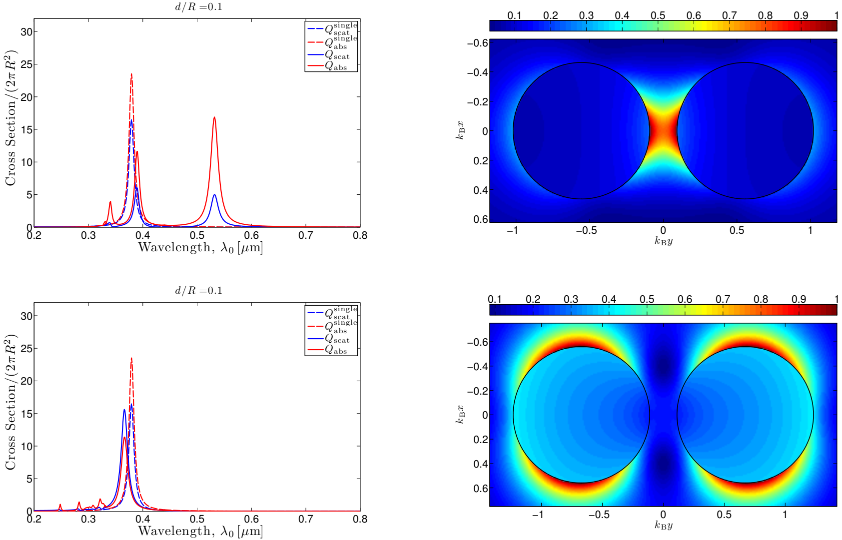

Dimer: Peak Shift Ratio (Longitudinal Polarization)

Peak shift ratio: $\Delta\lambda_0^{\mathrm{Res}} \equiv \frac{\lambda_0^{\mathrm{D}} - \lambda_0^{\mathrm{D,single}}}{\lambda_0^{\mathrm{D,single}}}$. $\Delta\lambda_0^{\mathrm{Res}} = f_{\mathrm{D}}(d; R) = ?$

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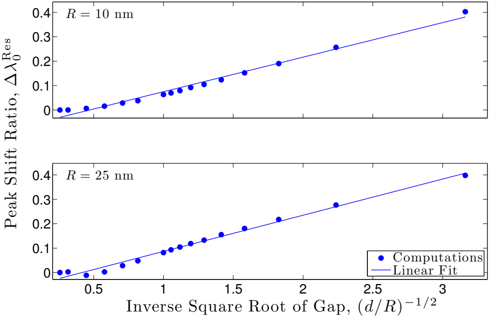

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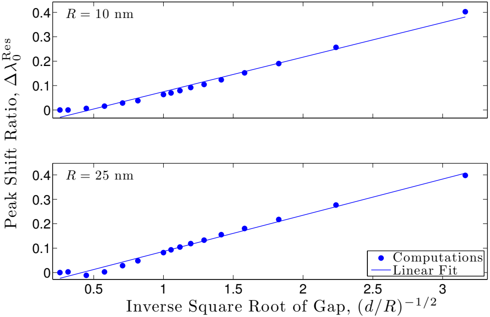
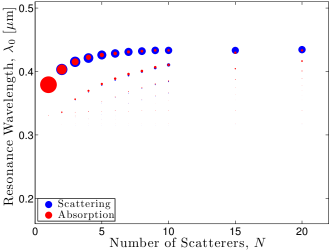
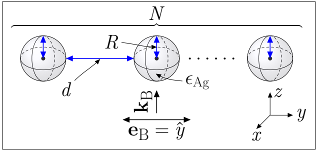
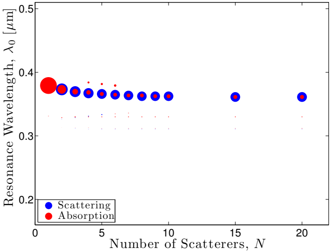


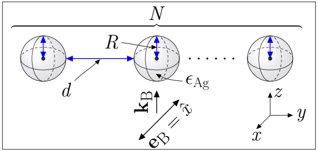
$\Delta\lambda_0^{\mathrm{Res}} \propto (d/R)^{-1/2}$; Softer dependence than reported in the literature.

Chain Resonance Wavelengths: $d = R = 10$ nm, Varying N









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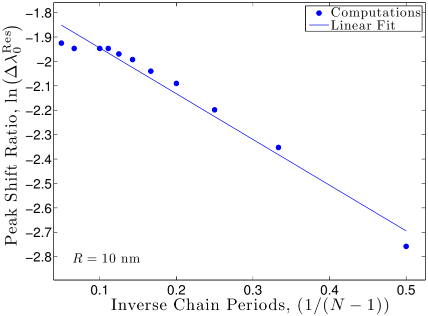

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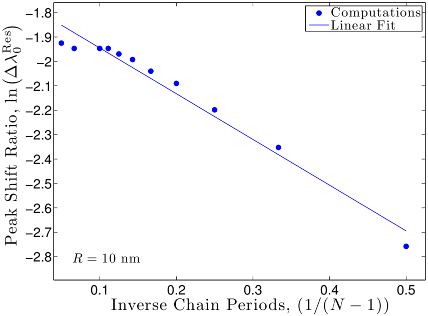

$\Delta\lambda_0^{\mathrm{Res}} = \Delta\lambda_0^{\mathrm{Asymp}} \exp\left(-\eta_N/(N-1)\right), \eta_N = 1.87$; Agreement with the literature; Next nearest neighbor interaction along the chain.

Summary and Outlook

Summary:

- Tool for determining analytically electric field in homogeneous 3D space with spherical scatterers.
- Dipole approximation: Careful if $d \gg R$ is not satisfied!
- Dimer: $(d/R)^{-1/2}$-dependence of peak shift ratio, $\Delta\lambda_0^{\mathrm{Res}}$.
- Chain: $\exp\left(-\eta_N/(N-1)\right)$-dependence of peak shift ratio, $\Delta\lambda_0^{\mathrm{Res}}$.

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Outlook:

- More systematic study of dimers and chain; Cover larger part of parameter space.
- Extension to layered geometry for modeling of plasmonic solar cells; New Green's tensor.
- Modeling of finite-sized 3D photonic crystals (cavity modes, Q-factors, LDOS, Purcell factors).

Thank you for your attention!