Derivation of an effective model for plasmonic coupling

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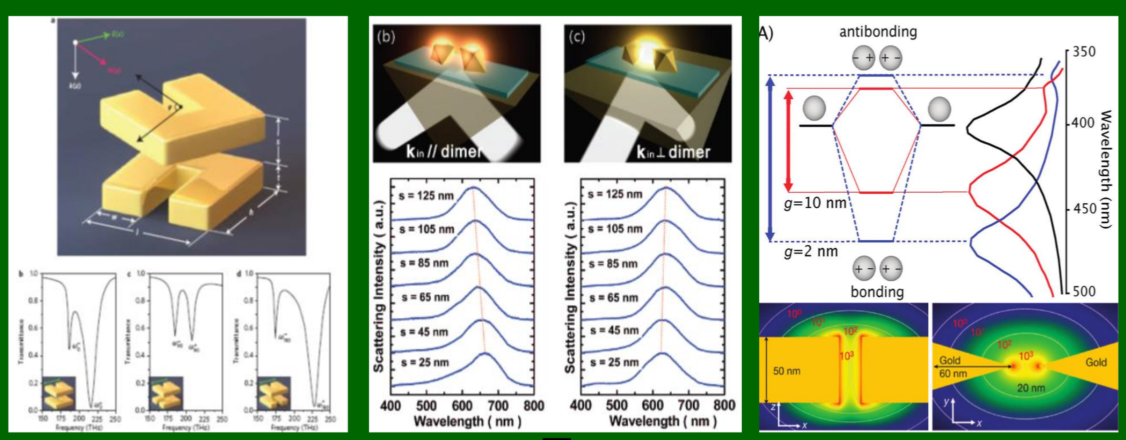
Abstract - Based on a recently developed **tight-binding theory** for dispersive photonic systems, we rigorously derived an **effective model** to describe the plasmonic **couplings between** nanoparticles of **general shape**. The effective model was **justified by full-wave simulations** in different plasmonic coupled systems with distinct geometry. We show that the coupling strength between certain plasmonic nanoparticles **can be tuned** through changing the orientations of nanoparticles, leading to many fascinating physical phenomena such as **ultra-slow-wave plasmon propagation** and Rabi-like oscillations.

Motivations:

Couplings are essential in many fascinating physical phenomena [2-4].



Problems

- Physical understandings are mostly based on full-wave simulations.
- Available theories are empirical (parameters from simulation) restricted to certain geometries

Question

- Find a complete effective model
  - From "ab-initio" theroy
  - Describing both electric and magnetic interactions

I. Theroy

- **Tight-binding method (TBM) [5]**

Hamiltonian operator:

$$\hat{\mathrm{H}}=\begin{pmatrix} 0 & i\mu^{-1}\nabla\times & 0 & 0 \\ i\varepsilon_\infty^{-1}\nabla\times & 0 & 0 & i\varepsilon_\infty^{-1} \\ 0 & 0 & 0 & -i \\ 0 & -i\omega_p^2\varepsilon_\infty & i\omega_e^2 & i\Gamma \end{pmatrix},\ |\varphi\rangle=\begin{pmatrix}\vec{E}\\ \vec{H}\\ \vec{V}\\ \vec{P}\end{pmatrix} \qquad (1)$$

For single particle:

$$\left(\hat{\mathbf{H}}_h+\hat{\mathbf{V}}_1\right)|\Phi(\vec{r})\rangle=2\pi f_0|\Phi(\vec{r})\rangle \qquad (2)$$

Eigen frequencies of coupled system:

$$\det\left[f_0\delta_{ij}+t_{i,j}-f\delta_{ij}\right]=0 \qquad (3)$$

Where

$$t_{i,j}=\langle\varphi_i|\sum_{l\neq j}\mathbf{V}_l|\varphi_j\rangle/\left(2\pi\langle\Phi|\Phi\rangle\right),\ (|\varphi_i\rangle=|\Phi(\vec{r}-\vec{R}_i)\rangle) \qquad (4)$$

Eq.(3) gives the frequency splitting:

$$\Delta f=f_+-f_-=2t_{1,2} \qquad (5)$$

From eq.(4) using multiple expansion:

$$t_{1,2}=\frac{f_r}{2\langle\Phi|\Phi\rangle_{GTBM}}\int_{S1}d\vec{r}\left[\left(\varepsilon_h-\varepsilon_s(\omega_r)\right)\vec{E}_r^*(\vec{r}-\vec{R}_1)\cdot\vec{E}_r(\vec{r}-\vec{R}_2)\right]$$

$$=-\frac{f_0}{2}\int_{S1}d\vec{r}\left[\vec{P}_1^*(\vec{r})\cdot\left(-\nabla\varphi_2(\vec{r})+(i\omega_0)\vec{A}_2(\vec{r})\right)\right]=t_{1,2}^{(E)}+t_{1,2}^{(H)} \qquad (6)$$

$$=t_{pp}-\frac{f_0}{2}\frac{(kd)^2}{8\pi\varepsilon_0}\left(\frac{\vec{p}_1^*\cdot\vec{p}_2+(\vec{p}_1^*\cdot\hat{d})(\vec{p}_2\cdot\hat{d})}{d^3}\right)+i\frac{f_0}{2}\frac{\omega_0}{4\pi\varepsilon_0c^2d^3}\vec{p}_1^*\cdot\left(\vec{m}_2\times\vec{d}\right)+t_{mm}$$

$$t_{1,2}=t_{pp}+t_{pp}^{rad}+t_{pm}+t_{mm} \qquad (7)$$

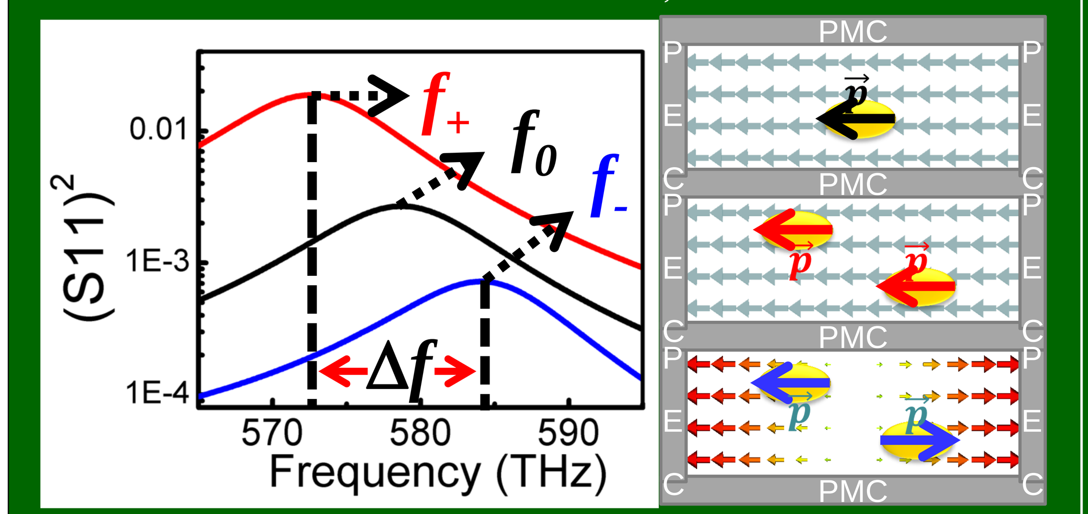
Electric dipolar interaction	Radiation correction	Interaction between P and M	Magnetic dipolar interaction

[1] B. Xi, et al. unpublished
[2] N. Liu, et al., Nature Photonics, 3, 157 (2009)
[3] S.-C. Yang, et al., Nano Lett., 10, 632 (2010)
[4] S. Kim, et al., Nature, 453, 757 (2008)
[5] B. Xi, *et al.*, Phys. Rev. B, 83, 165115 (2011)
[6] R. Marqués, et al., IEEE Trans. Antennas Propag, 51,2572 (2003)

II. Simulation

- **Frequency splitting**

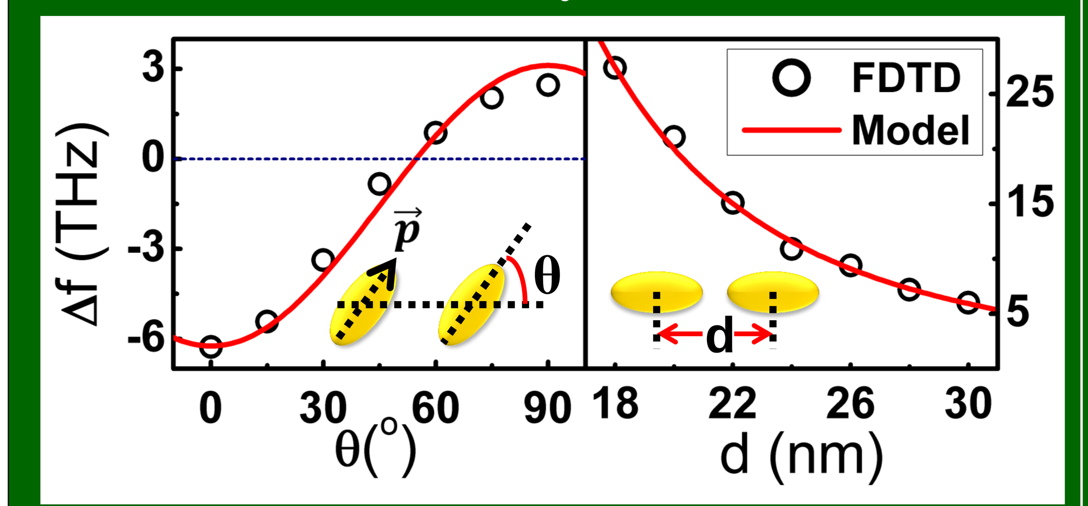
$$\Delta f=f_+-f_-=2t_{1,2}$$



- TEM mode → f_0 f_+
- TE10 mode → f_-
- Get two modes independently

- **Electric dipolar interaction**

$$\Delta f=2t_{pp}\approx\frac{f_0}{4\pi\varepsilon_0}\frac{(1-3\cos^2\theta)|\vec{p}|^2}{d^3}$$

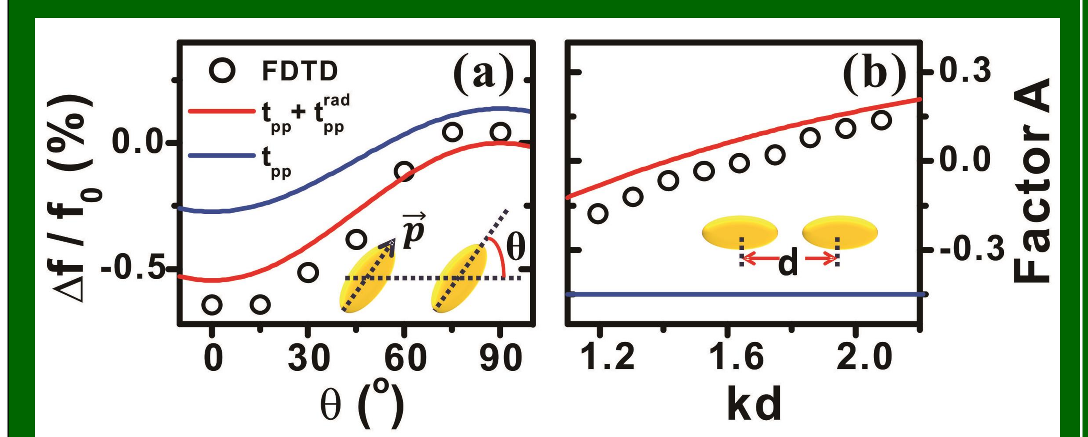


- gold nanorods deep subwavelength (16nm long and 8 nm wide)
- Coupling strength depends on: Orientations distance

- **Electric Radiation Correction**

$$t_{1,2}\approx t_{pp}+t_{pp}^{rad}=\frac{f_0|\vec{p}|^2}{8\pi\varepsilon_0\langle\Phi|\Phi\rangle d^3}\cdot\left[\left(1-\frac{(kd)^2}{2}\right)-\left(3+\frac{(kd)^2}{2}\right)\cos^2\theta\right]$$

$$A=\Delta f\left(\theta=90^\circ\right)/\Delta f\left(\theta=0^\circ\right)$$



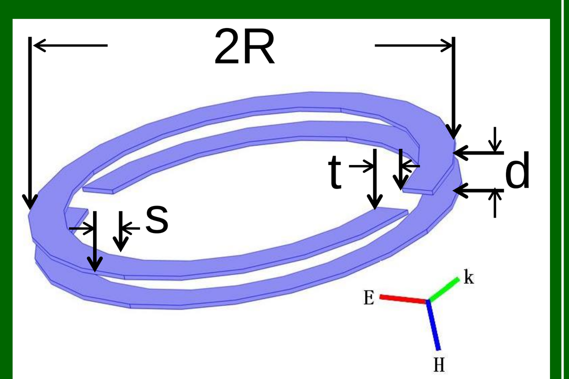
- gold nanorods **NOT** deep subwavelength (80nm long and 40 nm wide)

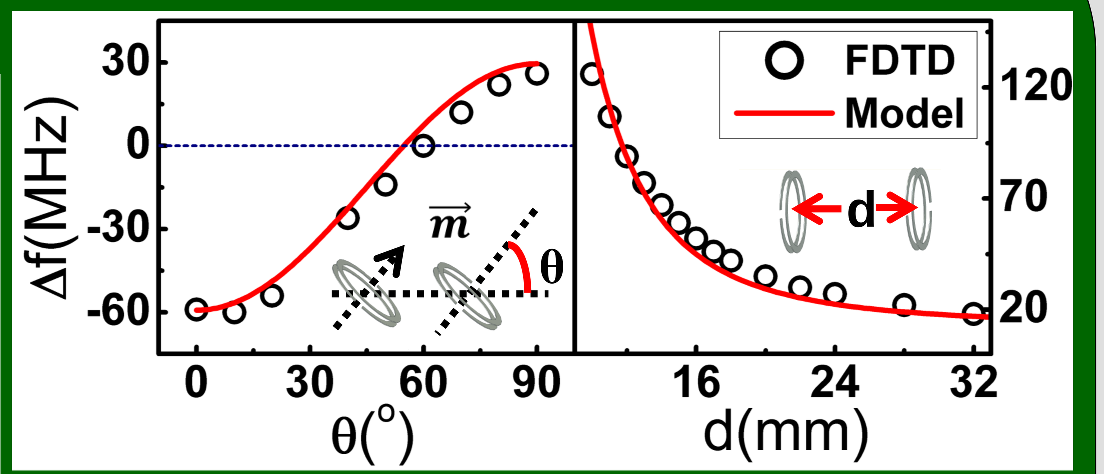
- **Magnetic dipolar interaction**

$$\Delta f=2t_{pp}\approx\frac{f_0\mu_0}{4\pi}\frac{(1-3\cos^2\theta)|\vec{m}|^2}{d^3}$$

- BC-SRR [6]:
  - Pure Magnetic resonance

R=4.8mm t=1.0mm
S=0.8mm d=0.7mm



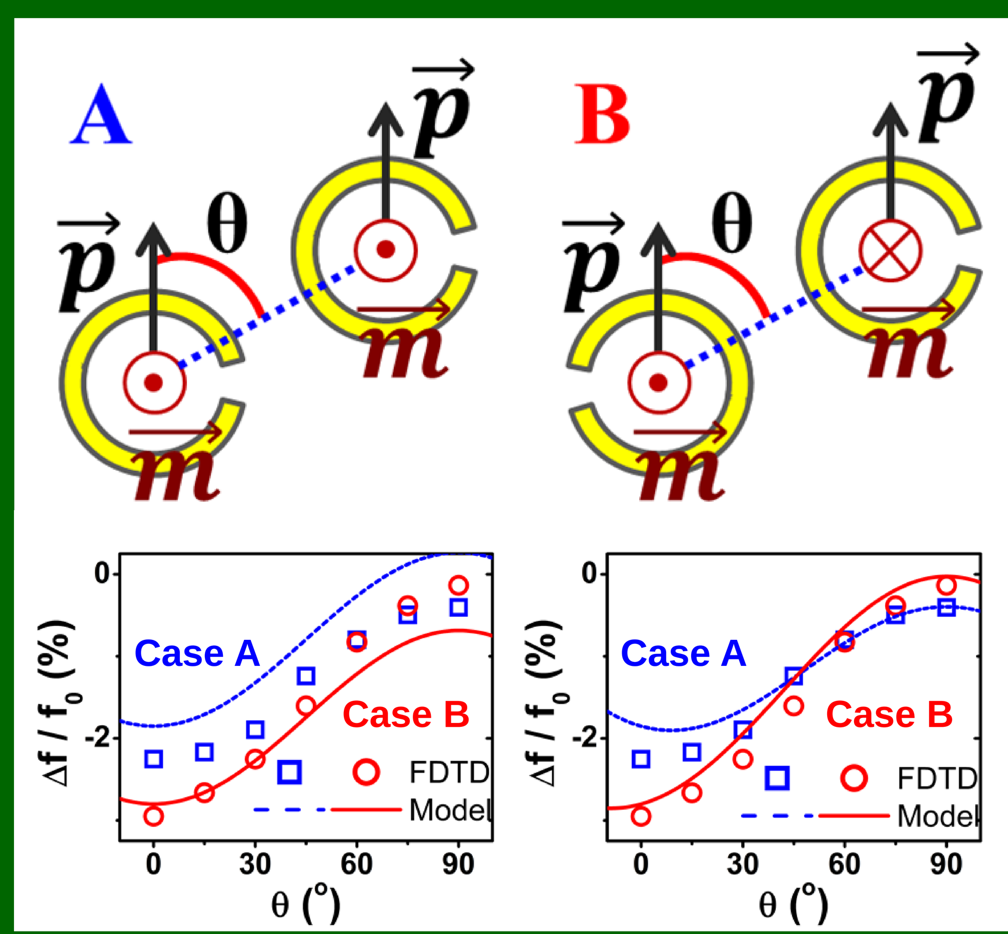


- Coupling strength depends on: Orientations Distance

- **EM Cross-interacting Term**

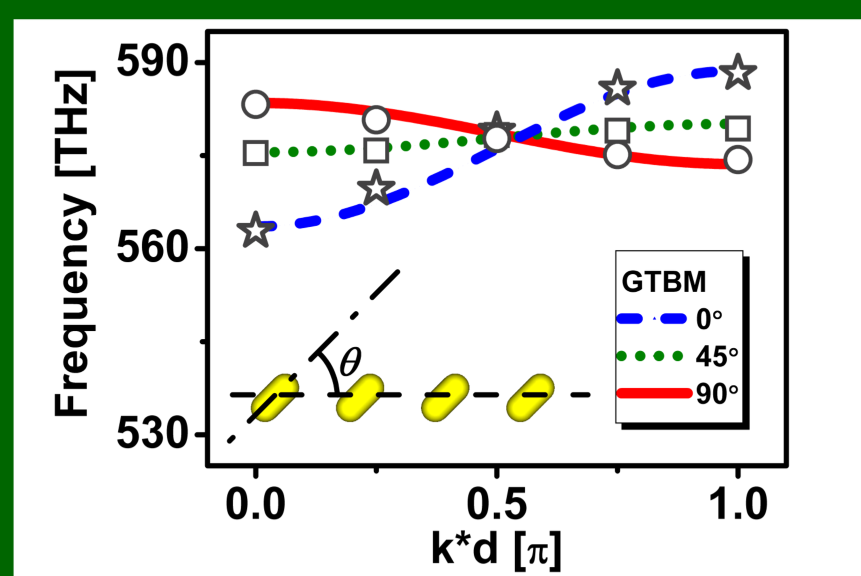
$$t_{1,2}\approx t_{pp}+t_{pp}^{rad}+t_{mm}+t_{pm}$$

$$=\frac{f_0}{8\pi\langle\Phi|\Phi\rangle d^3}\left\{\frac{|\vec{p}|^2}{\varepsilon_0}\cdot\left[\left(1-\frac{(kd)^2}{2}\right)-\left(3+\frac{(kd)^2}{2}\right)\cos^2\theta\right]\pm\mu_0|\vec{m}|^2\mp\frac{\omega_0|\vec{p}||\vec{m}|d}{\varepsilon_0c^2}\sin\theta\right\}$$



III. APPLICATIONS

- Dispersions of plasmonic modes in a gold nanorods chain with different orientation angle θ ($f=f_0-t_{1,2}\cos(ka)$, a is the lattice constant),



- ultra-slow plasmon transport velocity at particular angle near 45º
- Rabi-like oscillations between two nanorods

Conclusions

- An Effective model is derived for coupling in general plasmonic systems
- Derived from first principles (directly based on Maxwell Equations)
- Verified by full wave simulations
- Some fascinating phenomena demonstrated