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Characteristics of Plasmon Resonance Modes in Metallic Nanoparticles

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Abstract: Recently, dynamics of specific plasmon modes in nanoparticles have been studied numerically and experimentally, since they play an important role in developing ultra-high density recording, microfabrication technologies, and so on. We analyze plasmon resonance modes by using a boundary integral equation method and obtain resonance frequencies in metallic nanoparticles. Our method is error controllable and reliable simulation can be performed.

1. Introduction

Plasmon resonances in nanoparticles have been studied numerically and experimentally, since they play an important role in developing ultra-high density recording, microfabrication technologies, and so on[1]. Recently, dynamics of specific plasmon modes has been intensively studied in terms of femtosecond techniques. In this paper, we apply a boundary integral equation method together with the numerical inversion of Laplace transform to analyzing the time domain responses of specific plasmon modes. Our method is error controllable and stable for treating dispersive media.

2. Formulation

A Metallic nanoparticle such as in Figure 1 is assumed. Plasmon resonances are observed at specific frequencies for which the permittivity $\varepsilon(\omega)$ is negative and the free-space wavelength is large in comparison with particle dimensions. Resonant plasmon modes can be computed by solving the eigenvalue problem for the boundary integral equation[2]

$$\sigma_k(Q) = \frac{\lambda_k}{2\pi}\oint_S \sigma_k(M)\frac{\mathbf{r}_{MQ}\cdot\mathbf{n}_Q}{r_{MQ}^3}dS_M, \tag{1}$$

where $\sigma_k(M)$ indicates electric charges over the boundary S of the k-th plasmon mode. The resonance value of λ_k is related by

$$\lambda_k = \frac{\varepsilon_k - \varepsilon_0}{\varepsilon_k + \varepsilon_0}. \tag{2}$$

To express the time variation of the surface charge, the set of eigenfunctions $\sigma_k(M)$ can be used for the expansion of boundary charges $\sigma_k(M,t)$ which is induced on the object boundary during the excitation process[3]:

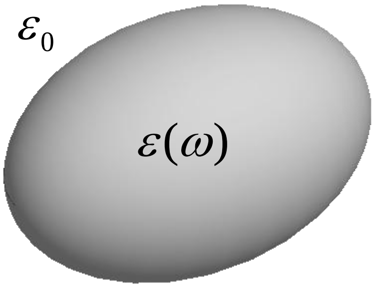

Figure 1. Dielectric Nonoparticle.

$$\sigma_k(M,t) = \sum_{k=1}^{\infty} a_k(t)\sigma_k(M), \tag{3}$$

where $a_k(t)$ is the expansion coefficient.

Considering the Laplace transform of Eq. (3), the image function can be represented in the complex frequency domain such as,

$$\hat{\sigma}_k(M,s) = \sum_{k=1}^{\infty} \hat{a}_k(s)\sigma_k(M). \tag{4}$$

In our method, surface electric charges in the complex frequency domain and they are numerically transformed into the time domain responses[4]. The numerical inversion of the Laplace transform is based on the approximation of the exponential function e^{st} in the Bromwich integral. The inverse of the Laplace transform can be approximated by

$$\begin{aligned}\sigma_k(Q,t) &\cong \frac{1}{2\pi j}\int_{\gamma-j\infty}^{\gamma+j\infty}\hat{\sigma}_k(Q,s)E_{ec}(st,\alpha)ds \\ &= \frac{e^{\alpha}}{t}\sum_{m=1}^{\infty}F_m,\end{aligned} \tag{5}$$

$$F_m = (-1)^m \operatorname{Im}\left[\hat{\sigma}_k\left\{Q, \frac{\alpha + j(m-0.5)\pi}{t}\right\}\right], \tag{6}$$

where α is the approximate parameter that is related to computational accuracy of the numerical inversion of the Laplace transform.

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3. Numerical results

Figure 2 shows the surface distribution of the plasmon mode first for a nanoscale single Au spheroid whose dispersion relation is assumed to be the Drude model[5]. The ratio of semimajor axis and semiminor axis is 3:2. The color bar indicates the normalized surface charge intensity. Charges have localized on the edge of a spheroid. The corresponding resonance wavelength is 278 nm.

Figure 3 shows the surface distribution of a plasmon mode for two Au spheroids. The corresponding resonance wavelength is 299 nm. It appears that charges have localized on the center of two spheroids.

To investigate the computational accuracy of our method, Figure 4 shows the convergence test for varying the truncation number l . We can confirm that the error converges to different values which depend on the approximate parameter α . Selecting proper truncation number, our method is fully error controllable.

4. Conclusions

We have applied the numerical inversion of the Laplace transform to analyzing the time domain responses of specific plasmon modes for metallic nanoparticles. The specific resonance wavelength and surface distribution of plasmon modes with Au nanospheroids have investigated by the proposed method. Our method is fully error controllable and reliable simulation can be performed.

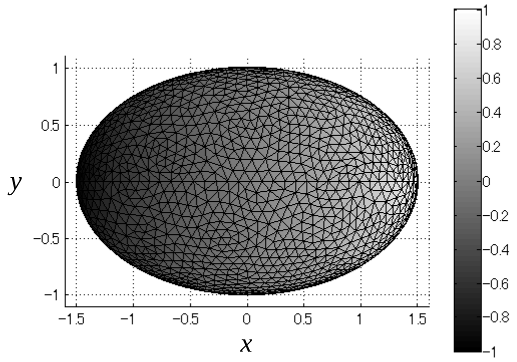

Figure 2. Surface distribution of plasmon mode for a single spheroid.

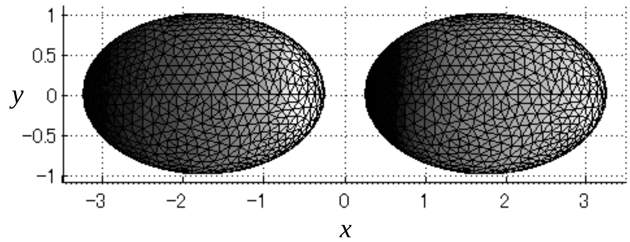

Figure 3. Surface distribution of plasmon mode for two spheroids.

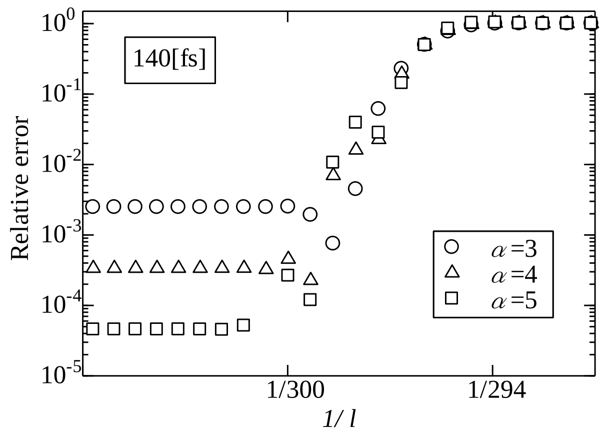

Figure 4. Computational error of the numerical Inversion of Laplace transform.

5. References

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