Nonlinear scattering optimization

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Background

We consider a hybrid dimer, formed by two nanoparticles: plasmonic (**gold nanoparticle**) and all-dielectric (**BaTiO3$_3$ nanoparticle**). The optical parameters are taken according to Ref. [1].

The full problem is shown in Fig. 1 - we have oblique incidence of pumping field with frequency ω, over particles of different size, and arbitrary interparticle distance. The first particle is nonlinear $\hat{\chi}(2)$ tensor with tetragonal lattice oriented arbitrary in space. **The problem:** for fixed angle of incidence we need to find the parameters of the system maximal generation of second harmonic in the fixed direction.

The fixed parameters are:

- the angles of incidence of pumping wave: 1 angle between the k-vector and dimer axis is required.
- the angle of polarization of the pumping wave (1 angle)
- the angle of the emitted wave
- the angle of polarization of the emitted wave (1 angle)

The free parameters are:

- angles of crystalline axis orientation (2 angles)
- radiuses of nanoparticles and distance between them (3 parameters)

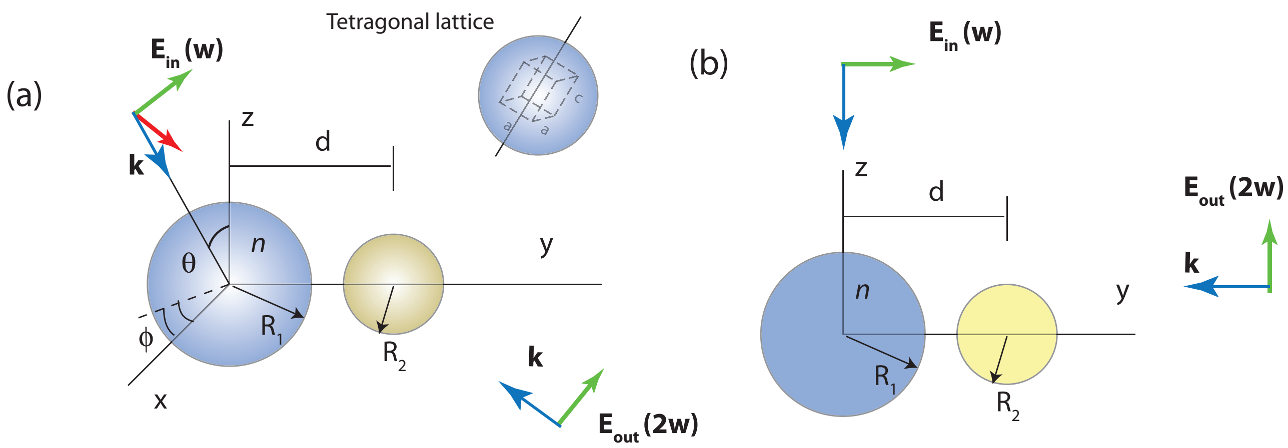

Figure 1: The geometry of the problem: (a) the general approach; (b) an example of simplified geometry.

To find the efficiency of the SHG generation we need to calculate the following function:

$$W = \frac{1}{2} Re \left(\int \mathbf{J}^{(2)}(\mathbf{r}(2\omega)) \cdot \mathbf{E}_{out}(\mathbf{r}) dV \right) = \frac{\omega}{2} Im \left(\int \mathbf{P}^{(2)}(\mathbf{r}, 2\omega) \cdot \mathbf{E}_{out}(\mathbf{r}, 2\omega) dV \right).$$

Here the $\mathbf{E}_{out}(\mathbf{r}, 2\omega)$ is the field distribution generated by plane wave, from the direction of wave emitted at second harmonic. The nonlinear polarization $\mathbf{P}^{(2)}(\mathbf{r}, (2\omega))$ can be expressed via the pumping field at first harmonic

$$P_i^{(2)}(\mathbf{r}, 2\omega) = \hat{\chi}_{ijk}^{(2)} E_j^{in}(\mathbf{r}, \omega) E_k^{in}(\mathbf{r}, \omega)$$

Alternatively it can be expressed as follows:

$$\begin{bmatrix} P_x(2\omega) \\ P_y(2\omega) \\ P_z(2\omega) \end{bmatrix} = 4 \begin{bmatrix} 0 & 0 & 0 & 0 & d_{15} & 0 \\ 0 & 0 & 0 & d_{15} & 0 & 0 \\ d_{31} & d_{31} & d_{33} & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} E_x^2(\omega) \\ E_y^2(\omega) \\ E_z^2(\omega) \\ 2E_y(\omega)E_z(\omega) \\ 2E_x(\omega)E_z(\omega) \\ 2E_x(\omega)E_y(\omega) \end{bmatrix}. \tag{1}$$

According to [2] the $\hat{d}$ tensor components equal to

$$\begin{aligned} d_{15} &= -41 \cdot 10^{-9} \text{ cm/statvolt}, \\ d_{31} &= -43 \cdot 10^{-9} \text{ cm/statvolt}, \\ d_{33} &= -16 \cdot 10^{-9} \text{ cm/statvolt}. \end{aligned}$$

That gives the following expression for the polarization vector

$$\begin{aligned} P_x(2\omega) &= 8d_{15}E_x(\omega)E_z(\omega), \\ P_y(2\omega) &= 8d_{15}E_y(\omega)E_z(\omega), \\ P_z(2\omega) &= 4\left(d_{31}E_x^2(\omega) + d_{31}E_y^2(\omega) + d_{33}E_z^2(\omega)\right). \end{aligned} \tag{2}$$

This gives us the $\chi^{(2)}$ tensor components:

$$\chi_{xxz}^{(2)} = \chi_{xzx}^{(2)} = 4d_{15} \quad \chi_{yyz}^{(2)} = \chi_{yzy}^{(2)} = 4d_{15}$$

$$\chi_{zxx}^{(2)} = \chi_{zyy}^{(2)} = 4d_{31} \quad \chi_{zzz}^{(2)} = 4d_{33}$$

The basic steps

The basic steps for approaching the result could the following:

1. Try to optimize *elastic scattering* of a single dielectric particle by tuning its size. This will allow check the feasibility of the approach and tot test the bass algorithms.

2. Try to optimize *elastic scattering* of a dimer dielectric and hybrid particles by tuning their sizes.

3. Try to optimize nonlinear scattering of a single dielectric particle by its size and the orientation of the crystalline axis.

4. Finally, optimize a hybrid nonlinear dimer by tuning all possible free parameters.

References

[1] http://refractiveindex.info/?shelf=main&book=BaTiO3&page=Wemple-e

[2] R. W. Boyd, Nonlinear optics. San Diego: Academic Press, 2003.