Supporting Information for

Analytical model for light scattering of plasmonic gold nanorods with size up to 200 nm

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In the supporting information section 1 - 4 we provide a full explicit calculation of electric field around an ellipsoid, and in section 5 for prolate spheroid, shown as Eqs. 4-5 in the main text. In section 6, we compare the result with previous results by Gersten and Nitzan[1].

1. Ellipsoidal coordinate system

From Stratton[2], the equation of an ellipsoid is

$$\frac{x^2}{a^2}+\frac{y^2}{b^2}+\frac{z^2}{c^2}=1, \qquad a>b>c, \tag{S1}$$

whose semiprincipal axes are of length a, b and c. Therefore, the equations

$$\frac{x^2}{a^2+\xi}+\frac{y^2}{b^2+\xi}+\frac{z^2}{c^2+\xi}=1, \quad \xi \geq -c^2, \tag{S2}$$

$$\frac{x^2}{a^2+\eta}+\frac{y^2}{b^2+\eta}+\frac{z^2}{c^2+\eta}=1, \quad -c^2 \geq \eta \geq -b^2, \tag{S3}$$

$$\frac{x^2}{a^2+\zeta}+\frac{y^2}{b^2+\zeta}+\frac{z^2}{c^2+\zeta}=1, \quad -b^2 \geq \zeta \geq -a^2, \tag{S4}$$

are respectively of an ellipsoid, a hyperboloid of one sheet, and a hyperboloid of two sheets, all confocal with the ellipsoid. Through each point of space there will pass just one surface of each kind, and to each point there will correspond a unique set of values for ξ, η, ζ. The variables (ξ, η, ζ) are the ellipsoidal coordinates. The surface, ξ = constant, is an ellipsoid, η = constant, is a hyperboloid of one sheet, ζ = constant, a hyperboloid of two sheets. From Eqs. (S2) and (S3), we can see that $\xi \geq -c^2 \geq \eta \geq -b^2 \geq \zeta \geq -a^2$; also $\xi > 0$ represents the external domain, $\xi < 0$ is for the internal domain and $\xi = 0$ represents the ellipsoid surface.

The transformation to rectangular coordinates is obtained by solving Eqs. (S2) to (S4) simultaneously for x, y, z, which gives

$$x^2=\frac{(\xi+a^2)(\eta+a^2)(\zeta+a^2)}{(b^2-a^2)(c^2-a^2)}, \quad x=\pm\sqrt{\frac{(\xi+a^2)(\eta+a^2)(\zeta+a^2)}{(b^2-a^2)(c^2-a^2)}}; \tag{S5}$$

$$y^2=\frac{(\xi+b^2)(\eta+b^2)(\zeta+b^2)}{(c^2-b^2)(a^2-b^2)}, \quad y=\pm\sqrt{\frac{(\xi+b^2)(\eta+b^2)(\zeta+b^2)}{(c^2-b^2)(a^2-b^2)}}; \tag{S6}$$

$$z^2 = \frac{(\xi + c^2)(\eta + c^2)(\zeta + c^2)}{(a^2 - c^2)(b^2 - c^2)}, \; z = \pm\sqrt{\frac{(\xi + c^2)(\eta + c^2)(\zeta + c^2)}{(a^2 - c^2)(b^2 - c^2)}}. \tag{S7}$$

The Làme coefficients are

$$\hbar_1 = \pm\frac{1}{2}\left[\frac{(\xi - \eta)(\xi - \zeta)}{(\xi + a^2)(\xi + b^2)(\xi + c^2)}\right]^{\frac{1}{2}}, \tag{S8}$$

$$\hbar_2 = \pm\frac{1}{2}\left[\frac{(\eta - \xi)(\eta - \zeta)}{(\eta + a^2)(\eta + b^2)(\eta + c^2)}\right]^{\frac{1}{2}}, \tag{S9}$$

$$\hbar_3 = \pm\frac{1}{2}\left[\frac{(\zeta - \xi)(\zeta - \eta)}{(\zeta + a^2)(\zeta + b^2)(\zeta + c^2)}\right]^{\frac{1}{2}}. \tag{S10}$$

2. Potentials

Let an ellipsoid described in Eq. (1) with dielectric constant ε_i be embedded in a constant electrostatic field $\boldsymbol{E}^{inc} = E_{0x}\mathbf{i} + E_{0y}\mathbf{j} + E_{0z}\mathbf{k}$ polarised any direction in the Cartesian coordinate system as shown in Fig. 1a where **(i, j, k)** are the unit vectors of the Cartesian coordinate system. It can be seen that in the ellipsoidal coordinate system described in Eqs. (S2) to (S4), $\xi = 0$ is the surface of the ellipsoid.

2.1 Potentials in the ellipsoidal coordinate system

The potential of the constant electrostatic field $\boldsymbol{E}^{inc}$ in the ellipsoidal coordinate system is

$$\phi_0 = \phi_{0x} + \phi_{0y} + \phi_{0z}, \tag{S11}$$

where

$$\phi_{0x} \equiv -E_{0x}x = \mp E_{0x}\left[\frac{(\xi + a^2)(\eta + a^2)(\zeta + a^2)}{(b^2 - a^2)(c^2 - a^2)}\right]^{\frac{1}{2}}, \tag{S12}$$

$$\phi_{0y} \equiv -E_{0y}y = \mp E_{0y}\left[\frac{(\xi + b^2)(\eta + b^2)(\zeta + b^2)}{(c^2 - b^2)(a^2 - b^2)}\right]^{\frac{1}{2}}, \tag{S13}$$

$$\phi_{0z} \equiv -E_{0z}z = \mp E_{0z}\left[\frac{(\xi+c^2)(\eta+c^2)(\zeta+c^2)}{(a^2-c^2)(b^2-c^2)}\right]^{\frac{1}{2}}. \tag{S14}$$

The potential inside the ellipsoid and the potential in the external medium are, respectively,

$$\phi_i = \phi_{0x}\left[\frac{\varepsilon_e}{\varepsilon_e+(\varepsilon_i-\varepsilon_e)L_1(0)}\right] + \phi_{0y}\left[\frac{\varepsilon_e}{\varepsilon_e+(\varepsilon_i-\varepsilon_e)L_2(0)}\right] + \phi_{0z}\left[\frac{\varepsilon_e}{\varepsilon_e+(\varepsilon_i-\varepsilon_e)L_3(0)}\right], \tag{S15}$$

and

$$\phi_e = \phi_{0x}\left[1+\frac{\frac{\varepsilon_e-\varepsilon_i}{\varepsilon_e}L_1(\xi)}{1+\frac{\varepsilon_i-\varepsilon_e}{\varepsilon_e}L_1(0)}\right] + \phi_{0y}\left[1+\frac{\frac{\varepsilon_e-\varepsilon_i}{\varepsilon_e}L_2(\xi)}{1+\frac{\varepsilon_i-\varepsilon_e}{\varepsilon_e}L_2(0)}\right] + \phi_{0z}\left[1+\frac{\frac{\varepsilon_e-\varepsilon_i}{\varepsilon_e}L_3(\xi)}{1+\frac{\varepsilon_i-\varepsilon_e}{\varepsilon_e}L_3(0)}\right] \tag{S16}$$

in which ε_e is the dielectric permittivity of the external medium.

Introducing a function

$$f(q) = \left[(q+a^2)(q+b^2)(q+c^2)\right]^{\frac{1}{2}}, \tag{S17}$$

we can define

$$L_1(\xi) = \frac{abc}{2}\int_\xi^\infty \frac{dq}{(a^2+q)f(q)}, \tag{S18}$$

$$L_2(\xi) = \frac{abc}{2}\int_\xi^\infty \frac{dq}{(b^2+q)f(q)}, \tag{S19}$$

$$L_3(\xi) = \frac{abc}{2}\int_\xi^\infty \frac{dq}{(c^2+q)f(q)} \tag{S20}$$

together with

$$L_1 \equiv L_1(0) = \frac{abc}{2}\int_0^\infty \frac{dq}{(a^2+q)f(q)}, \tag{S21}$$

$$L_2 \equiv L_2(0) = \frac{abc}{2}\int_0^{\infty} \frac{dq}{(b^2+q)f(q)}, \tag{S22}$$

$$L_3 \equiv L_3(0) = \frac{abc}{2}\int_0^{\infty} \frac{dq}{(c^2+q)f(q)}. \tag{S23}$$

2.2. Partial derivatives

In this subsection, we list some partial derivatives that are needed to obtain the ***E*** fields, which include

$$\frac{\partial(\phi_{0x},\phi_{0x},\phi_{0x})}{\partial\xi},\ \frac{\partial(\phi_{0x},\phi_{0x},\phi_{0x})}{\partial\eta},\ \frac{\partial(\phi_{0x},\phi_{0x},\phi_{0x})}{\partial\zeta},\ \text{and}\ \frac{d[L_1(\xi),L_2(\xi),L_3(\xi)]}{d\xi}. \tag{S24}$$

From Eqs. (S12) to (S14) and (S18) to (S20), we have

$$\frac{\partial\phi_{0x}}{\partial\xi} = \mp E_{0x}\left\{\frac{1}{2}\left[\frac{(a^2+\xi)(a^2+\eta)(a^2+\zeta)}{(b^2-a^2)(c^2-a^2)}\right]^{-\frac{1}{2}} \frac{(a^2+\eta)(a^2+\zeta)}{(b^2-a^2)(c^2-a^2)}\right\}, \tag{S25}$$

$$\frac{\partial\phi_{0x}}{\partial\eta} = \mp E_{0x}\left\{\frac{1}{2}\left[\frac{(a^2+\xi)(a^2+\eta)(a^2+\zeta)}{(b^2-a^2)(c^2-a^2)}\right]^{-\frac{1}{2}} \frac{(a^2+\xi)(a^2+\zeta)}{(b^2-a^2)(c^2-a^2)}\right\}, \tag{S26}$$

$$\frac{\partial\phi_{0x}}{\partial\zeta} = \mp E_{0x}\left\{\frac{1}{2}\left[\frac{(a^2+\xi)(a^2+\eta)(a^2+\zeta)}{(b^2-a^2)(c^2-a^2)}\right]^{-\frac{1}{2}} \frac{(a^2+\xi)(a^2+\eta)}{(b^2-a^2)(c^2-a^2)}\right\}, \tag{S27}$$

$$\begin{aligned}\frac{d[L_1(\xi)]}{d\xi} &\equiv \frac{d}{d\xi}\left[\frac{abc}{2}\int_0^{\infty}\frac{dq}{(a^2+q)f(q)}\right] = 0 - \frac{abc}{2(a^2+\xi)f(\xi)} \\ &= -\frac{abc}{2(a^2+\xi)[(a^2+\xi)(b^2+\xi)(c^2+\xi)]^{\frac{1}{2}}}\end{aligned}; \tag{S28}$$

$$\frac{\partial\phi_{0y}}{\partial\xi} = \mp E_{0y}\left\{\frac{1}{2}\left[\frac{(b^2+\xi)(b^2+\eta)(b^2+\zeta)}{(c^2-b^2)(a^2-b^2)}\right]^{-\frac{1}{2}} \frac{(b^2+\eta)(b^2+\zeta)}{(c^2-b^2)(a^2-b^2)}\right\}, \tag{S29}$$

$$\frac{\partial\phi_{0y}}{\partial\eta}=\mp E_{0y}\left\{\frac{1}{2}\left[\frac{(b^2+\xi)(b^2+\eta)(b^2+\zeta)}{(c^2-b^2)(a^2-b^2)}\right]^{-\frac{1}{2}}\frac{(b^2+\xi)(b^2+\zeta)}{(c^2-b^2)(a^2-b^2)}\right\}, \tag{S30}$$

$$\frac{\partial\phi_{0y}}{\partial\zeta}=\mp E_{0y}\left\{\frac{1}{2}\left[\frac{(b^2+\xi)(b^2+\eta)(b^2+\zeta)}{(c^2-b^2)(a^2-b^2)}\right]^{-\frac{1}{2}}\frac{(b^2+\xi)(b^2+\eta)}{(c^2-b^2)(a^2-b^2)}\right\}, \tag{S31}$$

$$\begin{aligned}\frac{d[L_2(\xi)]}{d\xi}&\equiv\frac{d}{d\xi}\left[\frac{abc}{2}\int_0^\infty\frac{dq}{(b^2+q)f(q)}\right]=0-\frac{abc}{2(b^2+\xi)f(\xi)}\\&=-\frac{abc}{2(b^2+\xi)[(a^2+\xi)(b^2+\xi)(c^2+\xi)]^{\frac{1}{2}}}\end{aligned}; \tag{S32}$$

$$\frac{\partial\phi_{0z}}{\partial\xi}=\mp E_{0z}\left\{\frac{1}{2}\left[\frac{(c^2+\xi)(c^2+\eta)(c^2+\zeta)}{(a^2-c^2)(b^2-c^2)}\right]^{-\frac{1}{2}}\frac{(c^2+\eta)(c^2+\zeta)}{(a^2-c^2)(b^2-c^2)}\right\}, \tag{S33}$$

$$\frac{\partial\phi_{0z}}{\partial\eta}=\mp E_{0z}\left\{\frac{1}{2}\left[\frac{(c^2+\xi)(c^2+\eta)(c^2+\zeta)}{(a^2-c^2)(b^2-c^2)}\right]^{-\frac{1}{2}}\frac{(c^2+\xi)(c^2+\zeta)}{(a^2-c^2)(b^2-c^2)}\right\}, \tag{S34}$$

$$\frac{\partial\phi_{0z}}{\partial\zeta}=\mp E_{0z}\left\{\frac{1}{2}\left[\frac{(c^2+\xi)(c^2+\eta)(c^2+\zeta)}{(a^2-c^2)(b^2-c^2)}\right]^{-\frac{1}{2}}\frac{(c^2+\xi)(c^2+\eta)}{(a^2-c^2)(b^2-c^2)}\right\}, \tag{S35}$$

$$\begin{aligned}\frac{d[L_3(\xi)]}{d\xi}&\equiv\frac{d}{d\xi}\left[\frac{abc}{2}\int_0^\infty\frac{dq}{(c^2+q)f(q)}\right]=0-\frac{abc}{2(c^2+\xi)f(\xi)}\\&=-\frac{abc}{2(c^2+\xi)[(a^2+\xi)(b^2+\xi)(c^2+\xi)]^{\frac{1}{2}}}\end{aligned}. \tag{S36}$$

3. Internal E field in the ellipsoidal coordinate system

The internal E field, when $0\geq\xi\geq-c^2$, is

$$\mathbf{E}_i \equiv (E_{i\xi}\mathbf{e}_\xi, E_{i\eta}\mathbf{e}_\eta, E_{i\zeta}\mathbf{e}_\zeta) = -\nabla_{(\xi,\eta,\zeta)}\phi_i = -\frac{1}{h_1}\frac{\partial\phi_i}{\partial\xi}\mathbf{e}_\xi - \frac{1}{h_2}\frac{\partial\phi_i}{\partial\eta}\mathbf{e}_\eta - \frac{1}{h_3}\frac{\partial\phi_i}{\partial\zeta}\mathbf{e}_\zeta. \quad \text{(S37)}$$

Using Eqs. (S8) to (S10) and (S25) to (S36),

$$\begin{aligned} E_{i\xi}(\xi,\eta,\zeta) = &\frac{E_{0x}\varepsilon_e}{\varepsilon_e + (\varepsilon_i - \varepsilon_e)L_1}\left[\frac{(a^2+\eta)(a^2+\zeta)(b^2+\xi)(c^2+\xi)}{(\xi-\eta)(\xi-\zeta)(b^2-a^2)(c^2-a^2)}\right]^{\frac{1}{2}} \\ &+ \frac{E_{0y}\varepsilon_e}{\varepsilon_e + (\varepsilon_i - \varepsilon_e)L_2}\left[\frac{(b^2+\eta)(b^2+\zeta)(c^2+\xi)(a^2+\xi)}{(\xi-\eta)(\xi-\zeta)(c^2-b^2)(a^2-b^2)}\right]^{\frac{1}{2}} \\ &+ \frac{E_{0z}\varepsilon_e}{\varepsilon_e + (\varepsilon_i - \varepsilon_e)L_3}\left[\frac{(c^2+\eta)(c^2+\zeta)(a^2+\xi)(b^2+\xi)}{(\xi-\eta)(\xi-\zeta)(a^2-c^2)(b^2-c^2)}\right]^{\frac{1}{2}}, \end{aligned} \quad \text{(S38)}$$

$$\begin{aligned} E_{i\eta}(\xi,\eta,\zeta) = &\frac{E_{0x}\varepsilon_e}{\varepsilon_e + (\varepsilon_i - \varepsilon_e)L_1}\left[\frac{(a^2+\xi)(a^2+\zeta)(b^2+\eta)(c^2+\eta)}{(\eta-\zeta)(\eta-\xi)(b^2-a^2)(c^2-a^2)}\right]^{\frac{1}{2}} \\ &+ \frac{E_{0y}\varepsilon_e}{\varepsilon_e + (\varepsilon_i - \varepsilon_e)L_2}\left[\frac{(b^2+\xi)(b^2+\zeta)(c^2+\eta)(a^2+\eta)}{(\eta-\zeta)(\eta-\xi)(c^2-b^2)(a^2-b^2)}\right]^{\frac{1}{2}} \\ &+ \frac{E_{0z}\varepsilon_e}{\varepsilon_e + (\varepsilon_i - \varepsilon_e)L_3}\left[\frac{(c^2+\xi)(c^2+\zeta)(a^2+\eta)(b^2+\eta)}{(\eta-\zeta)(\eta-\xi)(a^2-c^2)(b^2-c^2)}\right]^{\frac{1}{2}}, \end{aligned} \quad \text{(S39)}$$

$$\begin{aligned} E_{i\zeta}(\xi,\eta,\zeta) = &\frac{E_{0x}\varepsilon_e}{\varepsilon_e + (\varepsilon_i - \varepsilon_e)L_1}\left[\frac{(a^2+\xi)(a^2+\eta)(b^2+\zeta)(c^2+\zeta)}{(\zeta-\xi)(\zeta-\eta)(b^2-a^2)(c^2-a^2)}\right]^{\frac{1}{2}} \\ &+ \frac{E_{0y}\varepsilon_e}{\varepsilon_e + (\varepsilon_i - \varepsilon_e)L_2}\left[\frac{(b^2+\xi)(b^2+\eta)(c^2+\zeta)(a^2+\zeta)}{(\zeta-\xi)(\zeta-\eta)(c^2-b^2)(a^2-b^2)}\right]^{\frac{1}{2}} \\ &+ \frac{E_{0z}\varepsilon_e}{\varepsilon_e + (\varepsilon_i - \varepsilon_e)L_3}\left[\frac{(c^2+\xi)(c^2+\eta)(a^2+\zeta)(b^2+\zeta)}{(\zeta-\xi)(\zeta-\eta)(a^2-c^2)(b^2-c^2)}\right]^{\frac{1}{2}}. \end{aligned} \quad \text{(S40)}$$

4. External E field in the ellipsoidal coordinate system

Similarly, the external electric field E as $\xi \geq 0$, is

$$\mathbf{E}_e \equiv (E_{e\xi}\mathbf{e}_\xi, E_{e\eta}\mathbf{e}_\eta, E_{e\zeta}\mathbf{e}_\zeta) = -\nabla_{(\xi,\eta,\zeta)}\phi_e = -\frac{1}{h_1}\frac{\partial\phi_e}{\partial\xi}\mathbf{e}_\xi - \frac{1}{h_2}\frac{\partial\phi_e}{\partial\eta}\mathbf{e}_\eta - \frac{1}{h_3}\frac{\partial\phi_e}{\partial\zeta}\mathbf{e}_\zeta. \tag{S41}$$

Correspondingly,

$$\begin{aligned}
E_{e\xi}(\xi,\eta,\zeta) = {} & E_{0x}\left\{\begin{aligned}&\left[1+\frac{(\varepsilon_e-\varepsilon_i)L_1(\xi)}{\varepsilon_e+(\varepsilon_i-\varepsilon_e)L_1}\right]\left[\frac{(a^2+\eta)(a^2+\zeta)(b^2+\xi)(c^2+\xi)}{(\xi-\eta)(\xi-\zeta)(b^2-a^2)(c^2-a^2)}\right]^{\frac{1}{2}}\\ &-abc\left[\frac{(\varepsilon_e-\varepsilon_i)}{\varepsilon_e+(\varepsilon_i-\varepsilon_e)L_1}\right]\left[\frac{(a^2+\eta)(a^2+\zeta)}{(a^2+\xi)(\xi-\eta)(\xi-\zeta)(b^2-a^2)(c^2-a^2)}\right]^{\frac{1}{2}}\end{aligned}\right\}\\
&+E_{0y}\left\{\begin{aligned}&\left[1+\frac{(\varepsilon_e-\varepsilon_i)L_2(\xi)}{\varepsilon_e+(\varepsilon_i-\varepsilon_e)L_2}\right]\left[\frac{(b^2+\eta)(b^2+\zeta)(c^2+\xi)(a^2+\xi)}{(\xi-\eta)(\xi-\zeta)(c^2-b^2)(a^2-b^2)}\right]^{\frac{1}{2}}\\ &-abc\left[\frac{(\varepsilon_e-\varepsilon_i)}{\varepsilon_e+(\varepsilon_i-\varepsilon_e)L_2}\right]\left[\frac{(b^2+\eta)(b^2+\zeta)}{(b^2+\xi)(\xi-\eta)(\xi-\zeta)(c^2-b^2)(a^2-b^2)}\right]^{\frac{1}{2}}\end{aligned}\right\}^{\frac{1}{2}}\\
&+E_{0z}\left\{\begin{aligned}&\left[1+\frac{(\varepsilon_e-\varepsilon_i)L_3(\xi)}{\varepsilon_e+(\varepsilon_i-\varepsilon_e)L_3}\right]\left[\frac{(c^2+\eta)(c^2+\zeta)(a^2+\xi)(b^2+\xi)}{(\xi-\eta)(\xi-\zeta)(a^2-c^2)(b^2-c^2)}\right]^{\frac{1}{2}}\\ &-abc\left[\frac{(\varepsilon_e-\varepsilon_i)}{\varepsilon_e+(\varepsilon_i-\varepsilon_e)L_3}\right]\left[\frac{(b^2+\eta)(b^2+\zeta)}{(c^2+\xi)(\xi-\eta)(\xi-\zeta)(a^2-c^2)(b^2-c^2)}\right]^{\frac{1}{2}}\end{aligned}\right\}^{\frac{1}{2}},
\end{aligned} \tag{S42}$$

$$\begin{aligned}
E_{e\eta}(\xi,\eta,\zeta) = {} & E_{0x}\left[1+\frac{(\varepsilon_e-\varepsilon_i)L_1(\xi)}{\varepsilon_e+(\varepsilon_i-\varepsilon_e)L_1}\right]\left[\frac{(a^2+\xi)(a^2+\zeta)(b^2+\eta)(c^2+\eta)}{(\eta-\zeta)(\eta-\xi)(b^2-a^2)(c^2-a^2)}\right]^{\frac{1}{2}}\\
&+E_{0y}\left[1+\frac{(\varepsilon_e-\varepsilon_i)L_2(\xi)}{\varepsilon_e+(\varepsilon_i-\varepsilon_e)L_2}\right]\left[\frac{(b^2+\xi)(b^2+\zeta)(c^2+\eta)(a^2+\eta)}{(\eta-\zeta)(\eta-\xi)(c^2-b^2)(a^2-b^2)}\right]^{\frac{1}{2}}\\
&+E_{0z}\left[1+\frac{(\varepsilon_e-\varepsilon_i)L_3(\xi)}{\varepsilon_e+(\varepsilon_i-\varepsilon_e)L_3}\right]\left[\frac{(c^2+\xi)(c^2+\zeta)(a^2+\eta)(b^2+\eta)}{(\eta-\zeta)(\eta-\xi)(a^2-c^2)(b^2-c^2)}\right]^{\frac{1}{2}},
\end{aligned} \tag{S43}$$

$$
E_{e\zeta}(\xi,\eta,\zeta) = E_{0x}\left[1+\frac{(\varepsilon_e-\varepsilon_i)L_1(\xi)}{\varepsilon_e+(\varepsilon_i-\varepsilon_e)L_1}\right]\left[\frac{(a^2+\xi)(a^2+\eta)(b^2+\zeta)(c^2+\zeta)}{(\zeta-\xi)(\zeta-\eta)(b^2-a^2)(c^2-a^2)}\right]^{\frac{1}{2}}
$$

$$
+E_{0y}\left[1+\frac{(\varepsilon_e-\varepsilon_i)L_2(\xi)}{\varepsilon_e+(\varepsilon_i-\varepsilon_e)L_2}\right]\left[\frac{(b^2+\xi)(b^2+\eta)(c^2+\zeta)(a^2+\zeta)}{(\zeta-\xi)(\zeta-\eta)(c^2-b^2)(a^2-b^2)}\right]^{\frac{1}{2}} \quad . \tag{S44}
$$

$$
+E_{0z}\left[1+\frac{(\varepsilon_e-\varepsilon_i)L_3(\xi)}{\varepsilon_e+(\varepsilon_i-\varepsilon_e)L_3}\right]\left[\frac{(c^2+\xi)(c^2+\eta)(a^2+\zeta)(b^2+\zeta)}{(\zeta-\xi)(\zeta-\eta)(a^2-c^2)(b^2-c^2)}\right]^{\frac{1}{2}}
$$

5. Prolate Spheroid

Before we go to the details of prolate spheroids, let us introduce a system with polar angle θ and azimuthal angle ϕ to Eqs. (S5) and (S7),

$$
x^2 = \frac{(\xi+a^2)(\eta+a^2)(\zeta+a^2)}{(b^2-a^2)(c^2-a^2)} = (\xi+a^2)\cos^2\theta, \tag{S45}
$$

$$
y^2 = \frac{(\xi+b^2)(\eta+b^2)(\zeta+b^2)}{(c^2-b^2)(a^2-b^2)} = (\xi+b^2)\sin^2\theta\cos^2\phi, \tag{S46}
$$

$$
z^2 = \frac{(\xi+c^2)(\eta+c^2)(\zeta+c^2)}{(a^2-c^2)(b^2-c^2)} = (\xi+c^2)\sin^2\theta\sin^2\phi. \tag{S47}
$$

By using this coordinate system, the surface area of an ellipsoid when $\xi = 0$ can be obtained by integrating the following unit in the range of $0 \le \theta \le \pi$, and $0 \le \phi \le 2\pi$:

$$
dS = \sin\theta\sqrt{c^2a^2\sin^2\theta\cos^2\phi + b^2a^2\sin^2\theta\sin^2\phi + b^2c^2\cos^2\theta}\,d\theta d\phi \ . \tag{S48}
$$

We then introduce one symmetry of ellipsoid and make it to be a prolate spheroid (Fig. 1 in the main text). We have $b \rightarrow c$, and $\eta \rightarrow -b^2$. From Eqs. (S45) to (S47), we have

$$
(\zeta+a^2) = h^2\cos^2\theta, \tag{S49}
$$

$$
-(\zeta+b^2) = h^2\sin^2\theta\cos^2\phi, \tag{S50}
$$

$$
-(\zeta+c^2) = h^2\sin^2\theta\sin^2\phi. \tag{S51}
$$

where $h^2 = a^2 - b^2 = a^2 - c^2$.

Also, $L_1(\xi)$, $L_2(\xi)$, $L_3(\xi)$, and $L_1(0)$, $L_2(0)$, $L_3(0)$ become

$$L_1(\xi) = ac^2\left(-\frac{1}{2h^2\sqrt{a^2+\xi}} - \frac{1}{2h^3}\ln\left|\frac{\sqrt{a^2+\xi}+h}{\sqrt{a^2+\xi}-h}\right|\right), \tag{S52}$$

$$L_2(\xi) = L_3(\xi) = ac^2\left(\frac{\sqrt{a^2+\xi}}{2h^2(c^2+\xi)} - \frac{1}{4h^3}\ln\left|\frac{\sqrt{a^2+\xi}+h}{\sqrt{a^2+\xi}-h}\right|\right), \tag{S53}$$

$$L_1(0) = ac^2\left(-\frac{1}{h^2 a} - \frac{1}{2h^3}\ln\left|\frac{a+h}{a-h}\right|\right), \tag{S54}$$

$$L_2(0) = L_3(0) = ac^2\left(\frac{a}{2h^2c^2} - \frac{1}{4h^3}\ln\left|\frac{a+h}{a-h}\right|\right). \tag{S55}$$

Also the surface element Eq. S48 is reduced to

$$dS = c\sin\theta\sqrt{a^2 - h^2\cos^2\theta}\,d\theta d\phi. \tag{S56}$$

The components of the internal field in Eqs. 38 to 40 are reduced to two components as

$$\begin{aligned} E_{i\perp}(\xi,\theta,\phi) &= E_{0x}\frac{\varepsilon_e}{\varepsilon_e + (\varepsilon_i - \varepsilon_e)L_1}\left[\frac{(c^2+\xi)\cos^2\theta}{\xi - h^2\cos^2\theta + a^2}\right]^{\frac{1}{2}} \\ &+ (E_{0y}\cos\phi + E_{0z}\sin\phi)\frac{\varepsilon_e}{\varepsilon_e + (\varepsilon_i - \varepsilon_e)L_2}\left[\frac{(a^2+\xi)\sin^2\theta}{\xi - h^2\cos^2\theta + a^2}\right]^{\frac{1}{2}} \end{aligned}, \tag{S57}$$

$$\begin{aligned} E_{i\parallel}(\xi,\theta,\phi) &= E_{0x}\frac{\varepsilon_e}{\varepsilon_e + (\varepsilon_i - \varepsilon_e)L_1}\left[\frac{(a^2+\xi)\sin^2\theta}{\xi - h^2\cos^2\theta + a^2}\right]^{\frac{1}{2}} \\ &+ \left(E_{0y}\sqrt{1-\sin^2\theta\cos^2\phi} + E_{0z}\sqrt{1-\sin^2\theta\sin^2\phi}\right)\frac{\varepsilon_e}{\varepsilon_e + (\varepsilon_i - \varepsilon_e)L_2}\left[\frac{(c^2+\xi)}{\xi - h^2\cos^2\theta + a^2}\right]^{\frac{1}{2}} \end{aligned}. \tag{S58}$$

The components of the external field in Eqs. S42 to 44 are also reduced to

$$E_{e\perp}(\xi,\theta,\phi)=E_{0x}\left\{\begin{array}{l}\left[1+\dfrac{\dfrac{\varepsilon_e-\varepsilon_i}{\varepsilon_e}L_1(\xi)}{1+\dfrac{\varepsilon_i-\varepsilon_e}{\varepsilon_e}L_1}\right]\left[\dfrac{(c^2+\xi)\cos^2\theta}{\xi-h^2\cos^2\theta+a^2}\right]^{\frac{1}{2}}\\ -\left[\dfrac{\dfrac{\varepsilon_e-\varepsilon_i}{\varepsilon_e}ac^2}{1+\dfrac{\varepsilon_i-\varepsilon_e}{\varepsilon_e}L_1}\right]\left[\dfrac{\cos^2\theta}{(c^2+\xi)(a^2+\xi)(\xi-h^2\cos^2\theta+a^2)}\right]^{\frac{1}{2}}\end{array}\right\}$$

$$+(E_{0y}\cos\phi+E_{0z}\sin\phi)\left\{\begin{array}{l}\left[1+\dfrac{\dfrac{\varepsilon_e-\varepsilon_i}{\varepsilon_e}L_2(\xi)}{1+\dfrac{\varepsilon_i-\varepsilon_e}{\varepsilon_e}L_2}\right]\left[\dfrac{(a^2+\xi)\sin^2\theta}{\xi-h^2\cos^2\theta+a^2}\right]^{\frac{1}{2}}\\ -\left[\dfrac{\dfrac{\varepsilon_e-\varepsilon_i}{\varepsilon_e}ac^2}{1+\dfrac{\varepsilon_i-\varepsilon_e}{\varepsilon_e}L_1}\right]\left[\dfrac{\sin^2\theta}{(c^2+\xi)^2(\xi-h^2\cos^2\theta+a^2)}\right]^{\frac{1}{2}}\end{array}\right\}, \tag{S59}$$

$$E_{e\|}(\xi,\theta,\phi)=E_{0x}\left\{\left[1+\dfrac{\dfrac{\varepsilon_e-\varepsilon_i}{\varepsilon_e}L_1(\xi)}{1+\dfrac{\varepsilon_i-\varepsilon_e}{\varepsilon_e}L_1}\right]\left[\dfrac{(a^2+\xi)\sin^2\theta}{\xi-h^2\cos^2\theta+a^2}\right]^{\frac{1}{2}}\right\}$$

$$+(E_{0y}\sqrt{1-\sin^2\theta\cos^2\phi}+E_{0z}\sqrt{1-\sin^2\theta\sin^2\phi})\left\{\left[1+\dfrac{\dfrac{\varepsilon_e-\varepsilon_i}{\varepsilon_e}L_2(\xi)}{1+\dfrac{\varepsilon_i-\varepsilon_e}{\varepsilon_e}L_2}\right]\left[\dfrac{(c^2+\xi)}{\xi-h^2\cos^2\theta+a^2}\right]^{\frac{1}{2}}\right\}. \tag{S60}$$

Using Eqs. (S59) and (S60), the field enhancement factor at the surface can be defined and obtained as

$$\mathcal{L}(\xi,\theta,\varphi)=\frac{\sqrt{|E_{e\perp}|^2+|E_{e\|}|^2}}{\sqrt{|E_{0x}|^2+|E_{0y}|^2+|E_{0z}|^2}}, \tag{S61}$$

and the surface integrated field enhancement factors, when $\xi = 0$, as

$$\mathcal{L}_S=\frac{\iint_s\sqrt{|E_{e\perp}|^2+|E_{e\|}|^2}\,dS}{\iint_s\sqrt{|E_{0x}|^2+|E_{0y}|^2+|E_{0z}|^2}\,dS}. \tag{S62}$$

6. Comparison to Gersten and Nitzan[1]

Introduce a set of coordinate system, the prolate spheroidal coordinate system, (ξ_g, η_g, ψ_g), where

$$\xi_{\mathrm{g}}^2 = \frac{\xi + a^2}{h^2}, \tag{S63}$$

$$\eta_{\mathrm{g}}^2 = \frac{\zeta + a^2}{h^2}. \tag{S64}$$

Substituting Eqs. (S63) and (S64) into Eq. (S5) to (S7), noticing that $b \rightarrow c$, and $\eta \rightarrow -b^2$, and taking ψ_g as the angular coordinate, we have

$$x = h\xi_g\eta_g, \tag{S65}$$

$$y = h\left[\left(\xi_g^2 - 1\right)\left(1 - \eta_g^2\right)\right]^{\frac{1}{2}} \cos\psi_g, \tag{S66}$$

$$z = h\left[\left(\xi_g^2 - 1\right)\left(1 - \eta_g^2\right)\right]^{\frac{1}{2}} \sin\psi_g. \tag{S67}$$

Here (ξ_g, η_g, ψ_g) are identical to (ξ, η, ϕ), in Gersten and Nitzan [1], and h is the same as f in the paper. $\xi_{g,0} = a/h$ represents the surface of the prolate spheroid. Introducing Eq. (S63) into Eq. (S52), we get

$$L_1\left(\xi_g\right) = ab^2\left[-\frac{1}{h^3\xi_g} + \frac{1}{2h^3}\log\frac{\xi_g + 1}{\xi_g - 1}\right]. \tag{S68}$$

Introducing Eqs. (S63) and (S64) into Eq. (S16) using Eq. (S68), and setting $\eta \rightarrow -b^2$ for a prolate spheroid and $E_{0y} = E_{0z} = 0$, we get

$$\begin{aligned}\phi_e &= -E_{0x}h\left[\xi_g^2\eta_g^2\right]^{\frac{1}{2}}\left[1+\frac{\left(\varepsilon_e-\varepsilon_i\right)ab^2\left(-\frac{1}{h^3\xi_g}+\frac{1}{2h^3}\log\frac{\xi_g+1}{\xi_g-1}\right)}{\varepsilon_e+\left(\varepsilon_i-\varepsilon_e\right)ab^2\left(-\frac{1}{h^3a}+\frac{1}{2h^3}\log\frac{a+h}{a-h}\right)}\right] \\ &= -E_{0x}h\xi_g\eta_g+E_{0x}\eta_g\frac{\left(\varepsilon_e-\varepsilon_i\right)ab^2\left(-1+\frac{\xi_g}{2}\log\frac{\xi_g+1}{\xi_g-1}\right)}{\varepsilon_i\left(-\frac{1}{a}+\frac{1}{2h}\log\frac{a+h}{a-h}\right)-\varepsilon_e\left(-\frac{a}{a^2-h^2}+\frac{1}{2h}\log\frac{a+h}{a-h}\right)}\end{aligned} \quad . \tag{S69}$$

We would like to double check if the above expression of ϕ_e, is the same as that given in Gersten and Nitzan. Compared to the problem studied by Gersten and Nitzan, we do not have the polarized molecule or that molecule should be ignored in the first place (see the discussions in Liao and Wokaun [3]). As a result, the second term on the right-hand side of Eq. (2.3) in Gersten and Nitzan will vanish, which gives us

$$\varphi_e^g = -E_{0x}h\xi_g\eta_g + \sum_n c_n P_n(\eta_g)Q_n(\xi_g), \tag{S70}$$

where P_n and Q_n are Legendre Polynomial of the first kind and second kind, respectively. Also, from Eq. (2.14) in that paper, we notice that for the problem without the polarised molecule, only the term as n=1 is left. As such,

$$\phi_e^g = -E_{0x}h\xi_g\eta_g + c_1 P_1(\eta_g)Q_1(\xi_g)\,, \tag{S71}$$

where

$$P_1(\eta_g) = \eta_g\,, \tag{S72}$$

$$Q_1(\xi_g) = \frac{\xi_g}{2}\log\frac{\xi_g+1}{\xi_g-1} - 1\,, \tag{S73}$$

$$c_1 = \frac{(\varepsilon_i-\varepsilon_e)E_{0x}h\xi_{g,0}}{\varepsilon_i Q_1(\xi_{g,0}) - \varepsilon_e\xi_{g,0}Q_1'(\xi_{g,0})}\,, \tag{S74}$$

$$Q_1(\xi_{g,0}) = \frac{\xi_{g,0}}{2}\log\frac{\xi_{g,0}+1}{\xi_{g,0}-1} - 1\,, \tag{S75}$$

and

$$Q_1'(\xi_{g,0}) = \frac{1}{2}\log\frac{\xi_{g,0}+1}{\xi_{g,0}-1} - \frac{\xi_{g,0}}{\xi_{g,0}^2-1}\,. \tag{S76}$$

So that, when using $\xi_{g,0} = a/h$ we have

$$\frac{\varepsilon_i Q_1(\xi_{g,0})}{h\xi_{g,0}} - \frac{\varepsilon_i \xi_{g,0} Q_1'(\xi_{g,0})}{h\xi_{g,0}} = \varepsilon_i\left(\frac{1}{2h}\log\frac{a+h}{a-h} - \frac{1}{a}\right) - \varepsilon_e\left(\frac{1}{2h}\log\frac{a+h}{a-h} - \frac{a}{a^2-h^2}\right). \tag{S77}$$

Introducing Eq. (S77) into Eq. (S74) and substituting the result equation and Eqs. (S72), (S73) into Eq. (S71), we have

$$\phi_e^g = -E_{0x}h\xi_g\eta_g + E_{0x}\eta_g\frac{(\varepsilon_e-\varepsilon_i)ab^2\left(-1+\frac{\xi_g}{2}\log\frac{\xi_g+1}{\xi_g-1}\right)}{\varepsilon_i\left(-\frac{1}{a}+\frac{1}{2h}\log\frac{a+h}{a-h}\right)-\varepsilon_e\left(-\frac{a}{a^2-h^2}+\frac{1}{2h}\log\frac{a+h}{a-h}\right)}, \tag{S78}$$

which is identical to Eq. (S69).

Also, we can reproduce the formulations in Boyd. et. al.[4]. Using Eq. (S64), we can define

$$L_\perp^{out} = \frac{\varepsilon_i}{\varepsilon_e + (\varepsilon_i-\varepsilon_e)\left(-\frac{b^2}{h^2}+\frac{ab^2}{2h^3}\log\frac{a+h}{a-h}\right)}, \tag{S79}$$

$$L_\parallel^{out} = \frac{\varepsilon_e}{\varepsilon_e + (\varepsilon_i-\varepsilon_e)\left(-\frac{b^2}{h^2}+\frac{ab^2}{2h^3}\log\frac{a+h}{a-h}\right)}, \tag{S80}$$

together with

$$\sin\alpha = \left[\frac{a^2(1-\eta_s^2)}{a^2-h^2\eta_s^2}\right]^{\frac{1}{2}}, \tag{S81}$$

$$\cos\alpha = \left[\frac{a^2(1-\eta_s^2)}{a^2-h^2\eta_s^2}\right]^{\frac{1}{2}}. \tag{S82}$$

We then obtain Eq. (1) in Boyd et al.[4] directly. Following their definitions (note that there is a typo in the middle of page 521 of their paper as $L_{\parallel}^{out}$ should be $L_{\perp}^{out}$) and ignoring the damping term,

$$L_{\perp}^{out} = L_{LR} L_p, \tag{S83}$$

where

$$L_{LR} = \frac{1}{A}, \tag{S84}$$

and

$$L_p = \frac{\dfrac{\varepsilon_i}{\varepsilon_e}}{\dfrac{\varepsilon_i}{\varepsilon_e} - 1 + \dfrac{1}{A}}. \tag{S85}$$

We can then tell that

$$A = L_1(0) = -\frac{b^2}{h^2} + \frac{ab^2}{2h^3}\log\frac{a+h}{a-h}, \text{ and } L_{LR} = \frac{1}{L_1(0)}. \tag{S86}$$

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