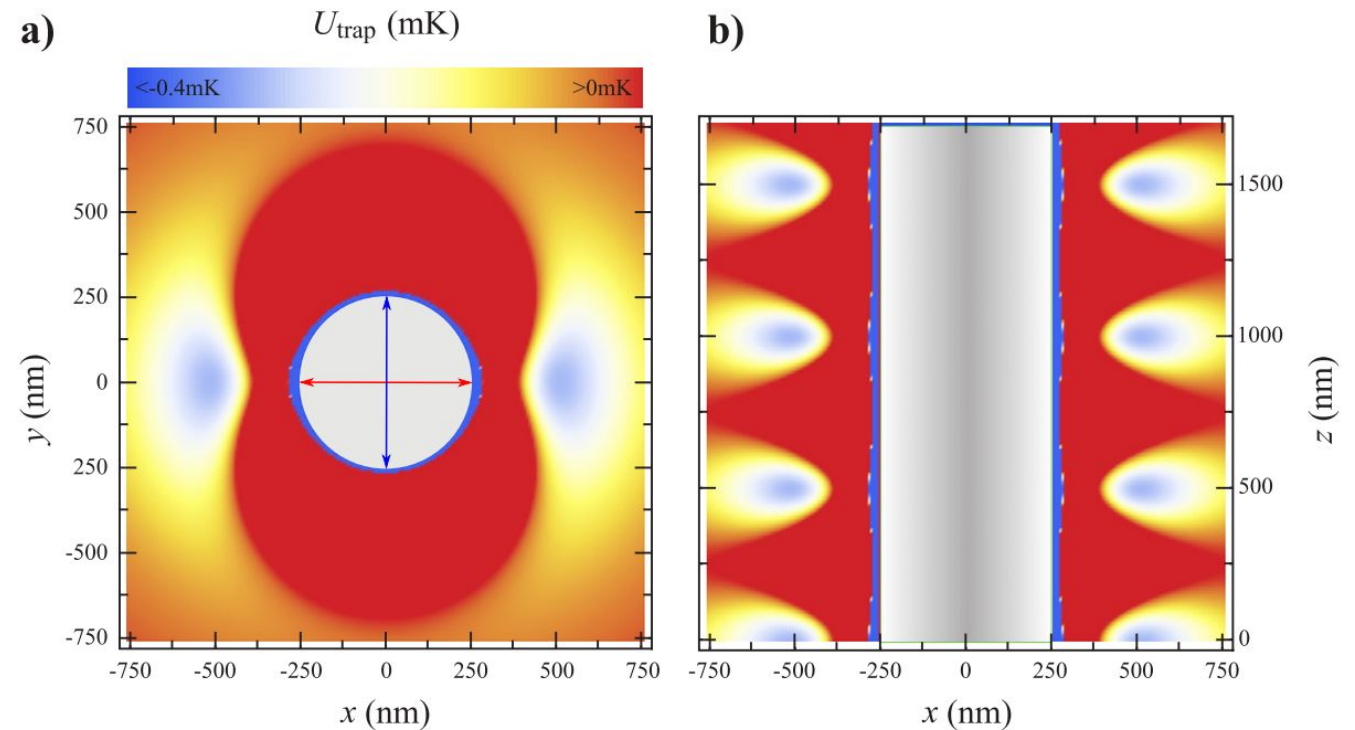


# **Optical lattice potential calculation and simulation**

Guanghui Su

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# Lorentz model

$$\mathbf{d}(t) = -e\mathbf{x}(t) = \alpha(\omega)\mathbf{E}(t)$$

$$U = -\frac{1}{2} \langle \mathbf{d}(t) \cdot \mathbf{E}(t) \rangle = -\frac{1}{4} |E_0|^2 \text{Re}[\alpha(\omega)].$$

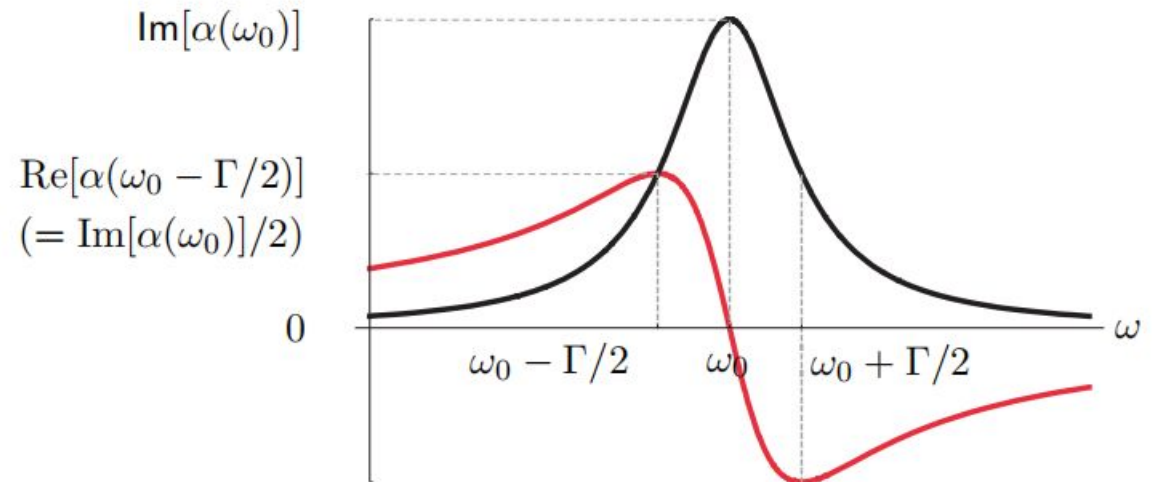
$$\ddot{\mathbf{x}}(t) + \Gamma_\omega \dot{\mathbf{x}}(t) + \omega_0^2 \mathbf{x}(t) = -\frac{e}{m_e} \mathbf{E}(t),$$

$$\Gamma_\omega = \frac{e^2 \omega^2}{6\pi \epsilon_0 m_e c^3},$$

$$\alpha(\omega) = \frac{e^2}{m_e} \frac{1}{\omega_0^2 - \omega^2 - i\Gamma_\omega \omega},$$

$$\text{Re}[\alpha(\omega)] = 6\pi\epsilon_0 c^3 \frac{(\omega_0^2 - \omega^2)\Gamma/\omega_0^2}{(\omega_0^2 - \omega^2)^2 + \Gamma^2(\omega^3/\omega_0^2)^2},$$

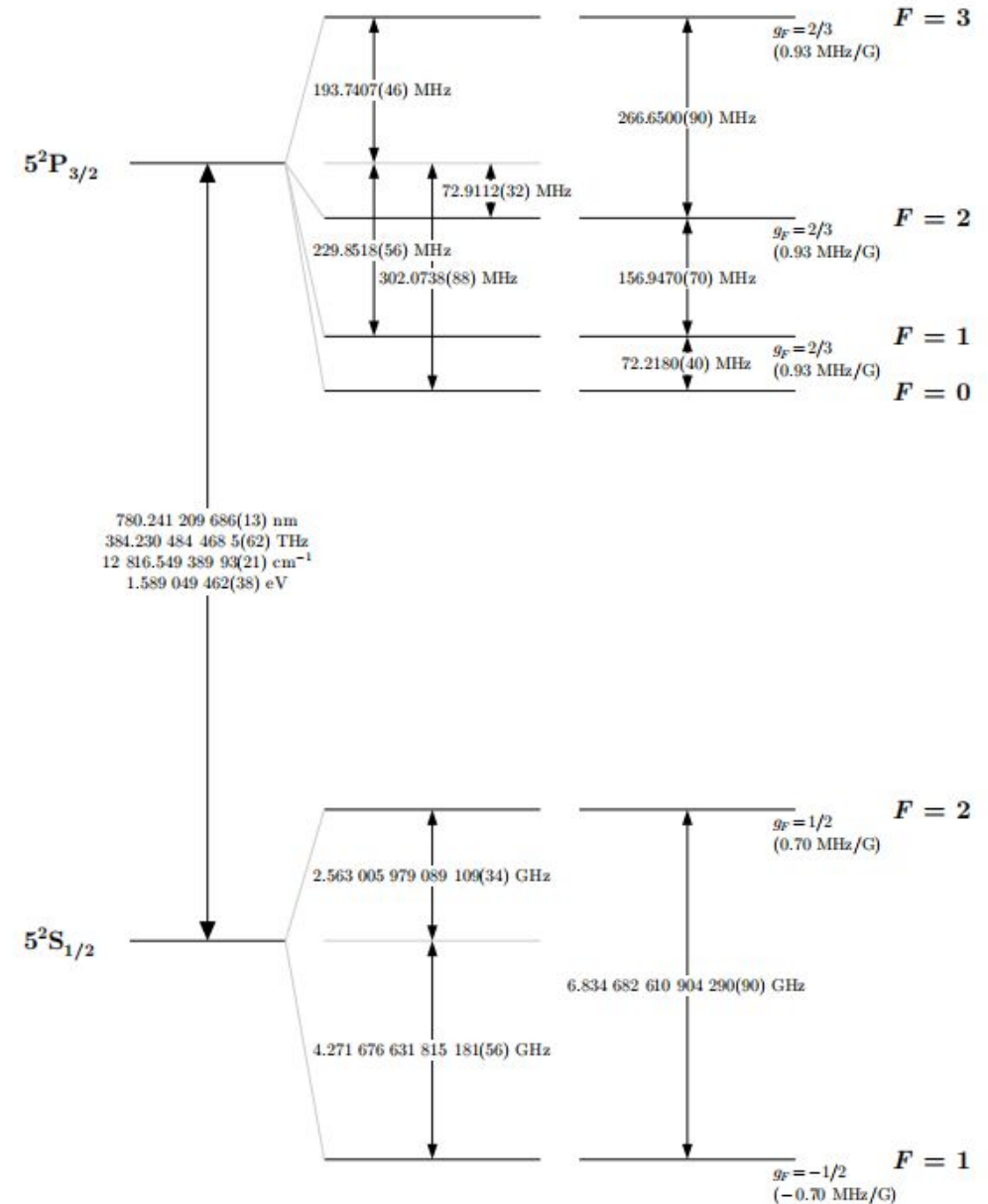
$$\text{Im}[\alpha(\omega)] = 6\pi\epsilon_0 c^3 \frac{\Gamma^2 \omega^3 / \omega_0^4}{(\omega_0^2 - \omega^2)^2 + \Gamma^2(\omega^3/\omega_0^2)^2}.$$



# Fine structure: J

$$\alpha(\omega) = \sum_{j=1}^n f_j \alpha_j(\omega).$$

$$\text{Re}[\alpha(\omega)] = 2\pi\epsilon_0 c^3 \sum_i \frac{2J' + 1}{2J + 1} \frac{(\omega_j^2 - \omega^2)\Gamma_j/\omega_j^2}{(\omega_j^2 - \omega^2)^2 + \Gamma_j^2(\omega^3/\omega_j^2)^2},$$



# Hyperfine structure

$$H_{\text{int}} = V^{\text{hfs}} + V^{EE}.$$

$$V^{\text{hfs}} = \hbar A_{\text{hfs}} \mathbf{I} \cdot \mathbf{J} + \hbar B_{\text{hfs}} \frac{6(\mathbf{I} \cdot \mathbf{J})^2 + 3\mathbf{I} \cdot \mathbf{J} - 2I^2 J^2}{2I(2I-1)2J(2J-1)}.$$

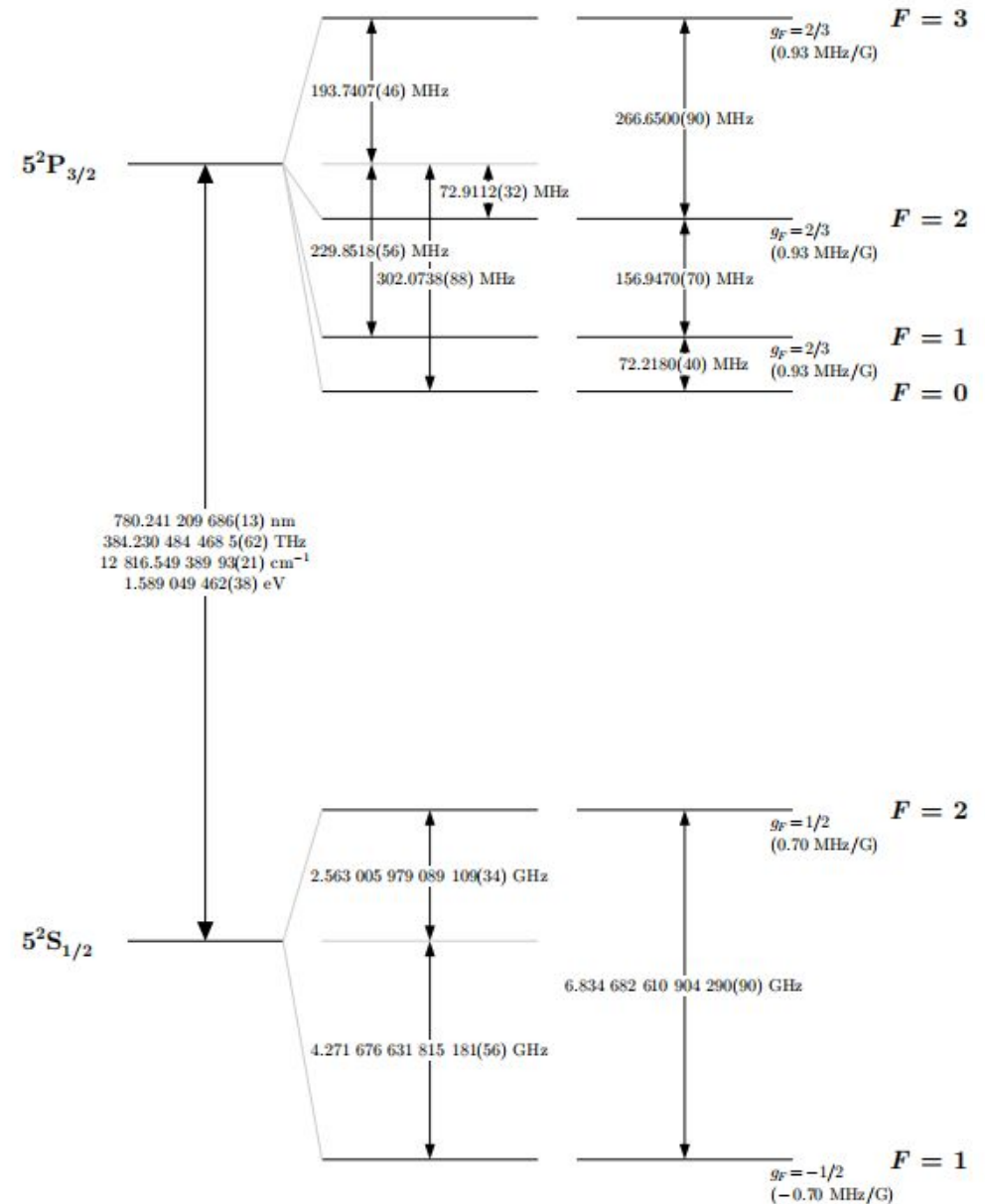
$$\langle nJFM | V^{\text{hfs}} | nJFM \rangle = \frac{1}{2} \hbar A_{\text{hfs}} G$$

$$+ \hbar B_{\text{hfs}} \frac{\frac{3}{2}G(G+1) - 2I(I+1)J(J+1)}{2I(2I-1)2J(2J-1)},$$

$$\text{where } G = F(F+1) - I(I+1) - J(J+1).$$

$$V^E = -\mathbf{E} \cdot \mathbf{d} = -\frac{1}{2} \mathcal{E} \mathbf{u} \cdot \mathbf{d} e^{-i\omega t} - \frac{1}{2} \mathcal{E}^* \mathbf{u}^* \cdot \mathbf{d} e^{i\omega t},$$

$$\mathbf{E} = \frac{1}{2} \mathcal{E} e^{-i\omega t} + \text{c.c.} = \frac{1}{2} \mathcal{E} \mathbf{u} e^{-i\omega t} + \text{c.c.},$$



# Second-order perturbation

$$V^E = -\mathbf{E} \cdot \mathbf{d} = -\frac{1}{2}\mathcal{E}\mathbf{u} \cdot \mathbf{d}e^{-i\omega t} - \frac{1}{2}\mathcal{E}^*\mathbf{u}^* \cdot \mathbf{d}e^{i\omega t},$$

$$\delta E_a = -\frac{|\mathcal{E}|^2}{4\hbar} \sum_b \operatorname{Re} \left( \frac{|\langle b|\mathbf{u} \cdot \mathbf{d}|a\rangle|^2}{\omega_b - \omega_a - \omega - i\gamma_{ba}/2} + \frac{|\langle a|\mathbf{u} \cdot \mathbf{d}|b\rangle|^2}{\omega_b - \omega_a + \omega + i\gamma_{ba}/2} \right).$$

$$V^{EE} = \frac{|\mathcal{E}|^2}{4} [(\mathbf{u}^* \cdot \mathbf{d})\mathcal{R}_+(\mathbf{u} \cdot \mathbf{d}) + (\mathbf{u} \cdot \mathbf{d})\mathcal{R}_-(\mathbf{u}^* \cdot \mathbf{d})]$$

with

$$\mathcal{R}_+ = -\frac{1}{\hbar} \sum_b \operatorname{Re} \left( \frac{1}{\omega_b - \omega_a - \omega - i\gamma_{ba}/2} \right) |b\rangle\langle b|,$$

$$\mathcal{R}_- = -\frac{1}{\hbar} \sum_b \operatorname{Re} \left( \frac{1}{\omega_b - \omega_a + \omega + i\gamma_{ba}/2} \right) |b\rangle\langle b|.$$

$$V_{EE}(\boldsymbol{\mathcal{E}}, \omega) = \frac{1}{4}\mathcal{E}^2 \sum_{K=0,1,2} \{\mathbf{e}^* \otimes \mathbf{e}\}_K \cdot \left[ \{\mathbf{d} \otimes R_{E_0}(\omega)\mathbf{d}\}_K + (-1)^K \{\mathbf{d} \otimes R_{E_0}(-\omega)\mathbf{d}\}_K \right],$$

$$\{\mathbf{e}^* \otimes \mathbf{e}\}_{0,0} = -\frac{1}{\sqrt{3}}(\mathbf{e}^* \cdot \mathbf{e}) = -\frac{1}{\sqrt{3}}$$

$$\{\mathbf{e}^* \otimes \mathbf{e}\}_{1,\mu} = -\frac{1}{\sqrt{2}}(\mathbf{e}^* \times \mathbf{e})_\mu = -\frac{A}{\sqrt{2}}\delta_{\mu,0}$$

$$\{\mathbf{e}^* \otimes \mathbf{e}\}_{2,\mu} = -\frac{1}{\sqrt{6}}\delta_{\mu,0} + \frac{l}{\sqrt{2}}\delta_{\mu,\pm 2}.$$

# polarizability and CG coefficients

$$\begin{aligned}
 V_{FMF'M'}^{EE} &= \frac{1}{4} |\mathcal{E}|^2 \sum_{\substack{K=0,1,2 \\ q=-K,\dots,K}} \alpha_{nJ}^{(K)} \{\mathbf{u}^* \otimes \mathbf{u}\}_{Kq} \\
 &\times (-1)^{J+I+K+q-M} \sqrt{(2F+1)(2F'+1)} \\
 &\times \begin{pmatrix} F & K & F' \\ M & q & -M' \end{pmatrix} \begin{Bmatrix} F & K & F' \\ J & I & J \end{Bmatrix}. \quad (10)
 \end{aligned}$$

$$\begin{aligned}
 \alpha_{nF}^{(K)}(\omega) &= (-1)^{I-J+F} \sqrt{2K+1} \sqrt{2F+1} \sqrt{2F'+1} \begin{Bmatrix} F & K & F' \\ J & I & J \end{Bmatrix} \\
 &\times \sum_{n''J''} \begin{Bmatrix} J & K & J \\ 1 & J'' & 1 \end{Bmatrix} \langle nJ \| \mathbf{d} \| n''J'' \rangle \langle n''J'' \| \mathbf{d} \| nJ \rangle \\
 &\times \left[ \frac{1}{E_{n,J} - E_{n'',J''} + \hbar\omega} + \frac{(-1)^K}{E_{n,J} - E_{n'',J''} - \hbar\omega} \right],
 \end{aligned}$$

$$\Delta E_{ac} = T_{M,M} = -\frac{1}{4} \mathcal{E}^2 \left[ \alpha_{nF}^s(\omega) + A \alpha_{nF}^a(\omega) \frac{M_F}{2F} - \alpha_{nF}^T(\omega) \frac{3M_F^2 - F(F+1)}{2F(2F-1)} \right],$$

$$\alpha_{nF}^s = \frac{1}{\sqrt{3(2F+1)}} \alpha_{nF}^{(0)},$$

$$\alpha_{nF}^a = -\sqrt{\frac{2F}{(F+1)(2F+1)}} \alpha_{nF}^{(1)},$$

$$\alpha_{nF}^T = -\sqrt{\frac{2F(2F-1)}{3(F+1)(2F+1)(2F+3)}} \alpha_{nF}^{(2)}.$$



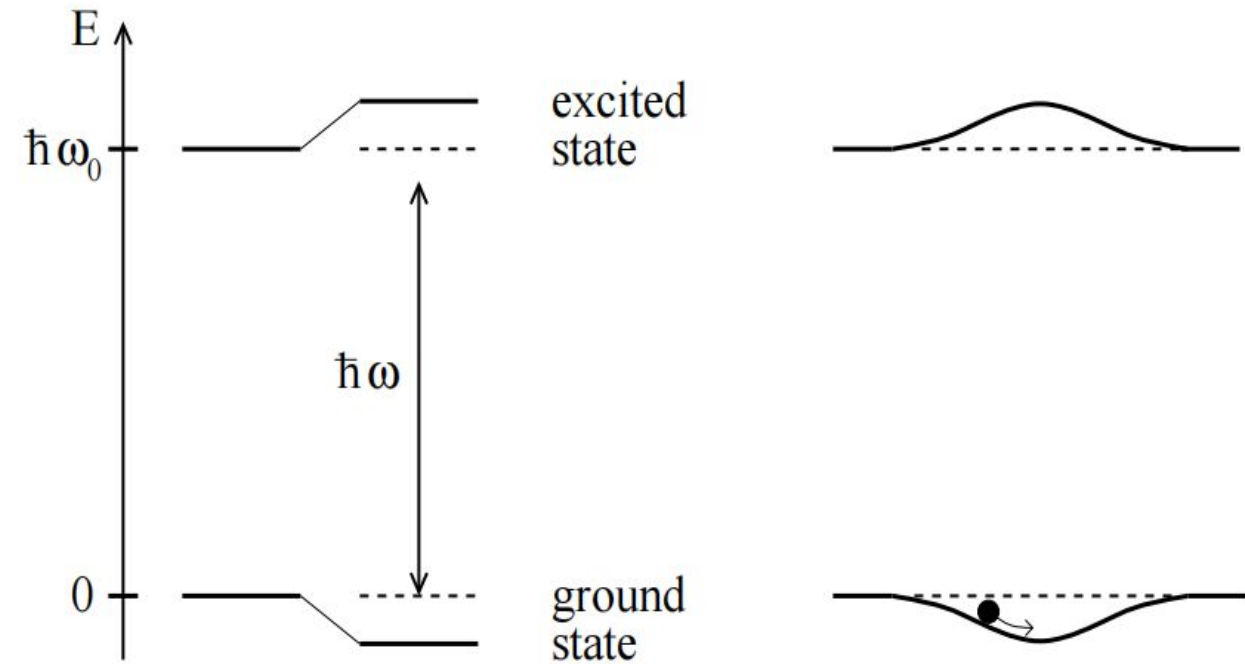
# Large detuning AC stark shift

$$\Delta E_i = \left( \frac{|\langle j | \mathbf{d} \cdot \boldsymbol{\varepsilon} | i \rangle|^2}{E_i - E_j + \hbar\omega} + \frac{|\langle j | \mathbf{d} \cdot \boldsymbol{\varepsilon} | i \rangle|^2}{E_i - E_j - \hbar\omega} \right) \left| \frac{E_0}{2} \right|^2$$

$$= \left( \frac{|\mathbf{r}_{ij}|^2}{E_i - E_j + \hbar\omega} + \frac{|\mathbf{r}_{ij}|^2}{E_i - E_j - \hbar\omega} \right) e^2 a_{ij}^2 \left| \frac{E_0}{2} \right|^2$$

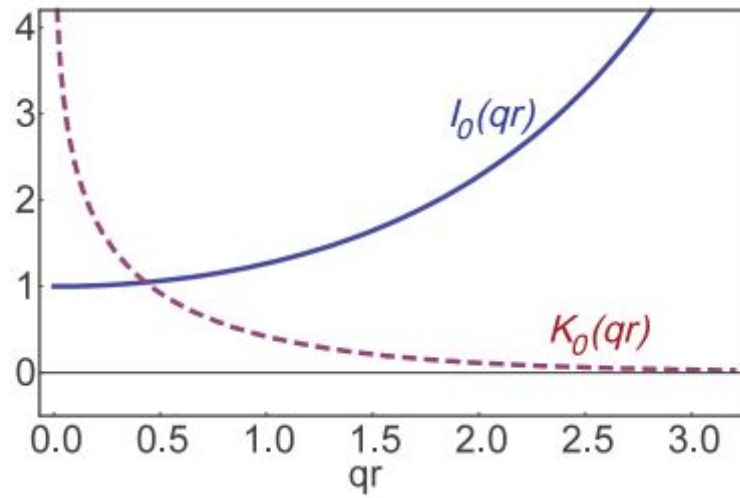
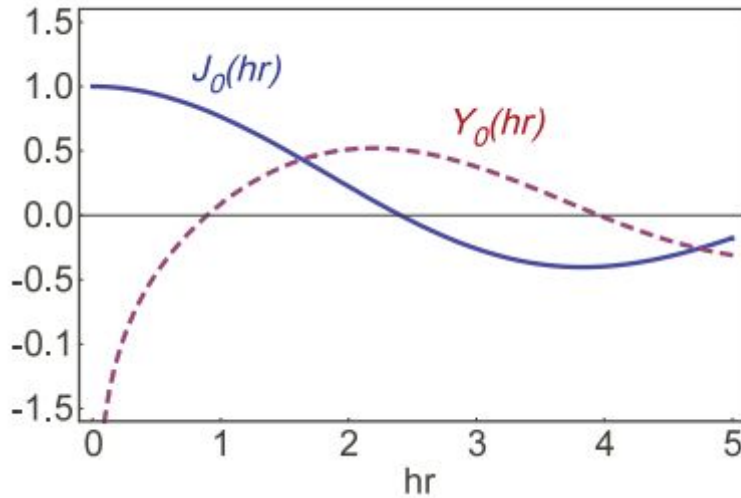
$$\Gamma_{ij} = \frac{e^2 |\omega_{ij}|^3}{3\pi \hbar \varepsilon_0 c^3} |\mathbf{r}_{ij}|^2$$

$$\Delta E_i = \left( \frac{1}{\omega_{ij} + \omega} + \frac{1}{\omega_{ij} - \omega} \right) a_{ij}^2 \frac{3\pi c^2}{2|\omega_{ij}|^3} \Gamma_{ij} I$$





# Bessel function



$$\vec{\nabla}^2 \vec{E} - \mu_0 \epsilon(r) \frac{\partial^2 \vec{E}}{\partial t^2} = -\vec{\nabla} \left( \frac{\vec{E}}{\epsilon(r)} \cdot \vec{\nabla} \epsilon(r) \right)$$

$$\vec{\nabla} \times \vec{H} = \epsilon(r) \frac{\partial \vec{E}}{\partial t}, \quad \vec{\nabla} \cdot \vec{H} = 0$$

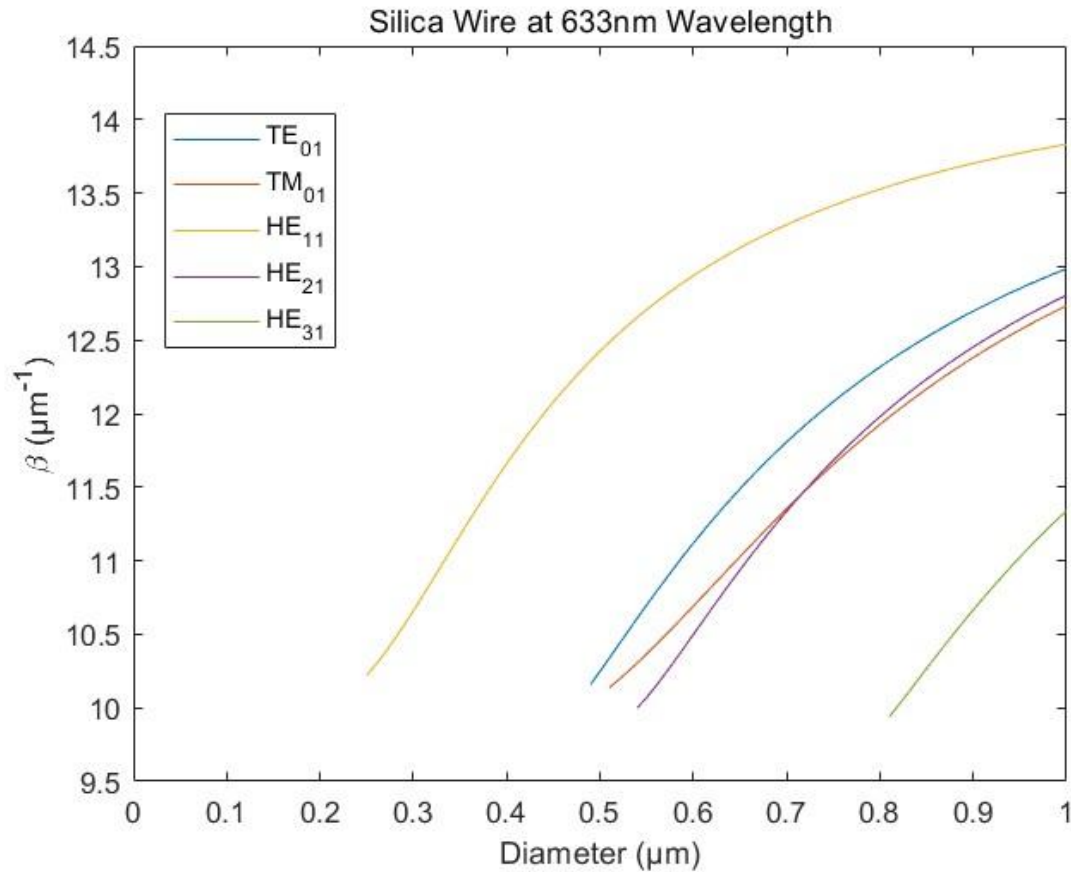
$$\vec{\nabla} \times \vec{E} = -\mu_0 \frac{\partial \vec{H}}{\partial t}, \quad \vec{\nabla} \cdot (\epsilon(r) \vec{E}) = 0$$

$$\begin{bmatrix} E_z(\vec{r}, t) \\ H_z(\vec{r}, t) \end{bmatrix} = \begin{bmatrix} E_z(r, \phi) \\ H_z(r, \phi) \end{bmatrix} \exp[i(\omega t - \beta z)],$$

$$\begin{bmatrix} E_z(r, \phi) \\ H_z(r, \phi) \end{bmatrix} = R(r) \exp[\pm i l \phi],$$

$$\left[ \partial_r^2 + \frac{1}{r} \partial_r + (k^2 - \beta^2 - \frac{l^2}{r^2}) \right] R(r) = 0.$$

# Propagation constant: beta



$$E_z(r, \phi, z, t) = AJ_l(hr) \exp[i(\omega t \pm l\phi - \beta z)],$$

$$H_z(r, \phi, z, t) = BJ_l(hr) \exp[i(\omega t \pm l\phi - \beta z)],$$

$$\text{with } h = \sqrt{n_1^2 k_0^2 - \beta^2}$$

( $r < a$ ), and

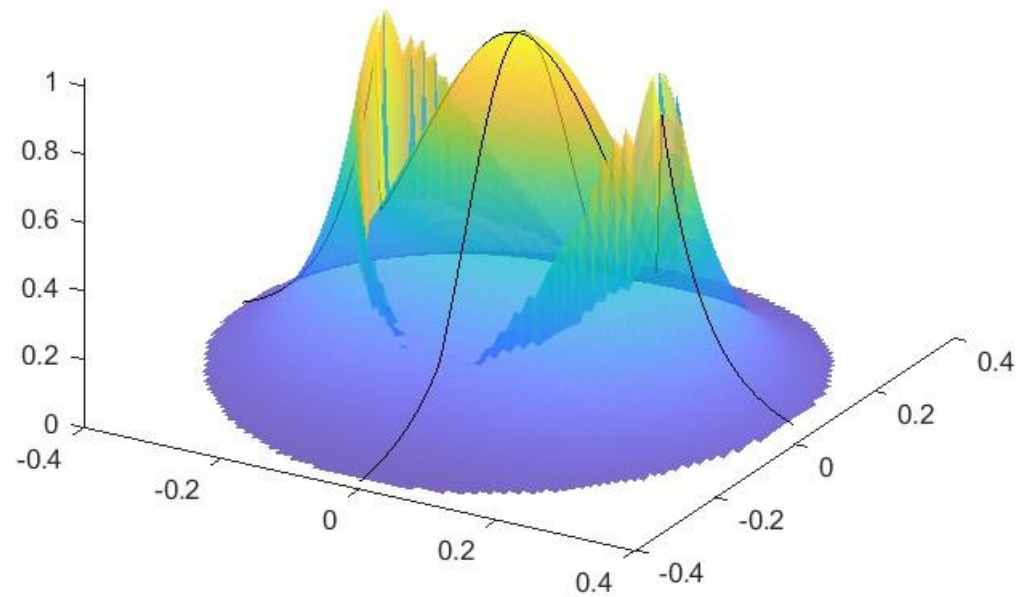
$$E_z(r, \phi, z, t) = CK_l(qr) \exp[i(\omega t \pm l\phi - \beta z)],$$

$$H_z(r, \phi, z, t) = DK_l(qr) \exp[i(\omega t \pm l\phi - \beta z)],$$

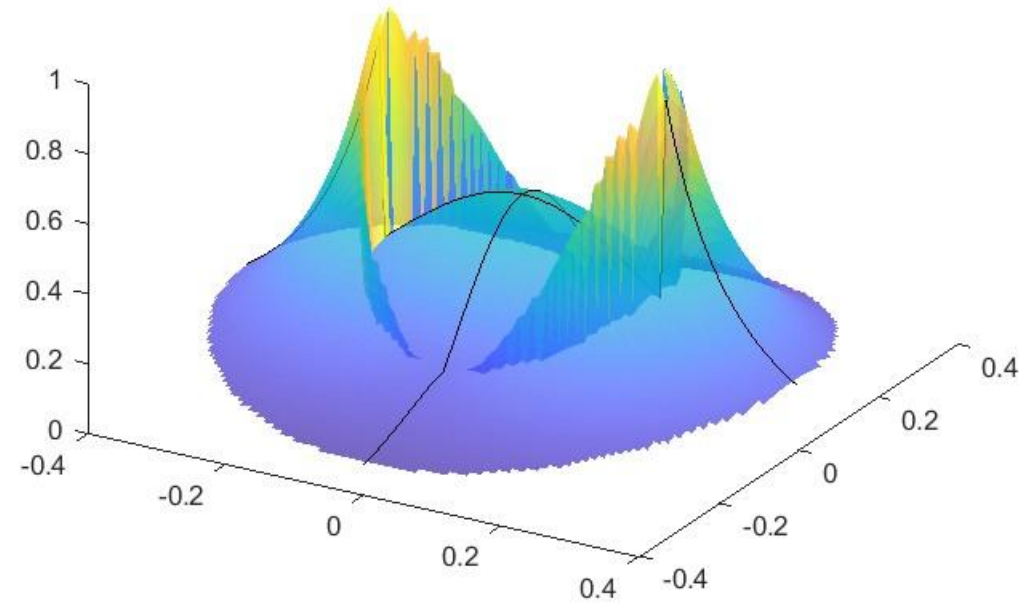
$$\text{with } q = \sqrt{\beta^2 - n_2^2 k_0^2}$$

core ( $r > a$ ).

# Cross-section intensity

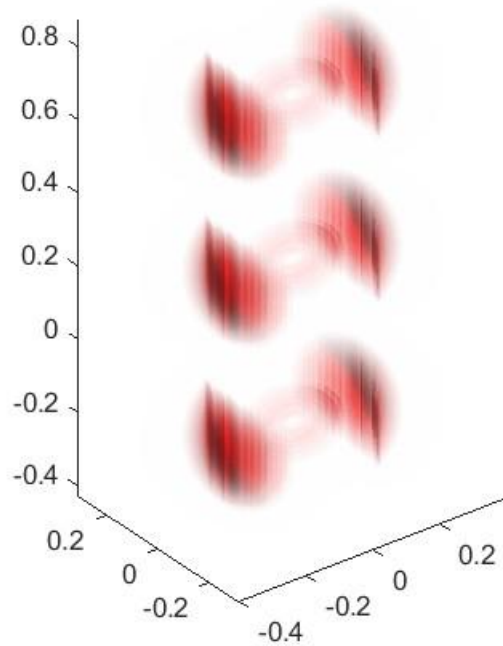


$\text{lam1} = 0.9352 \text{ um};$   
 $\text{dia} = 0.4 \text{ um}$ , parameters from Ground group



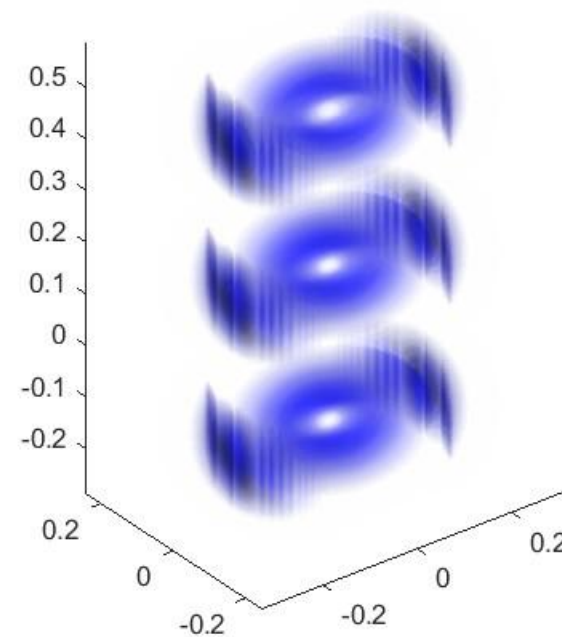
$\text{lam2} = 0.6865 \text{ um};$   
 $\text{lam3} = 0.6861 \text{ um};$

# 3D distribution of intensity



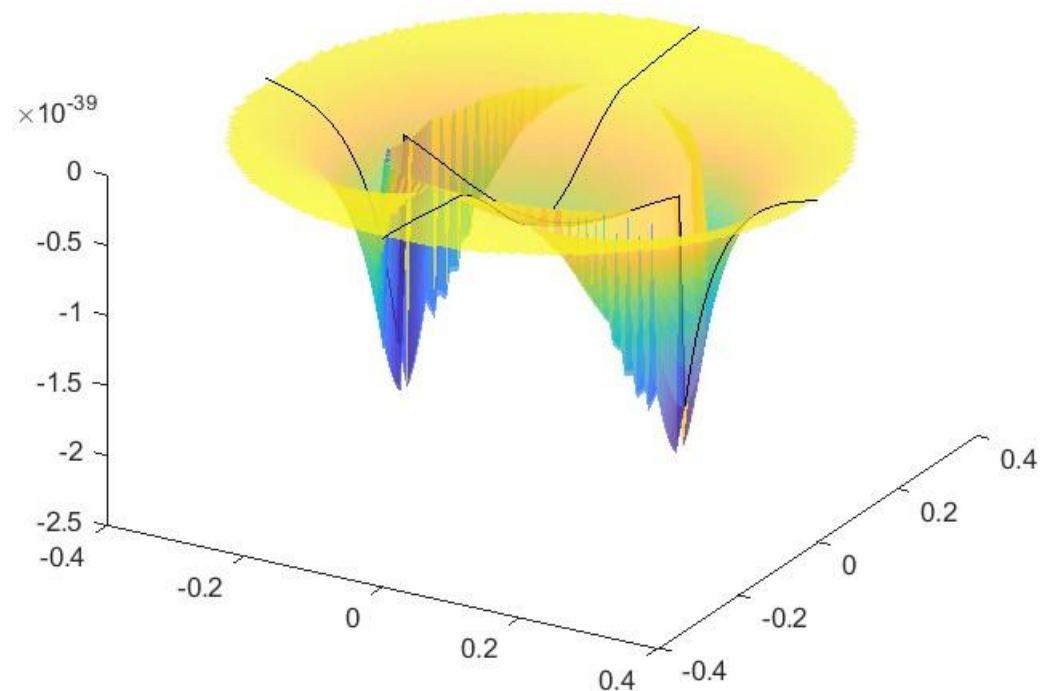
$\lambda_{m1} = 0.9352 \text{ } \mu\text{m};$

- $\text{dia} = 0.4 \text{ } \mu\text{m}$ , parameters from Ground group
- $z$  direction from  $-\pi/\beta$  to  $2\pi/\beta$



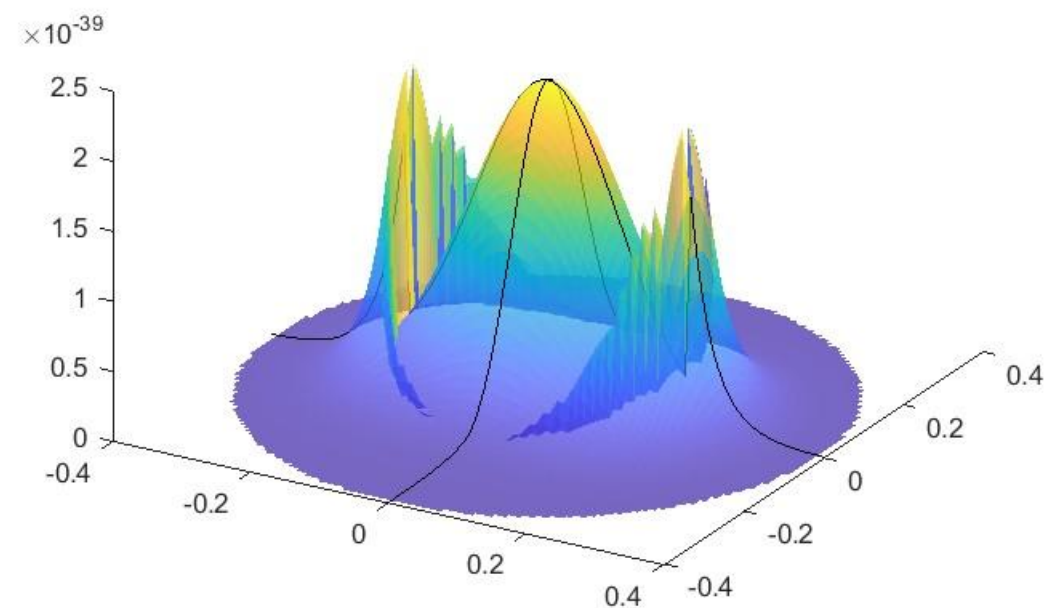
$\lambda_{m2} = 0.6865 \text{ } \mu\text{m};$   
 $\lambda_{m3} = 0.6861 \text{ } \mu\text{m};$

# Cross-section potential



$\text{lam1} = 0.9352 \text{ um};$

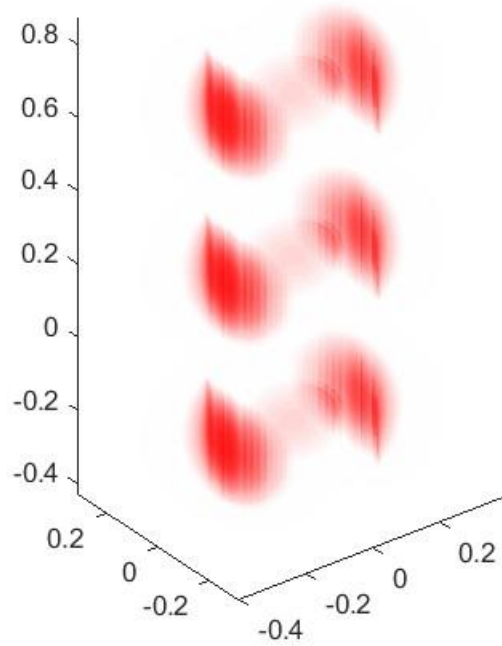
$\text{dia} = 0.4 \text{ um}$ , parameters from Ground group



$\text{lam2} = 0.6865 \text{ um};$

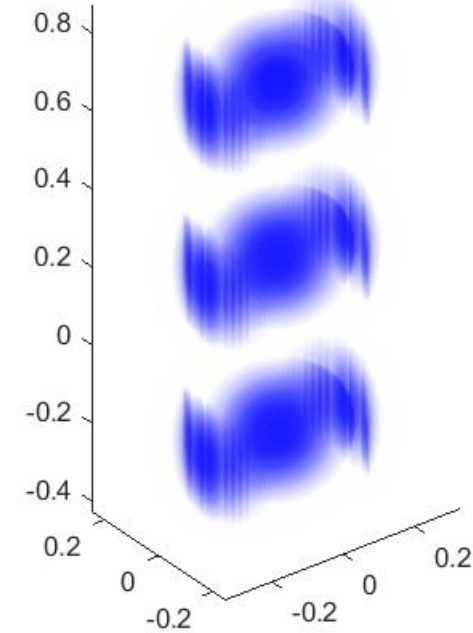
$\text{lam3} = 0.6861 \text{ um};$

# 3D potential



$\text{lam1} = 0.9352 \text{ um};$

- $\text{dia} = 0.4 \text{ um}$ , parameters from Ground group
- z direction from  $-\pi/\beta$  to  $2\pi/\beta$



$\text{lam2} = 0.6865 \text{ um};$

$\text{lam3} = 0.6861 \text{ um};$

**Total potential:  $2U_{\text{red}} + U_{\text{blue}}$**

