

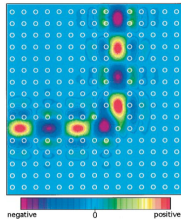
# Mathematical and Computational Methods in Photonics

Habib Ammari

Department of Mathematics, ETH Zürich

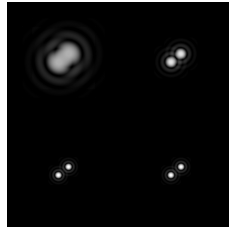
# Mathematics for photonics

- **Control, manipulate, reshape, guide, focus** electromagnetic waves at **sub-wavelength length scales** (beyond the **resolution limit**).
- **Direct, inverse, and optimal design** problems for electromagnetic wave propagation in **complex and resonant media**.
- Build **mathematical frameworks** and develop **effective numerical algorithms** for photonic applications.
- Partial differential equations, spectral analysis, integral equations, computational techniques, and multi-scale analysis.



# Resonances for plasmonic nanoparticles

- Key to **super-resolution**: push the **resolution limit** by reducing the **focal spot size**; confine light to a length scale significantly smaller than **half the wavelength**.
- **Resolution**: smallest detail that can be resolved.

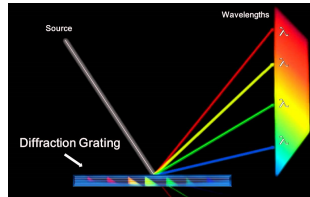
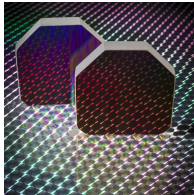


# Mathematics for photonics

- **Mathematical** and **computational** tools:
  - Diffraction gratings;
  - Photonic crystals;
  - Plasmonic resonant nanoparticles;
  - Metamaterials and metasurfaces.

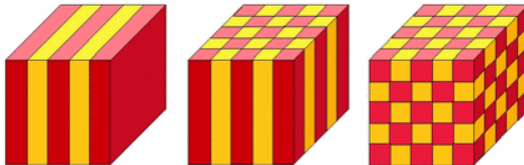
# Mathematics for photonics

- **Diffraction gratings:**
  - Scattering by **periodic structures**: dominated by diffraction; small features of the structure  $\rightarrow$  small number of **propagating modes** (other modes are **evanescent**).
  - **Spectroscopic**, telecommunications and laser applications.
  - Design problem: **grating profile** that give rise to a **specified diffraction pattern**.



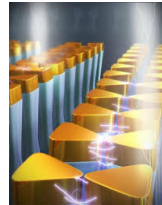
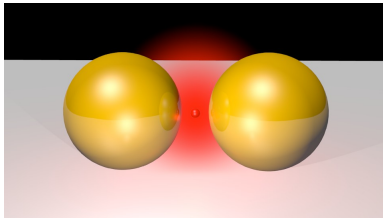
# Mathematics for photonics

- **Photonic crystals** (also known as **photonic band-gap materials**):
  - **Periodic dielectric structures** that have a **band gap** that forbids propagation of a certain frequency range of light.
  - **Band gap calculations**: **high-contrast** materials, periodicity of the **same order** as the wavelength; **efficient numerical schemes**.
  - **Control light** and produce effects that are impossible with conventional optics.
  - **Resonant cavities**: making **point defects** in a photonic crystal → light can be **localized**, **trapped** in the defect. The frequency, symmetry, and other properties of the **defect mode** can be easily **tuned** to anything desired.



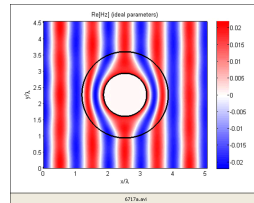
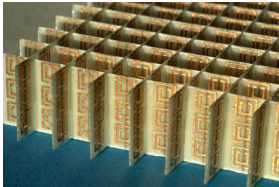
# Mathematics for photonics

- Plasmonic nanoparticles:
  - Sub-wavelength resonance: quasi-static regime.
  - Scattering and absorption enhancement.
  - Super-resolution: single particle imaging.
  - Nanoantenna, concentrate light at sub-wavelength scale.



# Mathematics for photonics

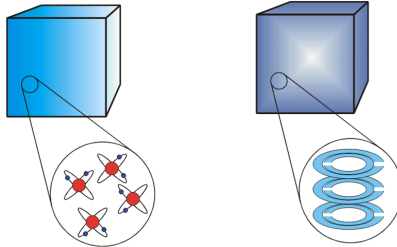
- **Metamaterials** and **metasurfaces**:
  - **Negative material** parameters.
  - **Electromagnetic invisibility and cloaking**: make a target invisible when probed by electromagnetic waves:
    - Interior cloaking: **scattering cancellations** techniques.
    - Exterior cloaking by **anomalous resonances**.
  - **Sub-wavelength band gap materials**: microstructure periodicity smaller than the wavelength.





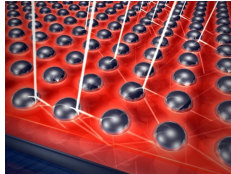
# Mathematics for photonics

- **Metamaterials and metasurfaces:**
  - **Microstructured** materials.
  - Building block microstructure: **sub-wavelength resonator**.



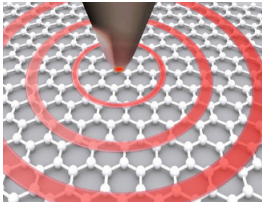
# Mathematics for photonics

- Effective medium theory:
  - High contrast materials: for some range of frequencies.
  - Super-resolution and super-focusing of electromagnetic waves.
- Unify the mathematical theory of super-resolution, photonic bandgap materials, metamaterials, and cloaking.



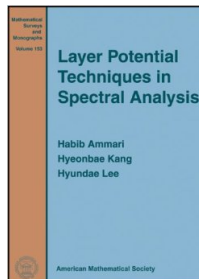
# Mathematics for photonics

- Near-field optics:
  - Interaction between the plasmonic probe and the sample.
  - Super-resolution imaging of the sample.
  - Mechanism → quantitative imaging.



# Mathematics for photonics

- Spectral analysis and integral equation formulations.
- Green's functions (free space, periodic, quasi-periodic, ...) → eigenvalue problems reduced to characteristic value problems (nonlinear eigenvalue problems).
- Gohberg-Sigal theory:
  - Generalization of Rouché theorem for operator valued function.
  - Sensitivity analysis (change in the shape, material parameters, environment, ...) of diffraction pattern, band gaps, resonance for plasmonic nanoparticles, ...



# Mathematics for photonics

- **2014 Kavli Prize in Nanoscience** (Norwegian Academy of Science & Letters): **T.W. Ebbesen**, **S.W. Hell**, and **J.B. Pendry**.
- "for their **transformative contributions** to the field of **nano-optics** that have broken long-held beliefs about the limitations of the **resolution limits** of optical microscopy and imaging.
  - "for the discovery of the **extraordinary transmission** of light through **sub-wavelength apertures**.
  - "for ground-breaking developments that have led to fluorescence microscopy with **nanometre scale resolution**, opening up nanoscale imaging to biological applications.
  - "for developing the theory underlying **new optical nanoscale materials** with unprecedented properties, such as the **negative index of refraction**, allowing for the formation of perfect lenses.



# Mathematics for photonics

- **Phononics:**
  - **Sound** /light.
  - **Elasticity equations**/ Maxwell's equations.
  - **Sub-wavelength resonances:** **Helmholtz resonator**, **Minnaert** bubble/ plasmonic nanoparticle.
- Similar **physical mechanisms** and mathematical and computational **frameworks** to those in photonics:
  - **Scattering enhancement** by sub-wavelength acoustic resonators.
  - **Phononic crystals.**
  - **Acoustic metamaterials** and metasurfaces, **sub-wavelength phononic band gap** materials.
  - **High contrast acoustic materials**, **super-resolution** and **super-focusing** for acoustic waves.

# Mathematics for photonics

- Gohberg-Sigal theory:
  - **Argument principle**:  $V \subset \mathbb{C}$ : bounded domain with smooth boundary  $\partial V$  positively oriented;  $f(z)$ : meromorphic function in a neighborhood of  $\overline{V}$ ;  $P$  and  $N$ : the **number of poles** and **zeros** of  $f$  in  $V$ , counted with their multiplicities. If  $f$  has no poles and never vanishes on  $\partial V$ , then

$$\frac{1}{2\pi i} \int_{\partial V} \frac{f'(z)}{f(z)} dz = N - P.$$

- **Rouché's theorem**:  $f(z)$  and  $g(z)$ : holomorphic in a neighborhood of  $\overline{V}$ . If  $|f(z)| > |g(z)|$  for all  $z \in \partial V$ , then  $f$  and  $f + g$  have the **same number of zeros** in  $V$ .

# Mathematics for photonics

- $\mathcal{L}(\mathcal{B}, \mathcal{B}')$ : linear bounded operators from  $\mathcal{B}$  into  $\mathcal{B}'$  (Banach spaces).
- $\mathfrak{U}(z_0)$ : set of all operator-valued functions in  $\mathcal{L}(\mathcal{B}, \mathcal{B}')$  which are holomorphic in some neighborhood of  $z_0$ , except possibly at  $z_0$ .
- $z_0$  **characteristic value** of  $A(z) \in \mathfrak{U}(z_0)$  if there exists a vector-valued function  $\phi(z)$  with values in  $\mathcal{B}$  such that
  - $\phi(z)$ : holomorphic at  $z_0$  and  $\phi(z_0) \neq 0$ ,
  - $A(z)\phi(z)$ : holomorphic at  $z_0$  and vanishes at this point.
  - $\phi(z)$ : **root function** of  $A(z)$  associated with the characteristic value  $z_0$ .



# Mathematics for photonics

- Generalized argument principle:

$$\mathcal{M}(A(z); \partial V) = \frac{1}{2\pi i} \operatorname{tr} \int_{\partial V} A^{-1}(z) \frac{d}{dz} A(z) dz.$$

- $\mathcal{M}(A(z); \partial V)$ : number of characteristic values of  $A(z)$  in  $V$ , counted with their multiplicities, minus the number of poles of  $A(z)$  in  $V$ , counted with their multiplicities.
- Generalized Rouché's theorem :

$$\mathcal{M}(A(z); \partial V) = \mathcal{M}(A(z) + S(z); \partial V).$$

- $S(z)$ : finitely meromorphic in  $V$  and continuous on  $\partial V$  s.t.

$$\|A^{-1}(z)S(z)\|_{\mathcal{L}(\mathcal{B}, \mathcal{B})} < 1, \quad z \in \partial V.$$

- Finitely meromorphic operator: coefficients of the principal part of its Laurent expansion are operators of finite rank.

# Mathematics for photonics

- $0 = \mu_1 < \mu_2 \leq \dots$ : eigenvalues of  $-\Delta$  in  $\Omega$  with Neumann conditions,

$$\begin{cases} \Delta u + \mu u = 0 & \text{in } \Omega, \\ \frac{\partial u}{\partial \nu} = 0 & \text{on } \partial\Omega, \end{cases}$$

- $(u_j)_{j \geq 1}$ : orthonormal basis of  $L^2(\Omega)$  of normalized eigenvectors.
- $\omega = \sqrt{\mu}$ ;  $\mathcal{S}_\Omega^\omega, \mathcal{D}_\Omega^\omega, \mathcal{K}_\Omega^\omega$ : **single- and double-layer potentials** and **Neumann-Poincaré operator** associated with the **outgoing fundamental solution**  $G_\omega(x, z)$  to the **Helmholtz operator**  $\Delta + \omega^2$ :

$$G_\omega(x, z) := \begin{cases} -\frac{i}{4} H_0^{(1)}(\omega|x-z|), & d = 2, \\ -\frac{e^{i|x-z|}}{4\pi|x-z|}, & d = 3. \end{cases}$$

- $H_0^{(1)}$ : Hankel function of the first kind of order 0.

# Mathematics for photonics

- **Sommerfeld radiation condition:**  $|x| \rightarrow +\infty$ ,

$$\frac{x}{|x|} \cdot \nabla G_\omega(x, z) - i\omega G_\omega(x, z) = \begin{cases} O(|x|^{-3/2}), & d = 2, \\ O(|x|^{-2}), & d = 3. \end{cases}$$

- **Layer potentials:**  $\varphi \in L^2(\partial\Omega)$ ,

$$\mathcal{S}_\Omega^\omega[\varphi](x) = \int_{\partial\Omega} G_\omega(x, y) \varphi(y) d\sigma(y), \quad x \in \mathbb{R}^d,$$

$$\mathcal{D}_\Omega^\omega[\varphi](x) = \int_{\partial\Omega} \frac{\partial G_\omega(x, y)}{\partial \nu(y)} \varphi(y) d\sigma(y), \quad x \in \mathbb{R}^d \setminus \partial\Omega,$$

$$\mathcal{K}_\Omega^\omega[\varphi](x) = \text{p.v.} \int_{\partial\Omega} \frac{\partial G_\omega(x, y)}{\partial \nu(y)} \varphi(y) d\sigma(y).$$

- $\sqrt{\mu_j}$ : **characteristic value** of  $\omega \mapsto ((1/2)I - \mathcal{K}_\Omega^\omega$ .
- **Muller's method:** compute **zeros** of  $\omega \mapsto 1/(((1/2)I - \mathcal{K}_\Omega^\omega)^{-1}[\varphi], \psi)$  for fixed  $\varphi$  and  $\psi$ .

# Mathematics for photonics

- $D$  conductive particle inside  $\Omega$ ,  $D = \varepsilon B + z$ ;  $k \neq 1$ : conductivity parameter;  $\varepsilon$ : characteristic size;  $d$ : space dimension.
- **Characteristic values** of the operator-valued function  $\mathcal{A}_\varepsilon(\omega)$ :

$$\omega \mapsto \mathcal{A}_\varepsilon(\omega) := \begin{pmatrix} \frac{1}{2}I - \mathcal{K}_\Omega^\omega & -S_D^\omega & 0 \\ \mathcal{D}_\Omega^\omega & S_D^\omega & -S_D^{\frac{\omega}{\sqrt{k}}} \\ \varepsilon \frac{\partial}{\partial \nu} \mathcal{D}_\Omega^\omega & \varepsilon(\frac{1}{2}I + (\mathcal{K}_D^\omega)^*) & -\varepsilon k(-\frac{1}{2}I + (\mathcal{K}_D^{\frac{\omega}{\sqrt{k}}})^*) \end{pmatrix}.$$

- **Generalized argument principle:**

$$\omega_\varepsilon - \omega_0 = \frac{1}{2\pi i} \operatorname{tr} \int_{\partial V_{\delta_0}} (\omega - \omega_0) \mathcal{A}_\varepsilon(\omega)^{-1} \frac{d}{d\omega} \mathcal{A}_\varepsilon(\omega) d\omega.$$

# Mathematics for photonics

- **Eigenvalue expansion:**

$$\mu_j^\varepsilon - \mu_j = \varepsilon^d \nabla u_j(z) \cdot M \nabla u_j(z) + o(\varepsilon^d).$$

- **Polarization tensor**  $M = (m_{ll'})$ :

$$m_{ll'} = (k-1) \int_{\partial B} \psi_l \frac{\partial x_{l'}}{\partial \nu} d\sigma.$$

$$\begin{cases} \nabla \cdot (1 + (k-1)\chi(B)) \nabla \psi_l = 0 & \text{in } \mathbb{R}^d, \\ \psi_l(x) - x_l = O(|x|^{1-d}) & \text{as } |x| \rightarrow +\infty. \end{cases}$$

- **Eigenfunction expansion** in  $\Omega$ :

$$u_j^\varepsilon(x) = u_j(z) + \varepsilon \sum_{l=1}^d \partial_l u_j(z) \psi_l \left( \frac{x-z}{\varepsilon} \right) + o(\varepsilon).$$

- $u_j^\varepsilon$ : normalized eigenfunction associated with  $\mu_j^\varepsilon$ .

# Mathematics for photonics

- Photonic crystals:
  - Floquet transform:

$$\mathcal{U}[f](x, \alpha) = \sum_{n \in \mathbb{Z}^d} f(x - n) e^{i\alpha \cdot n}.$$

- $f(x)$ : function decaying sufficiently fast.
- $\mathcal{U}$ : analogue of the Fourier transform for the periodic case.
- $\alpha \in \text{Brillouin zone } \mathbb{R}^d / (2\pi\mathbb{Z}^d)$ : quasi-momentum (analogue of the dual variable in the Fourier transform).
- Expansion of a periodic operator  $L$  in  $L^2(\mathbb{R}^d)$  into a direct integral of operators:

$$L = \int_{\mathbb{R}^d / (2\pi\mathbb{Z}^d)}^{\oplus} L(\alpha) d\alpha.$$

- $L(\alpha)[f] = \mathcal{U}[L[f]]$ .

# Mathematics for photonics

- **Spectral theorem** for a **self-adjoint** operator:

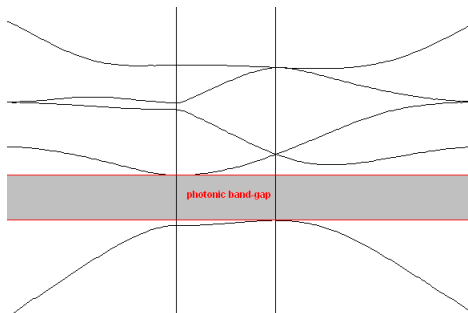
$$\sigma(L) = \bigcup_{\alpha \in \mathbb{R}^d / (2\pi\mathbb{Z}^d)} \sigma(L(\alpha)),$$

- $\sigma(L)$ : spectrum of  $L$ .
- $L$ : **elliptic**  $\rightarrow L(\alpha)$ : **compact resolvents**  $\rightarrow$  **discrete spectra**  $(\mu_l(\alpha))_l$ ,

$$\sigma(L) = \left[ \min_{\alpha} \mu_l(\alpha), \max_{\alpha} \mu_l(\alpha) \right].$$

# Mathematics for photonics

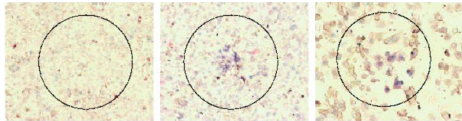
- Gohberg-Sigal theory:
  - Sensitivity analysis of band gaps with respect to changes of the coefficients of  $L$ .
  - Analysis of photonic crystal cavities: defect mode inside the band gap.





# Resonances for plasmonic nanoparticles

- **Gold nano-particles:** accumulate selectively in tumor cells; bio-compatible; reduced toxicity.
- Detection: localized enhancement in radiation dose (strong scattering).
- Ablation: **localized damage** (strong absorption).
- Functionalization: targeted drugs.



M.A. El-Sayed et al.

# Resonances for plasmonic nanoparticles

- Mechanisms of **scattering and absorption enhancements** and **supreresolution** using plasmonic nanoparticles.
- Spectral properties of **Neumann-Poincaré** operator.

# Resonances for plasmonic nanoparticles

- $D$ : nanoparticle in  $\mathbb{R}^d$ ,  $d = 2, 3$ ;  $C^{1,\alpha}$  boundary  $\partial D$ ,  $\alpha > 0$ .
- $\varepsilon_c(\omega)$ : complex permittivity of  $D$ ;  $\varepsilon_m > 0$ : permittivity of the background medium;
- Permittivity contrast:  $\lambda(\omega) = (\varepsilon_c(\omega) + \varepsilon_m)/(2(\varepsilon_c(\omega) - \varepsilon_m))$ .
- **Causality**  $\Rightarrow$  **Kramer-Krönig** relations (**Hilbert** transform),  
 $\varepsilon_c(\omega) = \varepsilon'(\omega) + i\varepsilon''(\omega)$ :

$$\varepsilon'(\omega) - \varepsilon_\infty = -\frac{2}{\pi} \text{p.v.} \int_0^{+\infty} \frac{s\varepsilon''(s)}{s^2 - \omega^2} ds,$$

$$\varepsilon''(\omega) = \frac{2\omega}{\pi} \text{p.v.} \int_0^{+\infty} \frac{\varepsilon'(s) - \varepsilon_\infty}{s^2 - \omega^2} ds.$$

- **Drude** model for the dielectric permittivity  $\varepsilon_c(\omega)$ :

$$\varepsilon_c(\omega) = \varepsilon_\infty \left(1 - \frac{\omega_p^2}{\omega^2 + i\tau\omega}\right), \quad \varepsilon'(\omega) \leq 0 \quad \text{for} \quad \omega \leq \omega_p.$$

$\omega_p$ ,  $\tau$ : positive constants.

# Resonances for plasmonic nanoparticles

- **Fundamental solution** to the Laplacian:

$$G(x) := \begin{cases} \frac{1}{2\pi} \ln |x|, & d = 2, \\ -\frac{1}{4\pi} |x|^{2-d}, & d = 3; \end{cases}$$

- **Single-layer potential**:

$$\mathcal{S}_D[\varphi](x) := \int_{\partial D} G(x-y)\varphi(y) \, ds(y), \quad x \in \mathbb{R}^d.$$

- **Neumann-Poincaré operator**  $\mathcal{K}_D^*$ :

$$\mathcal{K}_D^*[\varphi](x) := \int_{\partial D} \frac{\partial G}{\partial \nu(x)}(x-y)\varphi(y) \, ds(y), \quad x \in \partial D.$$

$\nu$ : normal to  $\partial D$ .

- $\mathcal{K}_D^*$ : **compact operator** on  $L^2(\partial D)$ ,

$$\frac{|\langle x-y, \nu(x) \rangle|}{|x-y|^d} \leq \frac{C}{|x-y|^{d-1-\alpha}}, \quad x, y \in \partial D.$$

- Spectrum of  $\mathcal{K}_D^*$  lies in  $(-\frac{1}{2}, \frac{1}{2}]$  (**Kellog**).

# Resonances for plasmonic nanoparticles

- $\mathcal{K}_D^*$  self-adjoint on  $L^2(\partial D)$  if and only if  $D$  is a disk or a ball.
- **Symmetrization** technique for **Neumann-Poincaré** operator  $\mathcal{K}_D^*$ :
  - **Calderón's** identity:  $\mathcal{K}_D \mathcal{S}_D = \mathcal{S}_D \mathcal{K}_D^*$ ;
  - In three dimensions,  $\mathcal{K}_D^*$ : **self-adjoint** in the Hilbert space  $\mathcal{H}^*(\partial D) = H^{-\frac{1}{2}}(\partial D)$  equipped with

$$(u, v)_{\mathcal{H}^*} = -(u, \mathcal{S}_D[v])_{-\frac{1}{2}, \frac{1}{2}}$$

$(\cdot, \cdot)_{-\frac{1}{2}, \frac{1}{2}}$ : duality pairing between  $H^{-\frac{1}{2}}(\partial D)$  and  $H^{\frac{1}{2}}(\partial D)$ .

- In **two dimensions**:  $\exists! \tilde{\varphi}_0$  s.t.  $\mathcal{S}_D[\tilde{\varphi}_0] = \text{constant on } \partial D$  and  $(\tilde{\varphi}_0, 1)_{-\frac{1}{2}, \frac{1}{2}} = 1$ .  $\mathcal{S}_D \rightarrow \tilde{\mathcal{S}}_D$ :

$$\tilde{\mathcal{S}}_D[\varphi] = \begin{cases} \mathcal{S}_D[\varphi] & \text{if } (\varphi, 1)_{-\frac{1}{2}, \frac{1}{2}} = 0, \\ -1 & \text{if } \varphi = \tilde{\varphi}_0. \end{cases}$$

# Resonances for plasmonic nanoparticles

- **Symmetrization** technique for **Neumann-Poincaré** operator  $\mathcal{K}_D^*$ :
  - Spectrum  $\sigma(\mathcal{K}_D^*)$  **discrete** in  $] -1/2, 1/2[$ ;
  - Ellipse:  $\pm \frac{1}{2}(\frac{a-b}{a+b})^j$ , elliptic harmonics ( $a, b$ : long and short axis).
  - Ball:  $\frac{1}{2(2j+1)}$ , spherical harmonics.
  - **Twin property** in two dimensions;
  - $(\lambda_j, \varphi_j)$ ,  $j = 0, 1, 2, \dots$ : eigenvalue and normalized eigenfunction pair of  $\mathcal{K}_D^*$  in  $\mathcal{H}^*(\partial D)$ ;  $\lambda_j \in (-\frac{1}{2}, \frac{1}{2}]$  and  $\lambda_j \rightarrow 0$  as  $j \rightarrow \infty$ ;
  - $\varphi_0$ : eigenfunction associated to  $1/2$  ( $\tilde{\varphi}_0$  multiple of  $\varphi_0$ );
  - **Spectral decomposition formula** in  $H^{-1/2}(\partial D)$ ,

$$\mathcal{K}_D^*[\psi] = \sum_{j=0}^{\infty} \lambda_j(\psi, \varphi_j)_{\mathcal{H}^*} \varphi_j.$$

# Resonances for plasmonic nanoparticles

- $u^i$ : incident plane wave; **Helmholtz** equation:

$$\begin{cases} \nabla \cdot (\varepsilon_m \chi(\mathbb{R}^d \setminus \bar{D}) + \varepsilon_c(\omega) \chi(\bar{D})) \nabla u + \omega^2 u = 0, \\ u^s := u - u^i \text{ satisfies the outgoing radiation condition.} \end{cases}$$

- **Uniform small volume expansion** with respect to the contrast:

$$D = z + \delta B, \delta \rightarrow 0, |x - z| \gg 2\pi/k_m,$$

$$u^s = -M(\lambda(\omega), D) \nabla_z G_{k_m}(x - z) \cdot \nabla u^i(z) + O\left(\frac{\delta^{d+1}}{\text{dist}(\lambda(\omega), \sigma(\mathcal{K}_D^*))}\right).$$

- $G_{k_m}$ : outgoing fundamental solution to  $\Delta + k_m^2$ ;  $k_m := \omega/\sqrt{\varepsilon_m}$ ;
- **Polarization tensor**:

$$M(\lambda(\omega), D) := \int_{\partial D} x(\lambda(\omega)I - \mathcal{K}_D^*)^{-1}[\nu](x) ds(x).$$

- **Scaling** and **translation** properties:  $M(\lambda(\omega), z + \delta B) = \delta^d M(\lambda(\omega), B)$ .

# Resonances for plasmonic nanoparticles

## Representation by equivalent ellipses and ellipsoids:

- Nanoparticle's permittivity:  $\varepsilon_c(\omega) = \varepsilon'(\omega) + i\varepsilon''(\omega)$ .
- $\varepsilon'(\omega) > 0$  and  $\varepsilon''(\omega) = 0$ : canonical representation; equivalent ellipse or ellipsoid with the same polarization tensor.
- Plasmonic nanoparticles: non Hermitian case.
- $\Im M(\lambda(\omega), D)$ : equivalent frequency depending ellipse or ellipsoid with the same imaginary part of the polarization tensor.



# Resonances for plasmonic nanoparticles

- Spectral decomposition:  $(l, m)$ -entry

$$M_{l,m}(\lambda(\omega), D) = \sum_{j=1}^{\infty} \frac{(\nu_m, \varphi_j)_{\mathcal{H}^*} (\nu_l, \varphi_j)_{\mathcal{H}^*}}{(1/2 - \lambda_j)(\lambda(\omega) - \lambda_j)}.$$

- $(\nu_m, \varphi_0)_{\mathcal{H}^*} = 0$ ;  $\varphi_0$ : eigenfunction of  $\mathcal{K}_D^*$  associated to  $1/2$ .
- **Quasi-static far-field approximation**:  $\delta \rightarrow 0$ ,

$$u^s = -\delta^d \mathbf{M}(\lambda(\omega), B) \nabla_z G_{k_m}(x - z) \cdot \nabla u^i(z) + O\left(\frac{\delta^{d+1}}{\text{dist}(\lambda(\omega), \sigma(\mathcal{K}_D^*))}\right).$$

- **Quasi-static plasmonic resonance**:  $\text{dist}(\lambda(\omega), \sigma(\mathcal{K}_D^*))$  minimal ( $\Re \varepsilon_c(\omega) < 0$ ).

# Resonances for plasmonic nanoparticles

- $M(\lambda(\omega), B) = \left( \frac{\varepsilon_c(\omega)}{\varepsilon_m} - 1 \right) \int_B \nabla v(y) dy$ :

$$\begin{cases} \nabla \cdot \left( \varepsilon_m \chi(\mathbb{R}^d \setminus \bar{B}) + \varepsilon_c(\omega) \chi(\bar{B}) \right) \nabla v = 0, \\ v(y) - y \rightarrow 0, \quad |y| \rightarrow +\infty. \end{cases}$$

- **Corrector**  $v$ :

$$v(y) = y + \mathcal{S}_B(\lambda(\omega)I - \mathcal{K}_B^*)^{-1}[\nu](y), \quad y \in \mathbb{R}^d.$$

- **Inner expansion**:  $\delta \rightarrow 0$ ,  $|x - z| = O(\delta)$ ,

$$u(x) = u^i(z) + \delta v\left(\frac{x - z}{\delta}\right) \cdot \nabla u^i(z) + O\left(\frac{\delta^2}{\text{dist}(\lambda(\omega), \sigma(\mathcal{K}_D^*))}\right).$$

- **Monitoring of temperature elevation due to nanoparticle heating**:

$$\begin{cases} \rho C \frac{\partial T}{\partial t} - \nabla \cdot \tau \nabla T = \frac{\omega}{2\pi} \Im(\varepsilon_c(\omega)) |u|^2 \chi(D), \\ T|_{t=0} = 0. \end{cases}$$

$\rho$ : mass density;  $C$ : thermal capacity;  $\tau$ : thermal conductivity.

# Resonances for plasmonic nanoparticles

- **Scattering amplitude:**

$$u^s(x) = -ie^{-\frac{\pi i}{4}} \frac{e^{ik_m|x|}}{\sqrt{8\pi k_m|x|}} A_\infty[D, \varepsilon_c, \varepsilon_m, \omega](\theta, \theta') + o(|x|^{-\frac{1}{2}}),$$

$|x| \rightarrow \infty$ ;  $\theta, \theta'$ : incident and scattered directions.

- **Scattering cross-section:**

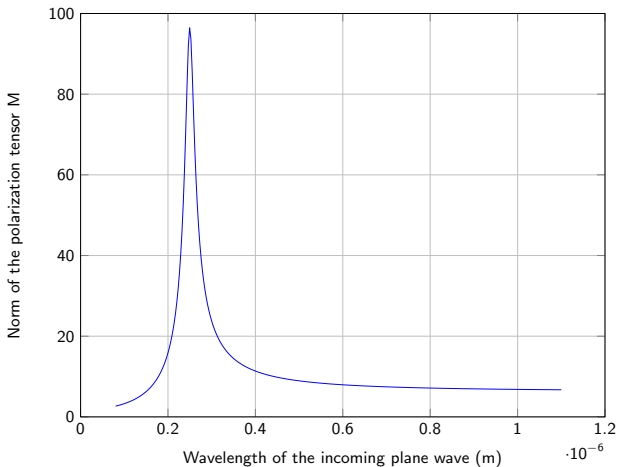
$$Q^s[D, \varepsilon_c, \varepsilon_m, \omega](\theta') := \int_0^{2\pi} \left| A_\infty[D, \varepsilon_c, \varepsilon_m, \omega](\theta, \theta') \right|^2 d\theta.$$

- Enhancement of the **absorption and scattering cross-sections**  $Q^a$  and  $Q^s$  at plasmonic resonances:

$$Q^a + Q^s (= \text{extinction cross-section } Q^e) \propto \Im \text{Trace}(M(\lambda(\omega), D));$$

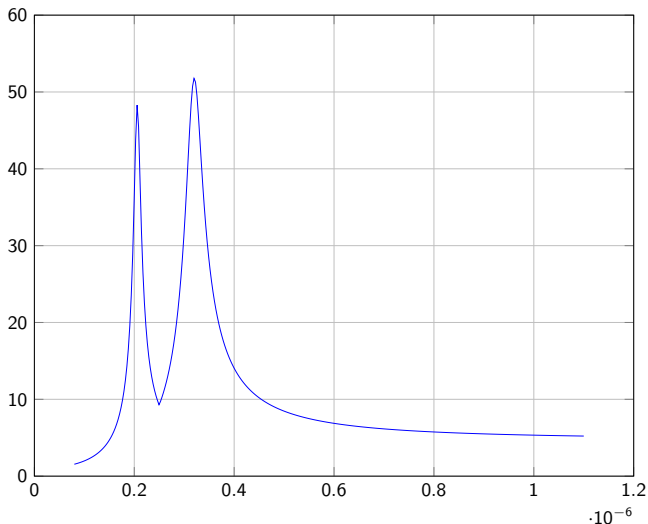
$$Q^s \propto |\text{Trace}(M(\lambda(\omega), D))|^2.$$

# Resonances for plasmonic nanoparticles



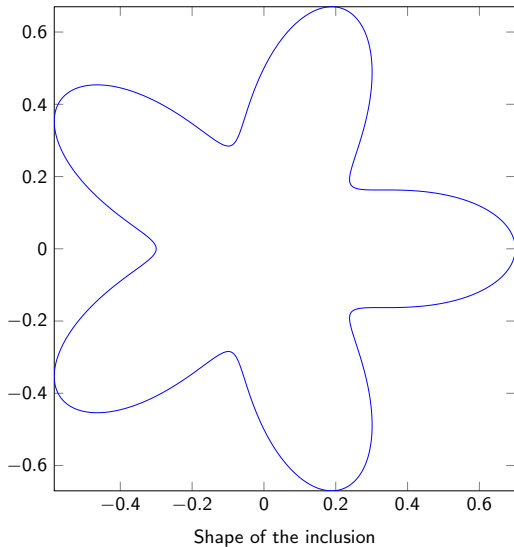
Norm of the polarization tensor for a circular inclusion.

# Resonances for plasmonic nanoparticles

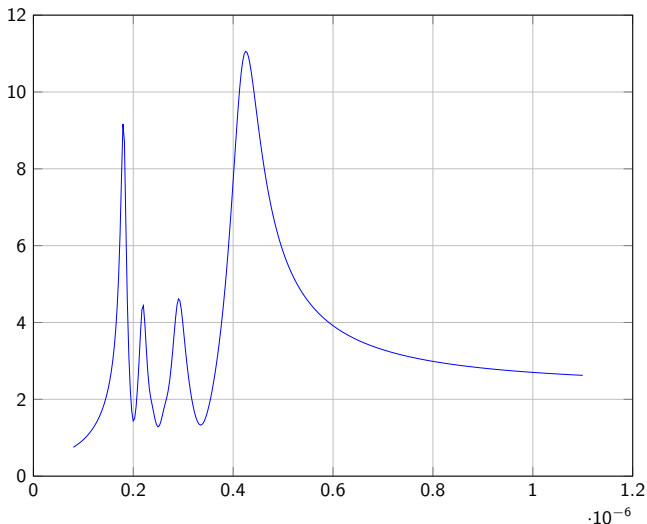


Norm of the polarization tensor for an elliptic inclusion.

# Resonances for plasmonic nanoparticles



# Resonances for plasmonic nanoparticles



Norm of the polarization tensor for a flower-shaped inclusion.

# Resonances for plasmonic nanoparticles

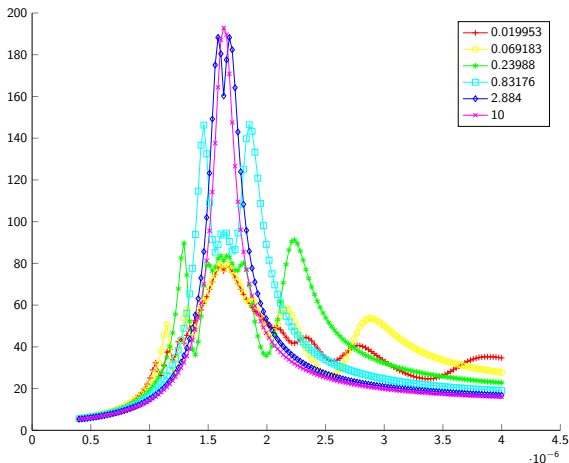
- Quasi-plasmonic resonances for **multiple particles**:  $D_1$  and  $D_2$ :  $C^{1,\alpha}$ -bounded domains;  $\text{dist}(D_1, D_2) > 0$ ;  $\nu^{(1)}$  and  $\nu^{(2)}$ : outward normal vectors at  $\partial D_1$  and  $\partial D_2$ .
- **Neumann-Poincaré** operator  $\mathbb{K}_{D_1 \cup D_2}^*$  associated with  $D_1 \cup D_2$ :

$$\mathbb{K}_{D_1 \cup D_2}^* := \begin{pmatrix} \mathcal{K}_{D_1}^* & \frac{\partial}{\partial \nu^{(1)}} \mathcal{S}_{D_2} \\ \frac{\partial}{\partial \nu^{(2)}} \mathcal{S}_{D_1} & \mathcal{K}_{D_2}^* \end{pmatrix}.$$

- **Symmetrization** of  $\mathbb{K}_{D_1 \cup D_2}^*$ .
- Behavior of the eigenvalues of  $\mathbb{K}_{D_1 \cup D_2}^*$  as  $\text{dist}(D_1, D_2) \rightarrow 0$ .



# Resonances for plasmonic nanoparticles



Norm of the polarization tensor for two disks for various separating distances.

# Resonances for plasmonic nanoparticles

- **Algebraic domains:** **finite number** of quasi-static plasmonic resonances:

$$\#\{j : (\nu_l, \varphi_j)_{\mathcal{H}^*} \neq 0\} : \text{finite.}$$

- Algebraic domains: **zero level sets of polynomials**; **dense** in Hausdorff metric among all planar domains.
- Blow-up of the polarization tensor for **finite number** of eigenvalues of the **Neumann-Poincaré** operator:

$$M_{l,m}(\lambda(\omega), D) = \sum_{j=1}^{\infty} \frac{(\nu_m, \varphi_j)_{\mathcal{H}^*} (\nu_l, \varphi_j)_{\mathcal{H}^*}}{(1/2 - \lambda_j)(\lambda(\omega) - \lambda_j)}.$$

- Two nearly touching disks: **infinite number** of quasi-static plasmonic resonances.

$$\lambda_j = \pm \frac{1}{2} e^{-2|j|\xi}, \xi = \sinh^{-1} \left( \sqrt{\frac{\delta}{r} \left(1 + \frac{\delta}{4r}\right)} \right);$$

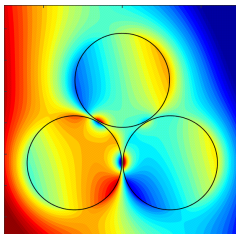
- $r$ : radius of the disks;  $\delta$ : separating distance.
- Separating distance  $\delta$  : estimated from the first plasmonic resonance (associated to  $\lambda_1$ ).

# Resonances for plasmonic nanoparticles

- **Singular** nature of the **interaction** between nearly touching plasmonic nanoparticles.
- Applications in nanosensing (beyond the resolution limit).
- **Blow-up** of  $\nabla u$  between the disks at plasmonic resonances:

$$\nabla u \propto \frac{r}{\Im(\lambda(\omega))\delta} e^{-2|j|\xi}.$$

- Accurate scheme for computing the field distribution between an arbitrary number of nearly touching plasmonic nanospheres: **transformation optics** + **method of image charges**.



# Resonances for plasmonic nanoparticles

- $(m, l)$ -entry of the polarization tensor  $M$ :

$$M_{l,m}(\lambda(\omega), D) = \sum_{j=1}^{\infty} \frac{\alpha_{l,m}^{(j)}}{\lambda(\omega) - \lambda_j},$$

$$\alpha_{l,m}^{(j)} := \frac{(\nu_m, \varphi_j) \mathcal{H}^*(\nu_l, \varphi_j) \mathcal{H}^*}{(1/2 - \lambda_j)}, \quad \alpha_{l,l}^{(j)} \geq 0, \quad j \geq 1.$$

- **Sum rules** for the polarization tensor:

$$\sum_{j=1}^{\infty} \alpha_{l,m}^{(j)} = \delta_{l,m} |D|; \quad \sum_{j=1}^{\infty} \lambda_j \sum_{l=1}^d \alpha_{l,l}^{(j)} = \frac{(d-2)}{2} |D|.$$

$$\sum_{j=1}^{\infty} \lambda_j^2 \sum_{l=1}^d \alpha_{l,l}^{(j)} = \frac{(d-4)}{4} |D| + \sum_{l=1}^d \int_D |\nabla \mathcal{S}_D[\nu_l]|^2 dx.$$

- $f$  holomorphic function in an open set  $U \subset \mathbb{C}$  containing  $\sigma(\mathcal{K}_D^*)$ :

$$f(\mathcal{K}_D^*) = \sum_{j=1}^{\infty} f(\lambda_j) (\cdot, \varphi_j) \mathcal{H}^* \varphi_j.$$

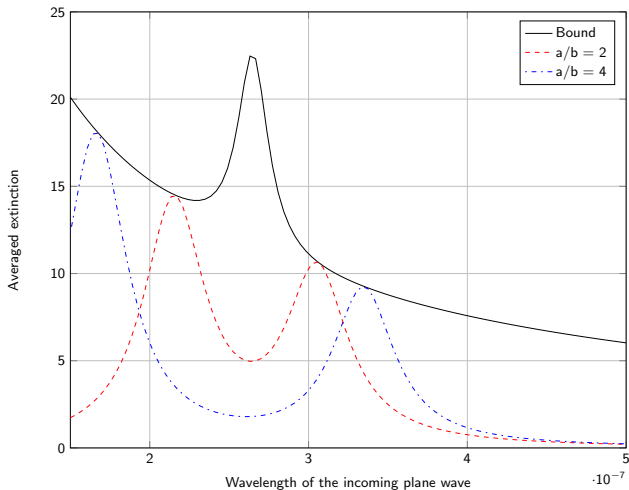
# Resonances for plasmonic nanoparticles

- **Upper bound** for the **averaged extinction cross-section**  $Q_m^e$  of a randomly oriented nanoparticle:

$$\begin{aligned} |\Im(\text{Trace}(M(\lambda, D)))| &\leq \frac{d|\lambda''||D|}{\lambda'^2 + 4\lambda'^2} \\ &+ \frac{1}{|\lambda''|(\lambda'^2 + 4\lambda'^2)} \left( d\lambda'^2 |D| + \frac{(d-4)}{4} |D| \right) \\ &+ \sum_{l=1}^d \int_D |\nabla S_D[\nu_l]|^2 dx + 2\lambda' \frac{(d-2)}{2} |D| + O\left(\frac{\lambda'^2}{4\lambda'^2 + \lambda'^2}\right). \end{aligned}$$

$$\lambda' = \Re\lambda, \lambda'' = \Im\lambda.$$

# Resonances for plasmonic nanoparticles



# Resonances for plasmonic nanoparticles

**Hadamard's formula** for  $\mathcal{K}_D^*$ :

- $\partial D$ : class  $\mathcal{C}^2$ ;  $\partial D := \{x = X(t), t \in [a, b]\}$ .
- $\Psi_\eta : \partial D \mapsto \partial D_\eta := \{x + \eta h(t)\nu(x)\}$ ;  $\Psi_\eta$ : diffeomorphism.
- **Hadamard's** formula for  $\mathcal{K}_D^*$ :

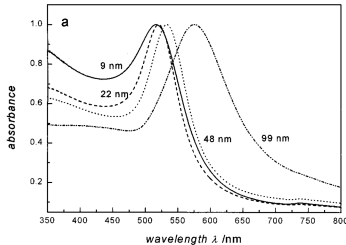
$$\|\mathcal{K}_{D_\eta}^*[\tilde{\phi}] \circ \Psi_\eta - \mathcal{K}_D^*[\phi] - \eta \mathcal{K}_D^{(1)}[\phi]\|_{L^2(\partial D)} \leq C\eta^2 \|\phi\|_{L^2(\partial D)},$$

$C$ : depends only on  $\|X\|_{\mathcal{C}^2}$  and  $\|h\|_{\mathcal{C}^1}$ ;  $\phi := \tilde{\phi} \circ \Psi_\eta$ .

- $\mathcal{K}_D^{(1)}$ : explicit kernel.
- **Hadamard's formula for the eigenvalues** of  $\mathcal{K}_D^*$ .
- **Shape derivative of plasmonic resonances** for nanoparticles.
- Generalization to **3D**.

# Resonances for plasmonic nanoparticles

- $\mathcal{K}_D^*$ : scale invariant  $\Rightarrow$  Quasi-static plasmonic resonances: **size independent**.
- Analytic formula for the **first-order correction** to quasi-static plasmonic resonances in terms of the particle's characteristic size  $\delta$ :



M.A. El-Sayed et al.



# Resonances for plasmonic nanoparticles

- **Helmholtz** equation:

$$\begin{cases} \nabla \cdot (\varepsilon_m \chi(\mathbb{R}^d \setminus \bar{D}) + \varepsilon_c(\omega) \chi(\bar{D})) \nabla u + \omega^2 u = 0, \\ u^s := u - u^i \text{ satisfies the outgoing radiation condition.} \end{cases}$$

$u^i$ : incident plane wave;  $k_m := \omega \sqrt{\varepsilon_m}$ ,  $k_c := \omega \sqrt{\varepsilon_c(\omega)}$ .

- **Integral formulation** on  $\partial D$ :

$$\begin{cases} \mathcal{S}_D^{k_c}[\phi] - \mathcal{S}_D^{k_m}[\psi] = u^i, \\ \varepsilon_c \left( \frac{1}{2} - (\mathcal{K}_D^{k_c})^* \right) [\phi] - \varepsilon_m \left( \frac{1}{2} + (\mathcal{K}_D^{k_m})^* \right) [\psi] = \varepsilon_m \partial u^i / \partial \nu. \end{cases}$$

- **Operator-Valued function**  $\delta \mapsto \mathcal{A}_\delta(\omega) \in \mathcal{L}(\mathcal{H}^*(\partial B), \mathcal{H}^*(\partial B))$ :

$$\mathcal{A}_\delta(\omega) = \overbrace{(\lambda(\omega)I - \mathcal{K}_B^*)}^{\mathcal{A}_0(\omega)} + (\omega\delta)^2 \mathcal{A}_1(\omega) + O((\omega\delta)^3).$$

- **Quasi-static limit**:

$$\mathcal{A}_0(\omega)[\psi] = \sum_{j=0}^{\infty} \tau_j(\omega) (\psi, \varphi_j)_{\mathcal{H}^*} \varphi_j, \quad \tau_j(\omega) := \frac{1}{2} (\varepsilon_m + \varepsilon_c(\omega)) - (\varepsilon_c(\omega) - \varepsilon_m) \lambda_j.$$

# Resonances for plasmonic nanoparticles

- Shift in the plasmonic resonance:

$$\arg \min_{\omega} \left| \frac{1}{2} (\varepsilon_m + \varepsilon_c(\omega)) - (\varepsilon_c(\omega) - \varepsilon_m) \lambda_j + (\omega \delta)^2 \tau_{j,1} \right|$$

- $\tau_{j,1} := (\mathcal{A}_1(\omega)[\varphi_j], \varphi_j)_{\mathcal{H}^*}$ .
- Gohberg-Sigal theory.

# Resonances for plasmonic nanoparticles

- Full Maxwell's equations:

$$\begin{cases} \nabla \times \nabla \times E - \omega^2 \left( \varepsilon_m \chi(\mathbb{R}^d \setminus \bar{D}) + \varepsilon_c(\omega) \chi(\bar{D}) \right) E = 0, \\ E^s := E - E^i \text{ satisfies the outgoing radiation condition.} \end{cases}$$

- Small-volume expansion:

$$E^s(x) = -\delta^3 \omega^2 G_{k_m}(x, z) M(\lambda(\omega), B) E^i(z) + O\left(\frac{\delta^4}{\text{dist}(\lambda(\omega), \sigma(\mathcal{K}_D^*))}\right)$$

- $G_{k_m}$ : fundamental (outgoing) solution to Maxwell's equations in free space.
- **Shift** in the plasmonic resonances due to the finite size of the nanoparticle.

# Resonances for plasmonic nanoparticles

- **Integral formulation:**

$$\begin{pmatrix} I + \mathcal{M}_D^{k_c} - \mathcal{M}_D^{k_m} & \mathcal{L}_D^{k_c} - \mathcal{L}_D^{k_m} \\ \mathcal{L}_D^{k_c} - \mathcal{L}_D^{k_m} & \frac{1}{2}(k_c^2 + k_m^2)I + k_c^2 \mathcal{M}_D^{k_c} - k_m^2 \mathcal{M}_D^{k_m} \end{pmatrix}$$

- **Integral operators:**

$$\begin{aligned} \mathcal{M}_D^k[\varphi] : H_T^{-\frac{1}{2}}(\text{div}, \partial D) &\longrightarrow H_T^{-\frac{1}{2}}(\text{div}, \partial D) \quad (\text{compact}) \\ \varphi &\longmapsto \int_{\partial D} \nu(x) \times \nabla_x \times G_k(x, y) \varphi(y) ds(y); \end{aligned}$$

$$\begin{aligned} \mathcal{L}_D^k[\varphi] : H_T^{-\frac{1}{2}}(\text{div}, \partial D) &\longrightarrow H_T^{-\frac{1}{2}}(\text{div}, \partial D) \\ \varphi &\longmapsto \nu(x) \times \left( k^2 \mathcal{S}_D^k[\varphi](x) + \nabla \mathcal{S}_D^k[\nabla_{\partial D} \cdot \varphi](x) \right). \end{aligned}$$

- **Key identities:**  $\mathcal{M}_D^{k=0}[\text{curl}_{\partial D} \varphi] = \text{curl}_{\partial D} \mathcal{K}_D[\varphi], \quad \forall \varphi \in H^{\frac{1}{2}}(\partial D),$

$$\mathcal{M}_D^{k=0}[\nabla_{\partial D} \varphi] = -\nabla_{\partial D} \Delta_{\partial D}^{-1} \mathcal{K}_D^*[\Delta_{\partial D} \varphi] + \mathcal{R}_D[\varphi],$$

$$\mathcal{R}_D = -\text{curl}_{\partial D} \Delta_{\partial D}^{-1} \text{curl}_{\partial D} \mathcal{M}_D \nabla_{\partial D}, \quad \forall \varphi \in H^{\frac{3}{2}}(\partial D).$$

# Resonances for plasmonic nanoparticles

- Quasi-static approximation:

$$\widetilde{\mathcal{M}}_B = \begin{pmatrix} -\Delta_{\partial B}^{-1} \mathcal{K}_B^* \Delta_{\partial B} & 0 \\ \mathcal{R}_B & \mathcal{K}_B \end{pmatrix}.$$

- $H(\partial B) := H_0^{\frac{3}{2}}(\partial B) \times H^{\frac{1}{2}}(\partial B)$ , equipped with the inner product

$$(u, v)_{H(\partial B)} = (\Delta_{\partial B} u^{(1)}, \Delta_{\partial B} v^{(1)})_{\mathcal{H}^*} + (u^{(2)}, v^{(2)})_{\mathcal{H}},$$

$$(u, v)_{\mathcal{H}^*} := -(u, \mathcal{S}_D[v])_{-\frac{1}{2}, \frac{1}{2}}, \quad (u, v)_{\mathcal{H}} = -(\mathcal{S}_D^{-1}[u], v)_{-\frac{1}{2}, \frac{1}{2}}.$$

- The spectrum  $\sigma(\widetilde{\mathcal{M}}_B) = \sigma(-\mathcal{K}_B^*) \cup \sigma(\mathcal{K}_B^*) \setminus \{-\frac{1}{2}\}$  in  $H(\partial B)$ .
- Only  $\sigma(\mathcal{K}_B^*)$  can be excited in the quasi-static approximation.

# Scattering coefficients

- Scattering coefficients: cloaking structures and dictionary matching approach for inverse scattering.
- Mechanism underlying plasmonic resonances in terms of the scattering coefficients corresponding to the nanoparticle.
- Scattering coefficients of order  $\pm 1$ : only scattering coefficients inducing the scattering-cross section enhancement.

# Scattering coefficients

- **Helmholtz** equation:

$$\begin{cases} \nabla \cdot (\varepsilon_m \chi(\mathbb{R}^d \setminus \bar{D}) + \varepsilon_c(\omega) \chi(\bar{D})) \nabla u + \omega^2 u = 0, \\ u^s := u - u^i \text{ satisfies the outgoing radiation condition.} \end{cases}$$

$u^i$ : incident plane wave;  $k_m := \omega \sqrt{\varepsilon_m}$ ,  $k_c := \omega \sqrt{\varepsilon_c(\omega)}$ .

- **Scattering coefficients**:

$$W_{mn}(D, \varepsilon_c, \varepsilon_m, \omega) = \int_{\partial D} \psi_m(y) J_n(\omega|y|) e^{-in\theta_y} ds(y).$$

- $\psi_m$ : electric current density on  $\partial D$  induced by the **cylindrical wave**  $J_m(\omega|x|)e^{im\theta_x}$ .
- $J_n$ : **Bessel** function.

# Scattering coefficients

## Properties of the scattering coefficients:

- $W_{mn}$  decays rapidly:

$$|W_{mn}| \leq \frac{O(\omega^{|m|+|n|})}{\min |\tau_j(\omega)|} \frac{C^{|m|+|n|}}{|m|!|n|!}, \quad m, n \in \mathbb{Z},$$

$C$ : independent of  $\omega$ ;  $\tau_j = \frac{1}{2}(\varepsilon_m + \varepsilon_c(\omega)) - (\varepsilon_c(\omega) - \varepsilon_m)\lambda_j$ .

- For any  $z \in \mathbb{R}^2, \theta \in [0, 2\pi), s > 0$ ,

$$W_{mn}(D^z) = \sum_{m', n' \in \mathbb{Z}} J_{n'}(\omega|z|) J_{m'}(\omega|z|) e^{i(m'-n')\theta_z} W_{m-m', n-n'}(D),$$

$$W_{mn}(D^\theta) = e^{i(m-n)\theta} W_{mn}(D),$$

$$W_{mn}(D^s, \omega) = W_{mn}(D, s\omega).$$



# Scattering coefficients

- **Scattering amplitude:**

$$u^s(x) = -ie^{-\frac{\pi i}{4}} \frac{e^{ik_m|x|}}{\sqrt{8\pi k_m|x|}} A_\infty[D, \varepsilon_c, \varepsilon_m, \omega](\theta, \theta') + o(|x|^{-\frac{1}{2}}),$$

$|x| \rightarrow \infty$ ;  $\theta, \theta'$ : incident and scattered directions.

- **Graf's formula:**

$$A_\infty[D, \varepsilon_c, \varepsilon_m, \omega](\theta, \theta') = \sum_{n,m \in \mathbb{Z}} (-i)^n i^m e^{in\theta'} W_{nm}(D, \varepsilon_c, \varepsilon_m, \omega) e^{-im\theta}.$$

- **Scattering cross-section:**

$$Q^s[D, \varepsilon_c, \varepsilon_m, \omega](\theta') := \int_0^{2\pi} \left| A_\infty[D, \varepsilon_c, \varepsilon_m, \omega](\theta, \theta') \right|^2 d\theta.$$

# Cloaking: scattering coefficient cancellation

- **Cloaking**: make a target **invisible** when **probed** by electromagnetic waves.
- **Scattering coefficient cancellation** technique:
  - **Small layered** object with vanishing first-order scattering coefficients.
  - **Transformation optics**:

$$(F_\rho)_*[\phi](y) = \frac{DF_\rho(x)\phi(x)DF_\rho(x)^t}{\det(DF_\rho(x))}, \quad x = F_\rho^{-1}(y).$$

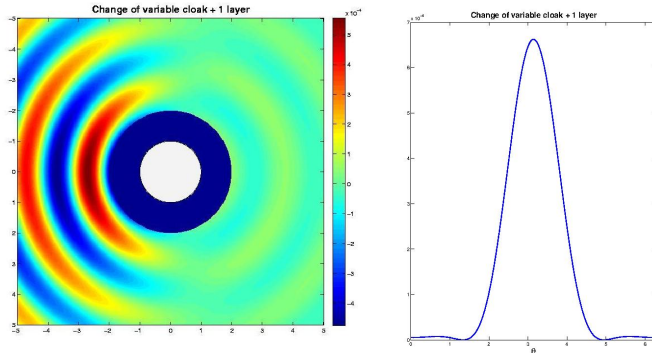
- Change of variables  $F_\rho$  sends the annulus  $[\rho, 2\rho]$  onto a fixed annulus.
- **Scattering coefficients vanishing structures** of order  $N$ :

$$Q^s \left[ D, (F_\rho)_*(\varepsilon \circ \Psi_{\frac{1}{\rho}}), \varepsilon_m, \omega \right] (\theta') = o(\rho^{4N}), \quad \Psi_{1/\rho}(x) = (1/\rho)x.$$

$\rho$ : **size of the small object**;  $N$ : **number of layers**.

- **Anisotropic** permittivity distribution.
- Invisibility at  $\omega \Rightarrow$  invisibility at all frequencies  $\leq \omega$ .

# Cloaking: scattering coefficient cancellation



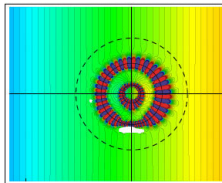
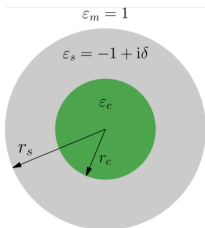
Cancellation of the scattered field and the scattering cross-section: 4 orders of magnitude (with wavelength of order 1,  $\rho = 10^{-1}$ , and  $N = 1$ ).

# Cloaking: anomalous resonance

- $\Omega$ : bounded domain in  $\mathbb{R}^2$ ;  $D \Subset \Omega$ .  $\Omega$  and  $D$  of class  $\mathcal{C}^{1,\mu}$ ,  $0 < \mu < 1$ . For a given loss parameter  $\delta > 0$ , the permittivity distribution in  $\mathbb{R}^2$  is given by

$$\varepsilon_\delta = \begin{cases} 1 & \text{in } \mathbb{R}^2 \setminus \overline{\Omega}, \\ -1 + i\delta & \text{in } \Omega \setminus \overline{D}, \\ 1 & \text{in } D. \end{cases}$$

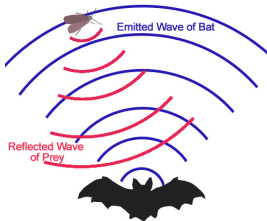
- Configuration (**plasmonic structure**): core with permittivity 1 coated by the shell  $\Omega \setminus \overline{D}$  with permittivity  $-1 + i\delta$ .



# Dictionary matching approach

## Dictionary matching approach:

- Form an image from the **echo** due to targets.
- Identify and **classify** the target, knowing by advance that it belongs to a **learned dictionary of shapes**.
  - Extract the **features** from the data.
  - Construct **invariants** with respect to rigid transformations and scaling.
  - Compare the invariants with precomputed ones for the **dictionary**.



# Dictionary matching approach

- **Feature extraction:**
  - Extract  $\mathbf{W}$  by solving a least-squares method

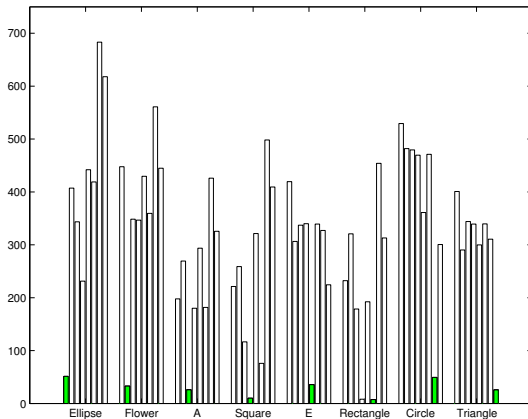
$$\mathbf{W} = \arg \min_{\mathbf{W}} \|\mathbf{L}(\mathbf{W}) - \mathbf{V}\|.$$

- $\mathbf{L}$  is ill-conditioned ( $\mathbf{W}$  decays rapidly).
- **Maximum resolving order  $K$ :**

$$K^{K+1/2} = C(\omega)\text{SNR}.$$

- Form a **multi-frequency shape descriptor**.
- Match in a **multi-frequency dictionary**.

# Dictionary matching approach



Shape descriptor matching in a multi-frequency dictionary.

# Resonances for plasmonic nanoparticles

- Asymptotic expansion of the scattering amplitude:

$$A_\infty \left( \frac{x}{|x|}, d \right) = \frac{x}{|x|}^t W_1 d + O(\omega^2),$$

$d$ : incident direction;  $x/|x|$ : observation direction;

$$W_1 = \begin{pmatrix} W_{-11} + W_{1-1} - 2W_{11} & i(W_{1-1} - W_{-11}) \\ i(W_{1-1} - W_{-11}) & -W_{-11} - W_{1-1} - 2W_{11} \end{pmatrix}.$$

- Blow up of the scattering coefficients:

$$W_{\pm 1 \pm 1} = \pm \pm \frac{k_m^2}{4} \frac{(\varphi_j, |x| e^{\mp i \theta_x})_{-\frac{1}{2}, \frac{1}{2}} (e^{\pm i \theta_\nu}, \varphi_j)_{\mathcal{H}^*}}{\lambda - \lambda_j} + O(1).$$



# Super-resolution

- Super-resolution for **plasmonic nanoparticles**:
  - **Sub-wavelength resonators**;
  - **High contrast: effective medium theory**;
  - **Single nanoparticle imaging**.

# Super-resolution

- **Resolution**: determined by the behavior of the **imaginary part of the Green function**. **Helmholtz-Kirchhoff identity**:

$$\Im G_{k_m}(x, x_0) = k_m \int_{|y|=R} \overline{G_{k_m}(y, x_0)} G_{k_m}(x, y) ds(y), \quad R \rightarrow +\infty.$$

- **The sharper** is  $\Im G_{k_m}$ , the better is the resolution.
- **Local resonant media** used to make shape peaks of  $\Im G_{k_m}$ .
- Mechanism of **super-resolution** in **resonant media**:
  - Interaction of the point source  $x_0$  with the resonant structure excites **high-modes**.
  - Resonant modes encode the information about the point source and can **propagate** into the **far-field**.
  - Super-resolution: only limited by the **resonant structure** and the **signal-to-noise ratio** in the data.

# Super-resolution

- System of **weakly coupled plasmonic nanoparticles**.
- Size of the nanoparticle  $\delta \ll$  wavelength  $2\pi/k_m$ ; distance between the nanoparticles of order one.
- $\Im G^\delta = \Im G_{k_m} +$  exhibits **sub-wavelength peak with width of order one**.
- Break the resolution limit.



S. Nicosia & C. Ciraci, Cover, Science 2012

# Super-resolution

- Sub-wavelength resonator:



M. Fink et al.

- Asymptotic expansion of the Green function ( $\delta$ : size of the resonator openings;  $z_j$ : center of aperture for  $j$ th resonator;  $J$ : number of resonators;  $\omega = O(\sqrt{\delta})$ ):

$$\Im m G^\delta(x, x_0, \omega) \approx \frac{\sin \omega |x - x_0|}{2\pi |x - x_0|} + \sqrt{\delta} \sum_{j=1}^J \frac{c_j}{|x - z_j| |x_0 - z_j|}.$$

# Super-resolution

- Effective medium theory:

$$\varepsilon_{\text{eff}}(\omega) = \varepsilon_m \left( I + f M(\lambda(\omega), B) \left( I - \frac{f}{3} M(\lambda(\omega), B) \right)^{-1} \right) + O\left( \frac{f^{8/3}}{\text{dist}(\lambda(\omega), \sigma(\mathcal{K}_D^*))^2} \right).$$

- $f$ : volume fraction;  $B$ : rescaled particle.
- $\varepsilon_{\text{eff}}(\omega)$ : **anisotropic**.
- Validity of the effective medium theory:

$$f \ll \text{dist}(\lambda(\omega), \sigma(\mathcal{K}_D^*))^{3/5}.$$

# Super-resolution

- **High contrast** effective medium at plasmonic resonances:

$$\nabla \times \nabla \times E - \omega^2 \left( \varepsilon_m \chi(\mathbb{R}^d \setminus \bar{\Omega}) + \varepsilon_{\text{eff}}(\omega) \chi(\bar{\Omega}) \right) E = 0.$$

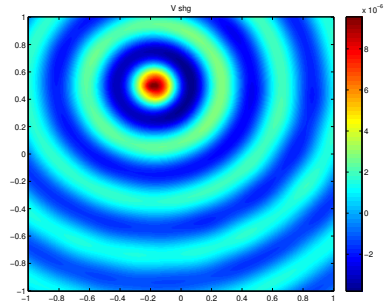
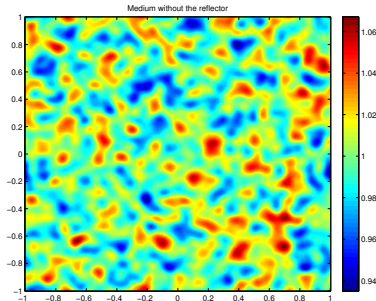
- $E|_{\Omega} \mapsto \int_{\Omega} (\varepsilon_{\text{eff}}(\omega) - \varepsilon_m) E(y) G_{k_m}(x, y) dy, \quad x \in \Omega.$
- **Mixing of resonant modes**: intrinsic nature of **non-hermitian** systems.
- **Sub-wavelength resonance modes** excited  $\Rightarrow$  dominate over the other ones in the expansion of the Green function.
- **Imaginary part of the Green function** may have sharper peak than the one of  $G$  due to the excited **sub-wavelength resonant modes**.
- Sub-wavelength modes: determine the super-resolution.

# Super-resolution

- Single nanoparticle imaging:

$$\max_{z^S} I(z^S, \omega)$$

- $I(z^S, \omega)$ : imaging functional;  $z^S$ : search point.
- Resolution: limited only by the signal-to-noise-ratio.
- Cross-correlation techniques: robustness with respect to medium noise.



# Plan

- Part I: **Mathematical and computational tools**
  - Gohberg-Sigal theory
  - Layer potentials, Green's functions (free space, grating, quasi-periodic), integral formulations, Helmholtz-Kirchhoff identities, scattering coefficients, Floquet theory, Muller's method, Ewald's method for grating and quasi-periodic Green's functions.
- Part II: **Diffraction gratings and photonic crystals**
  - Diffraction gratings: radiation condition, existence and uniqueness of a solution, optimal design problem.
  - Photonic crystals: sensitivity of band gaps, analysis of photonic crystal cavities.



# Plan

- Part III: **Sub-wavelength resonators and super-resolution**
  - Plasmonic nanoparticles.
  - Scattering and absorption enhancement.
  - Resolution enhancement.
  - Super-resolution in high contrast media.
  - Effective medium theory for sub-wavelength resonators.
  - Near-field optics.
- Part IV: **Metamaterials, metasurfaces, and sub-wavelength photonic crystals**
  - Metamaterials and cloaking.
  - Metasurfaces with superabsorption effect: layers of periodically distributed plasmonic nanoparticles.
  - Sub-wavelength photonic crystals.

# Plan

- Part V: Minnaert bubbles
  - Minnaert resonance for bubbles.
  - Acoustic metasurfaces.
  - Effective medium theory and super-resolution.
  - Sub-wavelength phononic crystals.
  - Double-negative acoustic metamaterials.