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LIA ALPhA

Spectral expansions of open and dispersive optical systems: Gaussian regularization and convergence

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http://www.fresnel.fr/perso/stout/

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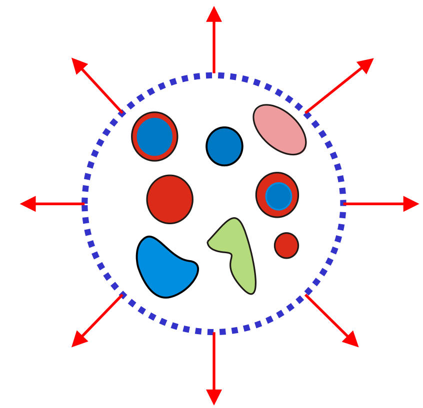
Construct open system response functions using Resonant States (QNMs)

Maxwell electromagnetic equation :

$$(\mathbb{L} - \omega\Gamma_\omega)|\Psi\rangle = -i|J\rangle$$

$$|\Psi\rangle = \begin{pmatrix} \vec{\boldsymbol{E}}(\vec{\boldsymbol{r}},\omega) \\ \vec{\boldsymbol{H}}(\vec{\boldsymbol{r}},\omega) \end{pmatrix}, \quad \mathbb{L} = ic\begin{pmatrix} 0 & \nabla\times \\ \nabla\times & 0 \end{pmatrix}, \quad \Gamma_\omega \equiv \begin{pmatrix} \overleftrightarrow{\varepsilon}(\vec{\boldsymbol{r}},\omega) & 0 \\ 0 & -\overleftrightarrow{\mu}(\vec{\boldsymbol{r}},\omega) \end{pmatrix}$$

Outgoing boundary conditions



Response function : $\mathbb{G}$

$$|\Psi\rangle = -i(\mathbb{L} - \omega\Gamma_\omega)^{-1}|J\rangle \equiv -\mathbb{G}|J\rangle$$

Resonant States : $|\Psi_\alpha\rangle$

$$\mathbb{L}|\Psi_\alpha\rangle = \omega_\alpha\Gamma_\alpha|\Psi_\alpha\rangle$$

$$\omega_\alpha = \omega'_\alpha + i\omega''_\alpha$$

$$\alpha = -\infty, \dots, -1, 0, 1, 2, \dots, \infty$$

$$\mathbb{G} = i\sum_\alpha \frac{1}{\langle\Psi_\alpha|\left[\frac{d}{d\omega}\omega\Gamma_\omega\right]_{\omega_\alpha}|\Psi_\alpha\rangle} \frac{|\Psi_\alpha\rangle\langle\Psi_\alpha|}{\omega - \omega_\alpha} + \mathbb{G}_{\text{n.r.}}$$

Construct the response operator $\mathbb{G}$ (Green's "function")

$$\mathbb{G} = (\mathbb{L} - \omega\Gamma_\omega)^{-1} \quad \Longrightarrow \quad \mathbb{G} = i \sum_{\alpha=-L_{\max}}^{L_{\max}} \frac{1}{\langle\Psi_\alpha| \left[\frac{d}{d\omega}\omega\Gamma_\omega\right]_{\omega_\alpha} |\Psi_\alpha\rangle} \frac{|\Psi_\alpha\rangle\langle\Psi_\alpha|}{\omega - \omega_\alpha} + \mathbb{G}_{\text{n.r.}}$$

$$L_{\max} = \infty$$

Three important problems must be resolved :

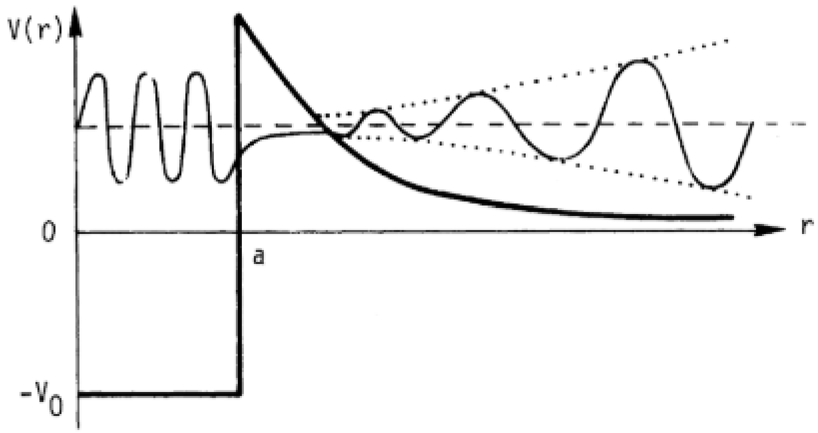
1) Render $\langle\Psi_\alpha| \left[\frac{d}{d\omega}\omega\Gamma_\omega\right]_{\omega_\alpha} |\Psi_\alpha\rangle$ well defined (normalization)

2) Determine the non-resonant contribution $\mathbb{G}_{\text{n.r.}}$?

3) Truncate the RS expansion ($L_{\max}$ finite) in a meaningful manner

Why are Resonant States scalar products, $\langle \Psi_\alpha | \hat{\Gamma} | \Psi_\beta \rangle$, problematic ?

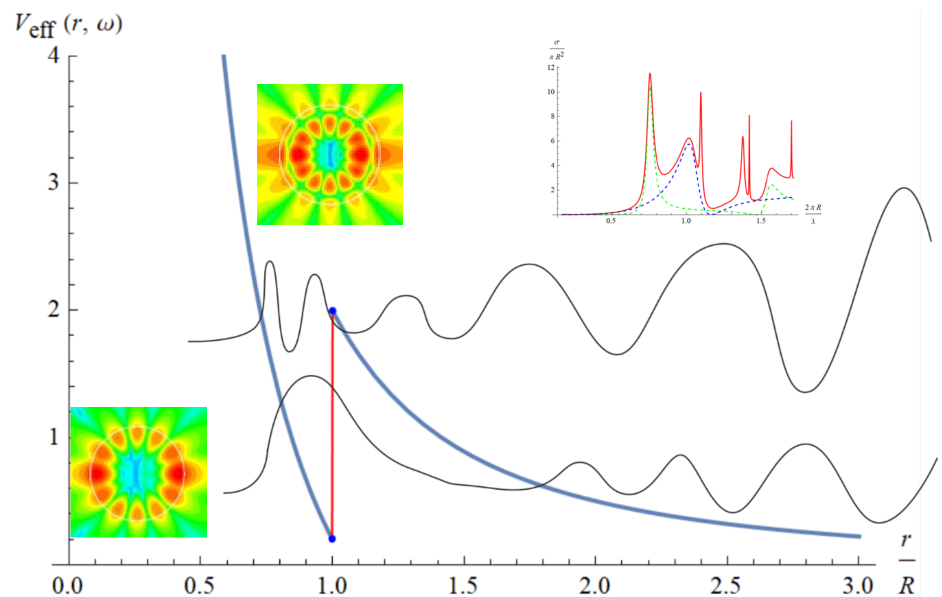
Gamow theory α-decay



Complex energy : $E_q = E'_q + iE''_q$

"… for the running wave the amplitude in the direction of the diverging wave will increase. This means nothing more than that if the vibrations are damped at the source of the wave, the amplitude of the wave segment that left earlier must be larger."

Dielectrics light scatterering

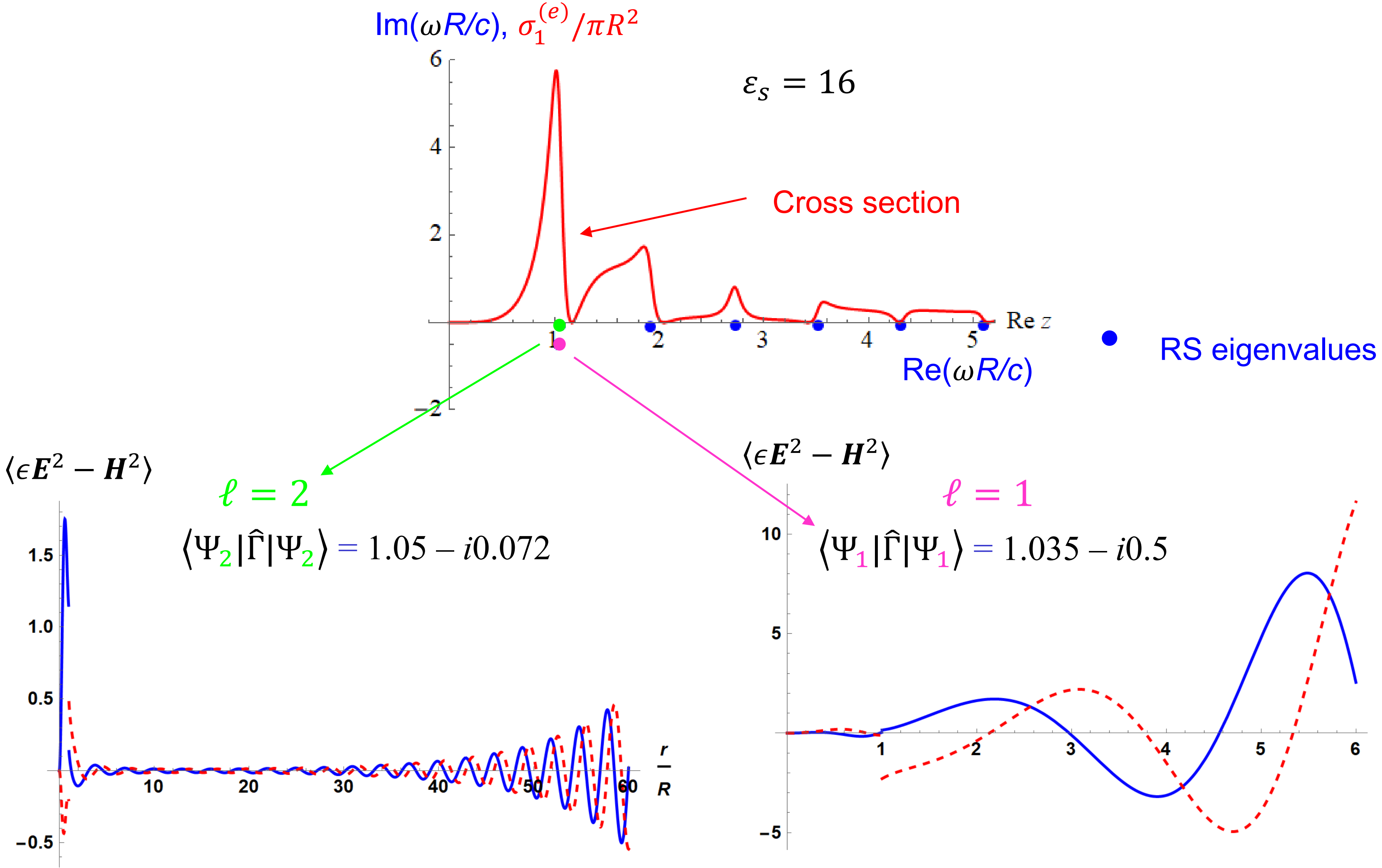


"Whispering gallery" resonances

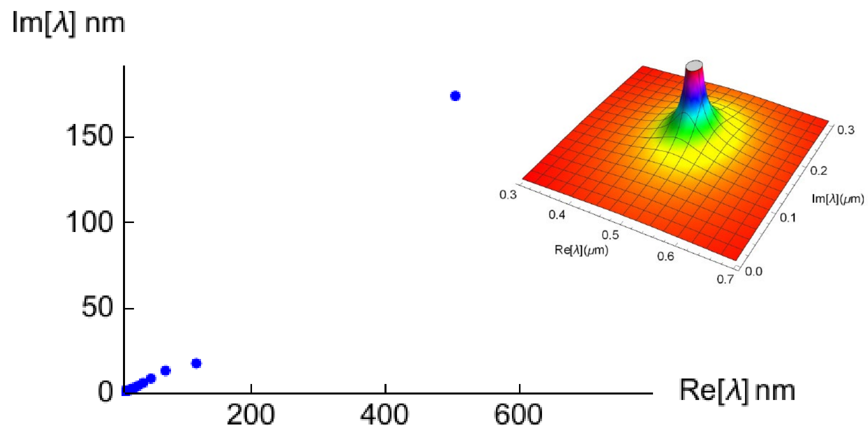
$\omega_\alpha = \omega'_\alpha + i\omega''_\alpha$

Gaussian regularization for RS scalar products :

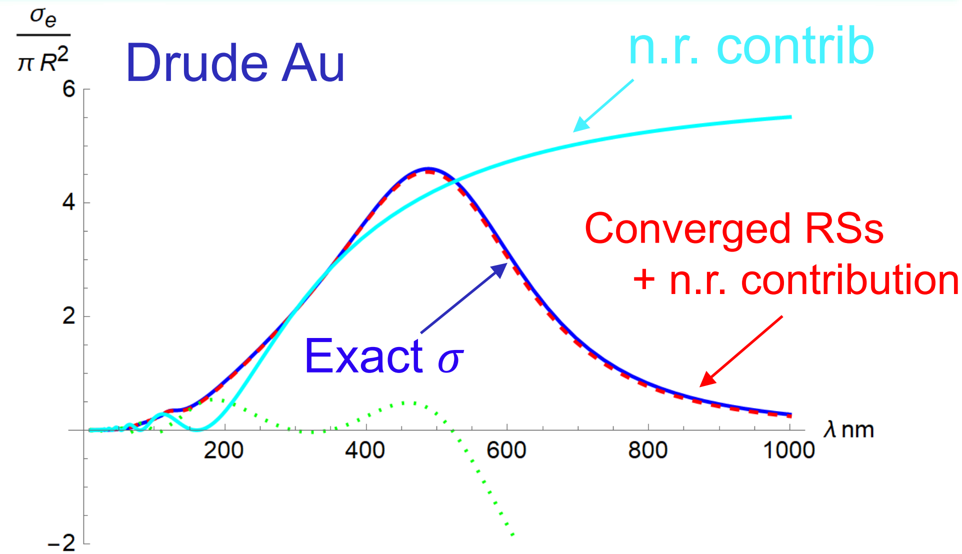
$$\langle \Psi_\ell | \hat{\Gamma} | \Psi_\ell \rangle = \lim_{\eta \to 0} \int e^{-\eta r^2} (\epsilon \boldsymbol{E}_\ell^2 - \boldsymbol{H}_\ell^2) d\boldsymbol{r} = \omega_\ell \frac{R}{c}$$

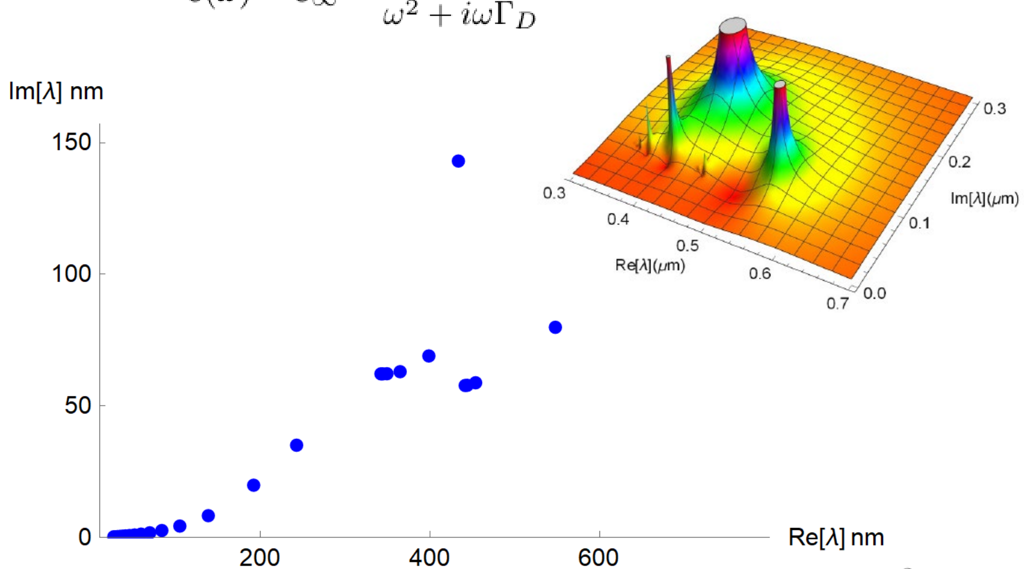


Dispersion materials are particularly challenging
But we can formulate response functions !

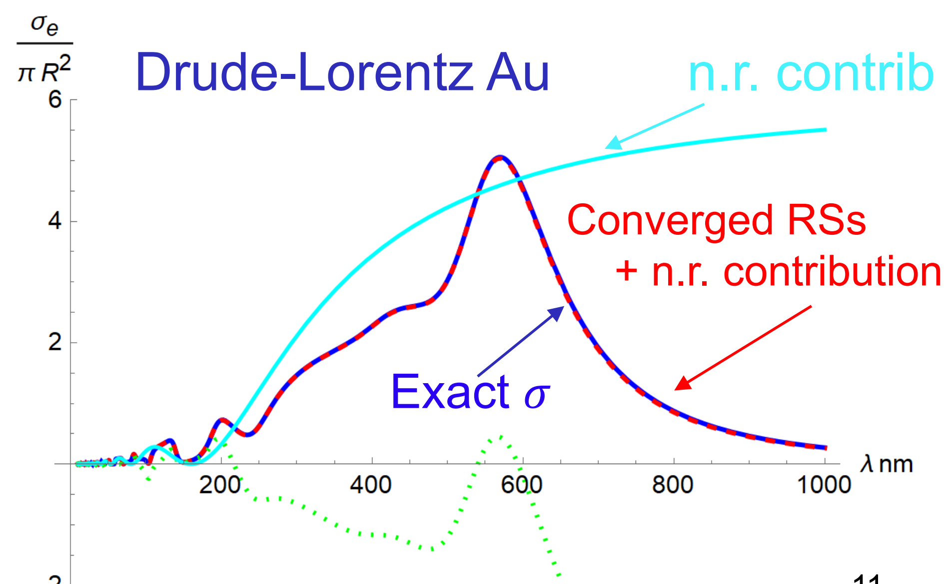


$$\varepsilon(\omega) = \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\omega\Gamma_D}$$





$$\varepsilon(\omega) = \varepsilon_\infty - \frac{\omega_{pD}^2}{\omega^2 + i\omega\Gamma_D} - s_1\frac{\omega_{p1,L}^2}{\omega^2 - \omega_{p1,L}^2 + i\Gamma_{1,L}\omega} - s_2\frac{\omega_{p2,L}^2}{\omega^2 - \omega_{p2,L}^2 + i\Gamma_{2,L}\omega}$$



Conclusion : RS Spectral expansions work !

But handle with care ! (non-resonant states, corrected normalizations, …)

1) ***Spectral expansions of open and dispersive optical systems: Gaussian regularization and convergence,*** B.Stout, R.Colom, N.Bonod and R.C.McPhedran, New Journal of Physics (2021)

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5) ***Egocentric physics : Just about Mie,*** Brian Stout and Ross McPhedran, European Physics Letters, **119**(4), 44002(7), (2017).

6) ***Time dynamics of open optical cavities and Quasi-normal modes*** Submitted R.Colom, B.Stout, N.Bonod

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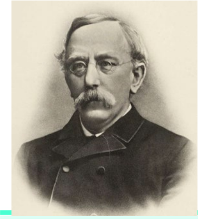
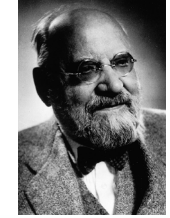
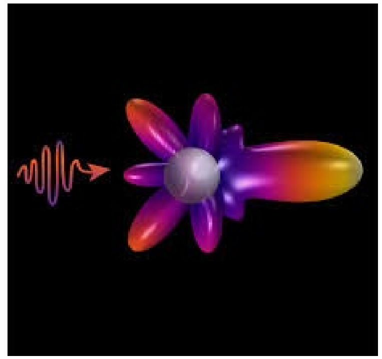


Lorenz(1890)-Mie(1908) theory
“Exact” response functions of a spherical scatterer





T-matrix coefficients

$$\begin{cases} f_p^{(e)} = -a_n e_p^{(e)} = \overbrace{t_n^{(e)}} e_p^{(e)} \\ f_p^{(h)} = -b_n e_p^{(h)} = t_n^{(h)} e_p^{(h)} \end{cases}$$

Lorenz-Mie coefficients

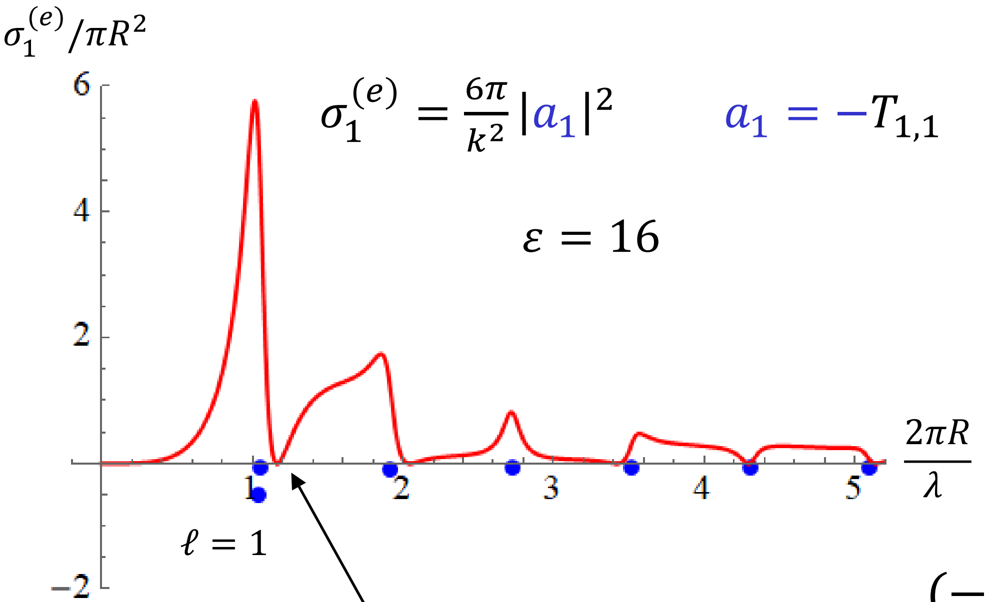
$$a_n = \frac{\frac{\varepsilon_s}{\varepsilon_b} j_n(k_s R)\psi'_n(kR) - \psi'_n(k_s R) j_n(kR)}{\frac{\varepsilon_s}{\varepsilon_b} j_n(k_s R)\xi'_n(kR) - \psi'_n(k_s R) h_n(kR)}$$

$$b_n = \frac{\frac{\mu_s}{\mu_b} j_n(k_s R)\psi'_n(kR) - \psi'_n(kR) j_n(kR)}{\frac{\mu_s}{\mu_b} \psi_n(k_s R)\xi'_n(kR) - \psi'_n(k_s R) h_n(kR)}$$

Gustav Mie (1868-1957) **“Contributions to the Optics of Turbid Media, particularly of colloidal metal solutions”** Translation (Royal Aircraft Establishment (1976). **(1908)**

Ludvig Lorenz (1829–91) **“Light scattering and reflection by a transparent sphere (surface)”** in Oeuvres scientifiques de **L. Lorenz**. 1898, p 403-529 **(1890)**.

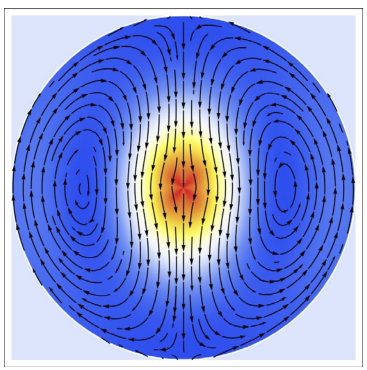
Explain physical phenomena using RS (QNMs) with well-defined normalizations



$$\sigma_1^{(e)} = \frac{6\pi}{k^2}|a_1|^2 \qquad a_1 = -T_{1,1}$$

$$\varepsilon = 16$$

"Anapole"



$$a_1 = \frac{\frac{\varepsilon_s}{\varepsilon_b} j_1(k_s R)\psi'_1(kR) - \psi'_1(k_s R) j_1(kR)}{\frac{\varepsilon_s}{\varepsilon_b} j_1(k_s R)\xi'_1(kR) - \psi'_1(k_s R) h_1(kR)}$$

$$T_{n,q}(\omega) = \underbrace{\frac{(-1)^{n+q} e^{-2iR\omega/c} - 1}{2}}_{\text{Non-resonant term !}} + \underbrace{\frac{c e^{-2iz}}{R} \sum_{\ell=-\infty}^{\infty} \frac{r_\alpha}{\omega - \omega_\alpha}}_{\text{resonant state spectral expansion}}$$

Non-resonant term !

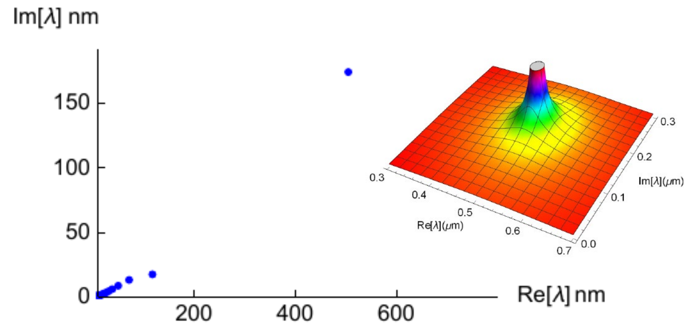
resonant state spectral expansion

$$r_\alpha = \frac{i e^{2iR\omega_\alpha/c}}{\mathcal{N}_\alpha^2}$$

Egocentric physics : Just about Mie, ,
Stout et al, EPL **119**(4), 44002(7), (2017).

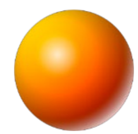
The problem of spectral RS expansion convergence (case of a gold sphere)

$$T_{n,q}(\omega) = \frac{(-1)^{n+q} e^{-2iR\omega/c} - 1}{2} + \frac{c e^{-2iz}}{R} \sum_{\ell=-L_{\max}}^{L_{\max}} \frac{r_\alpha}{\omega - \omega_\alpha}$$



$$\lambda_\alpha = 2\pi c/\omega_\alpha$$

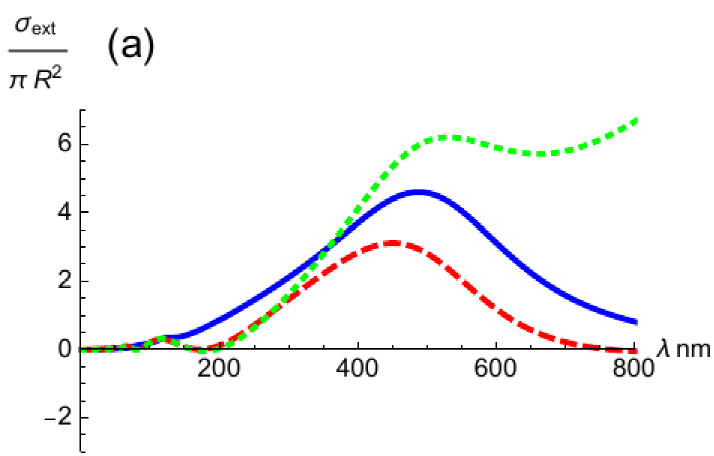
Drude model $\varepsilon(\omega) = \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\omega\Gamma_D}$



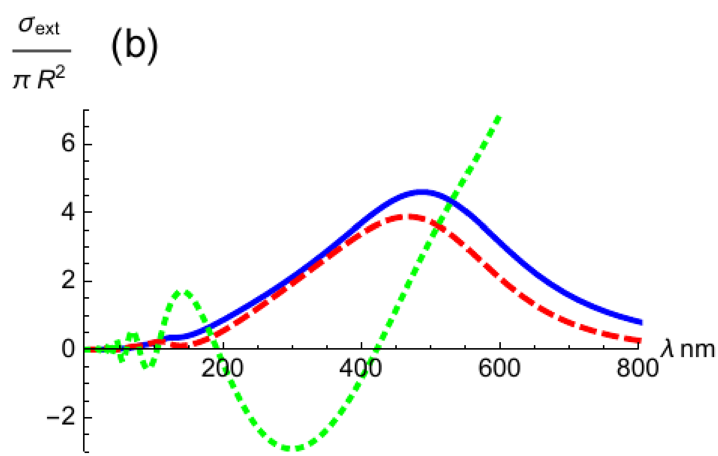
$R = 80\text{nm}$

Direct cutoff for a Drude model sphere is disastrous

$L_{\max} = 1$



$L_{\max} = 4$

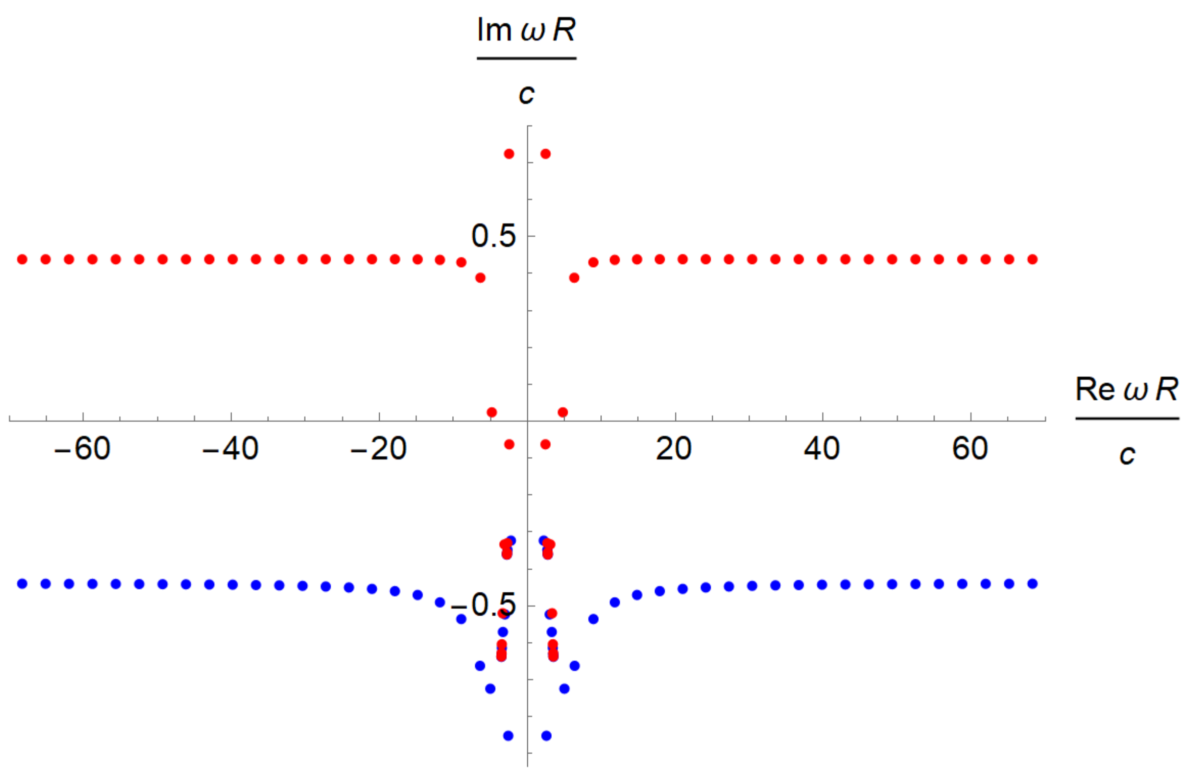


Solving the spectral convergence problem

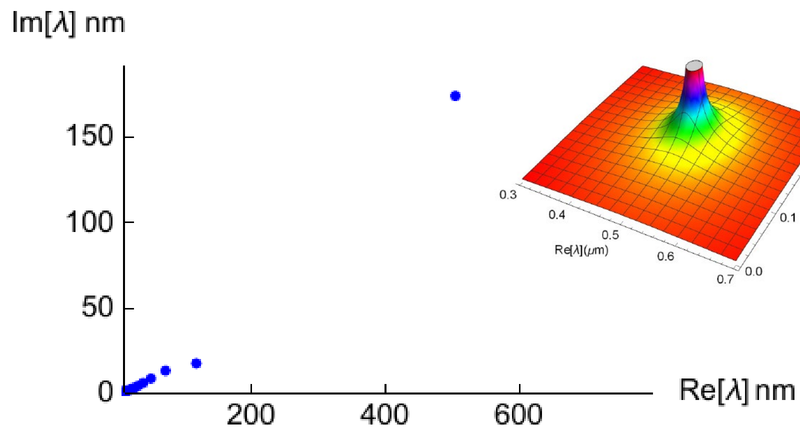
$$\tilde{r}_{\alpha(q,n,\ell)} = \frac{R}{2c_b} \frac{\prod_{\ell'=-L_{\max}}^{L_{\max}} \left(\omega^{(+)}_{\alpha(q,n,\ell)} - \omega^{(-)}_{\alpha(q,n,\ell')}\right)}{\prod_{\ell'=-L_{\max},\ell'\neq\ell}^{L_{\max}} \left(\omega^{(+)}_{\alpha(q,n,\ell)} - \omega^{(+)}_{\alpha(q,n,\ell')}\right)}$$

$\omega^{(-)}_{\alpha(q,n,\ell)}$ ●

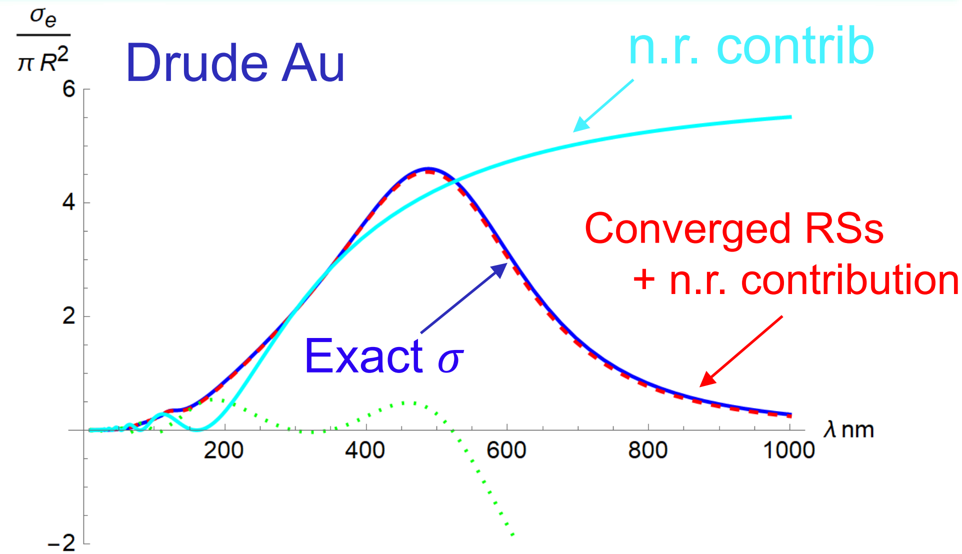
$\omega^{(+)}_{\alpha(q,n\ell)}$ ●

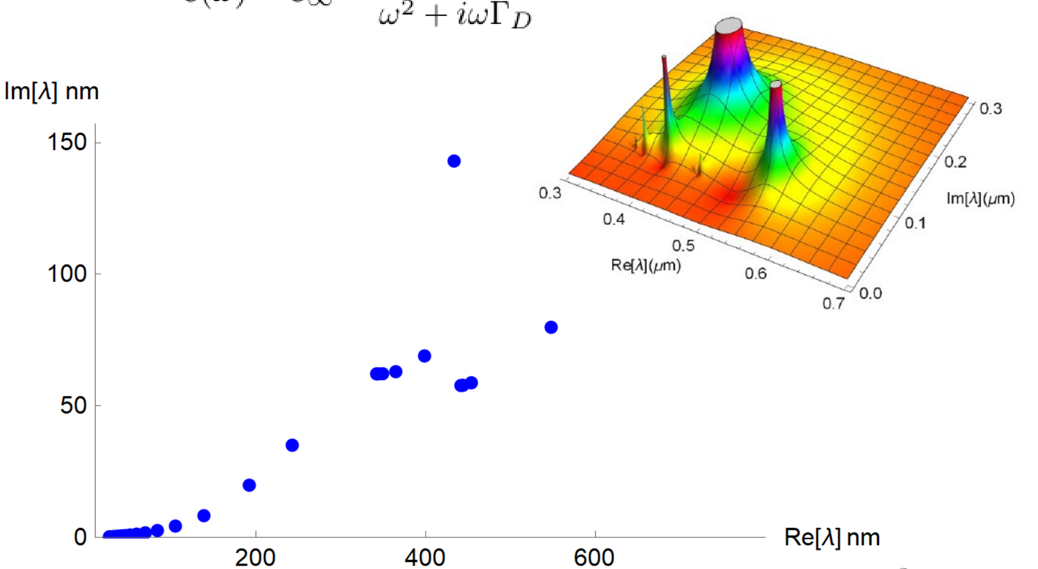


Response of dispersive gold sphere – Dispersion models

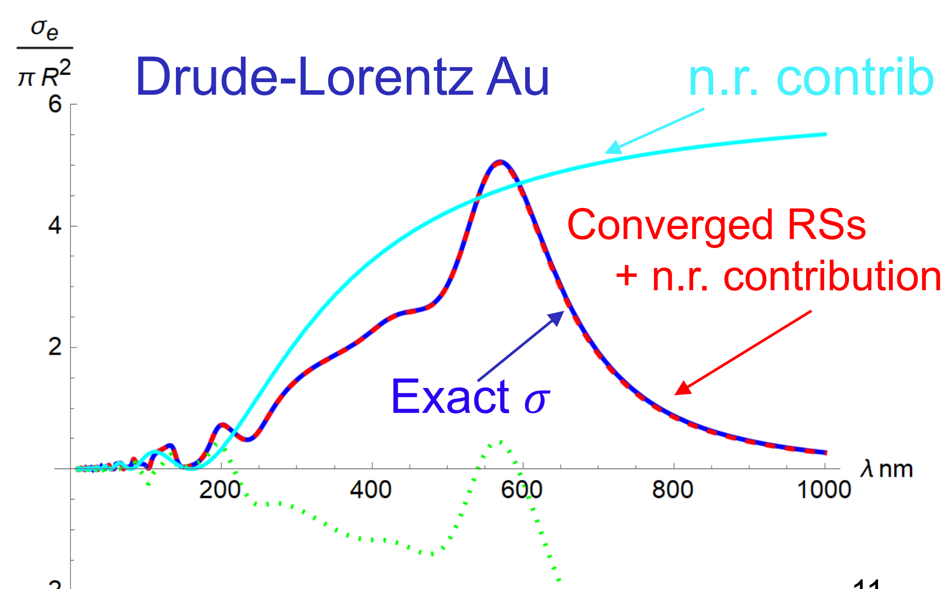


$$\varepsilon(\omega) = \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\omega\Gamma_D}$$





$$\varepsilon(\omega) = \varepsilon_\infty - \frac{\omega_{pD}^2}{\omega^2 + i\omega\Gamma_D} - s_1\frac{\omega_{p1,L}^2}{\omega^2 - \omega_{p1,L}^2 + i\Gamma_{1,L}\omega} - s_2\frac{\omega_{p2,L}^2}{\omega^2 - \omega_{p2,L}^2 + i\Gamma_{2,L}\omega}$$



Conclusion : Spectral expansions work !

But handle with care ! (non-resonant states, corrected normalizations, …)

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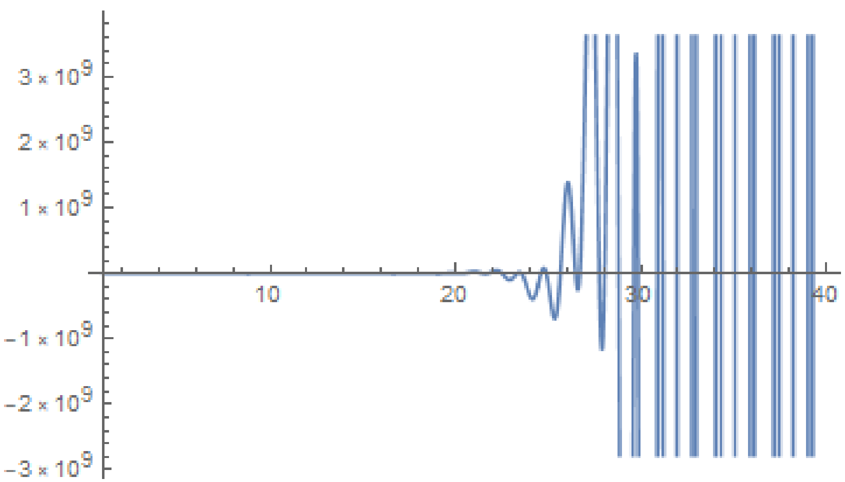
The regularization technique remains valid even for complex K and k where integrals diverge for large r

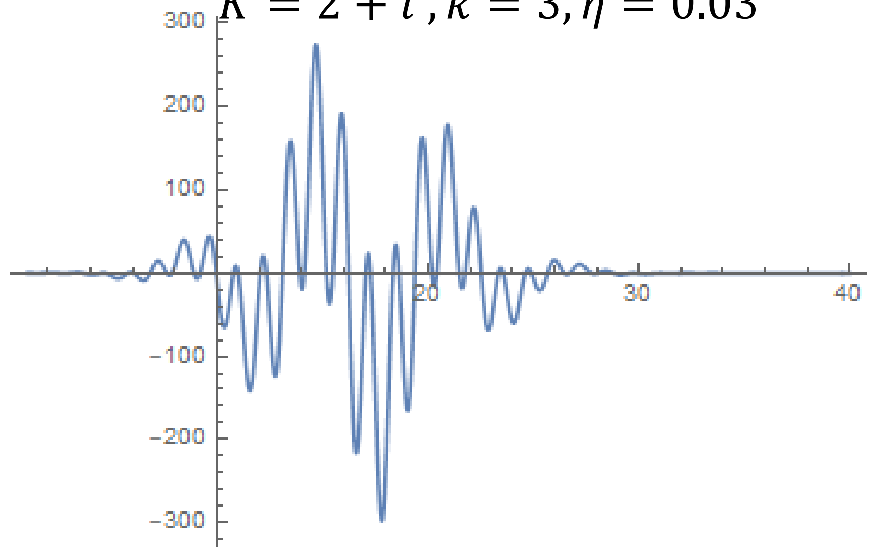
$$\lim_{\eta\to 0}\int_0^\infty r^2 e^{-\eta r^2} j_n(Kr)y_n(kr)dr = -\frac{K^n}{k^{n+1}(K^2-k^2)}$$

$$\lim_{\eta\to 0}\int_0^\infty r^2 e^{-\eta r^2} j_0(Kr)y_0(kr)dr = \lim_{\eta\to 0}\int_0^\infty e^{-\eta r^2}\sin(Kr)\cos(kr)dr = -\frac{1}{k(K^2-k^2)}$$

$K = 2+i\,, k = 3, \eta = 0$



$K = 2+i\,, k = 3, \eta = 0.03$



For a sphere there are exact expressions for RS normalization

$$\widetilde{\mathcal{N}}^2_{\alpha(e,n,\ell)} = z_\alpha^2(\mu_\alpha - 1) + (\varepsilon_\alpha - 1)\left\{\left[\varphi_n^{(+)}(z_\alpha)\right]^2 + \frac{n(n+1)}{\varepsilon_\alpha}\right\}$$

$$+ \frac{\omega_\alpha}{2}\left\{\widetilde{\Xi}^{(+)}_{\alpha(e,n,\ell)}\,\frac{d}{d\omega}\ln\varepsilon_\alpha(\omega)\bigg|_{\omega_\alpha} + \widetilde{\Xi}^{(-)}_{\alpha(e,n,\ell)}\,\frac{d}{d\omega}\ln\mu_\alpha(\omega)\bigg|_{\omega_\alpha}\right\}$$

$$\widetilde{\mathcal{N}}^2_{\alpha(h,n,\ell)} = z_\alpha^2(\varepsilon_\alpha - 1) + (\mu_\alpha - 1)\left\{\left[\varphi_n^{(+)}(z_\alpha)\right]^2 - \frac{n(n+1)}{\mu_\alpha}\right\}$$

$$+ \frac{\omega_\alpha}{2}\left\{\widetilde{\Xi}^{(-)}_{\alpha(h,n,\ell)}\,\frac{d}{d\omega}\ln\varepsilon(\omega)\bigg|_{\omega_\alpha} + \widetilde{\Xi}^{(+)}_{\alpha(h,n,\ell)}\,\frac{d}{d\omega}\ln\mu(\omega)\bigg|_{\omega_\alpha}\right\},$$

$$\widetilde{\Xi}^{(\pm)}_{\alpha(e,n,\ell)} \equiv \varepsilon_\alpha\left[\varphi_n^{(+)}(z_\alpha)\right]^2 + \mu_\alpha z_\alpha^2 - \frac{n(n+1)}{\varepsilon_\alpha} \pm \varphi_n^{(+)}(z_\alpha)$$

$$\widetilde{\Xi}^{(\pm)}_{\alpha(h,n,\ell)} \equiv \mu_\alpha\left[\varphi_n^{(+)}(z_\alpha)\right]^2 + \varepsilon_\alpha z_\alpha^2 - \frac{n(n+1)}{\mu_\alpha} \pm \varphi_n^{(+)}(z_\alpha),$$

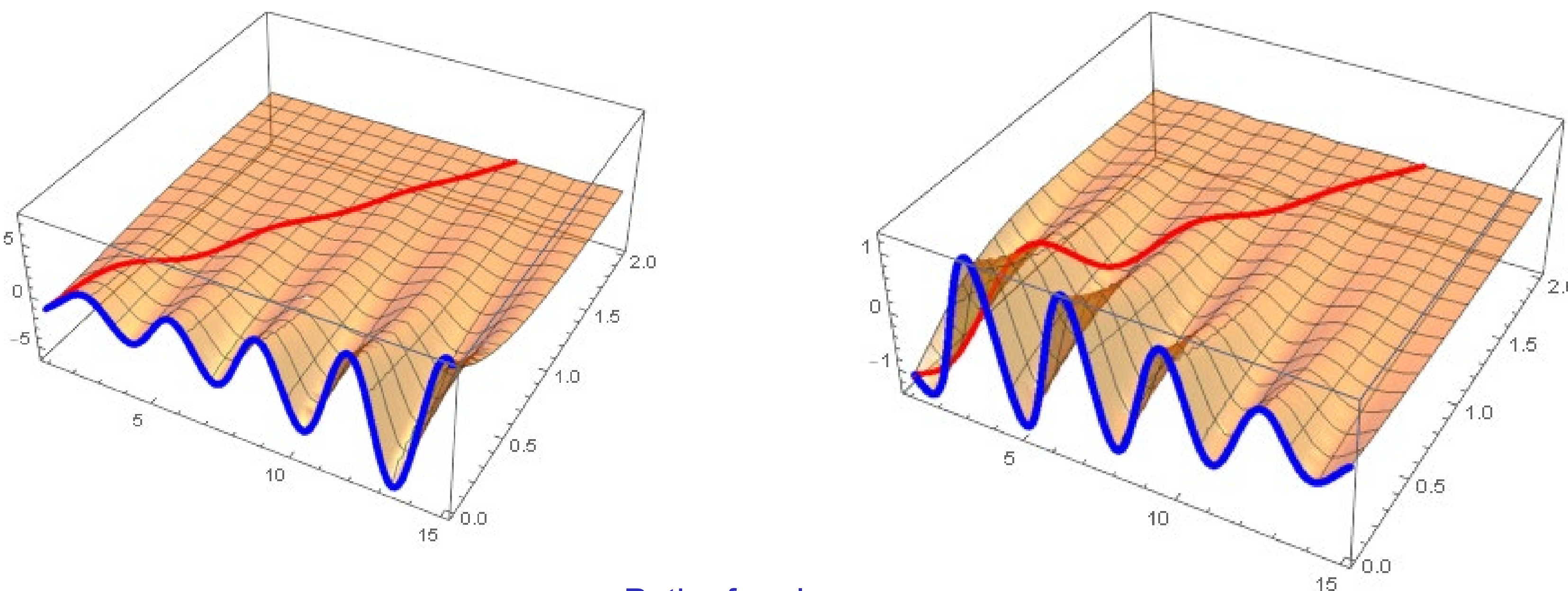
Gaussian vs PML regularization scheme

`Killing Mie softly' - Regularization !

$$\lim_{\eta\to 0}\int_1^\infty r^2 e^{-\eta r^2}\left[h_n^{(+)}(zr)\right]dr = -\frac{1}{2}z\frac{[\xi_n'(z)]^2+\xi_n^2(z)-n(n+1)h_n^2(z)-h_n(z)\xi_n'(z)}{k^3}$$

$z_{e,1,2} = 1.05 - i0.07$ High Q

$\eta = 0$ $\ell = 2$ $\eta = 0.015$



Path of real r

`PML' path in the complex plane

What is the “secret” to analytic results ?

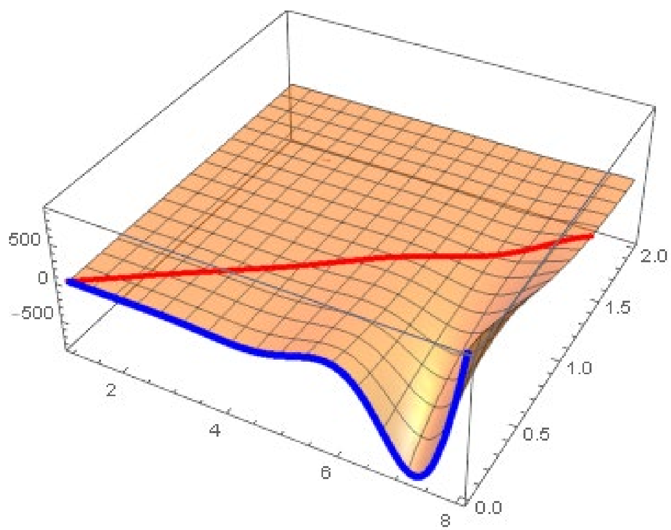
`Killing Mie softly’ - Regularization !

$$\lim_{\eta\to 0}\int_1^\infty r^2 e^{-\eta r^2}\left[h_n^{(+)}(zr)\right]dr = -\frac{1}{2}z\frac{[\xi_n'(z)]^2+\xi_n^2(z)-n(n+1)h_n^2(z)-h_n^{(+)}(z)\xi_n'(z)}{k^3}$$

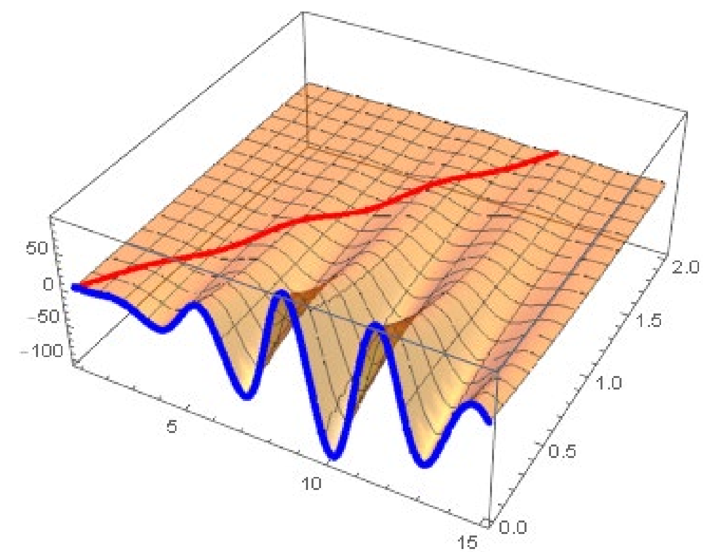
$z_{\alpha(e,1,1)} = 1.04 - i0.5$ Low Q

$\ell = 1$

$\eta = 0$



$\eta = 0.5$



Path of real r

`PML’ path in the complex plane

Some more resonant state history

Thomson modes (1884)

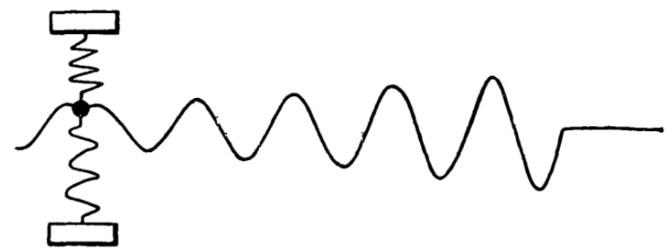
Outgoing modes of a perfectly conducting sphere are associated with complex frequencies

$$\omega_q = \omega'_q - i\gamma_q$$

J. J. Thomson, *Proceedings of the London Mathematical Society* 1.1 (1883)

Lamb (1900)

Exponential catastrophe avoided by causality



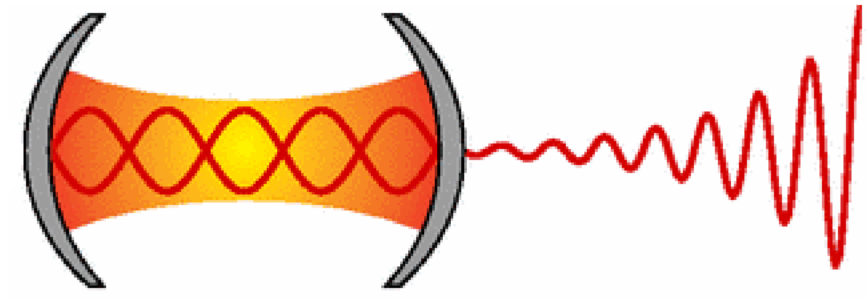
H. Lamb, *Proceedings of the London Mathematical Society* 1.1 (1900)

Modal Expansion of the Scattered Field: Causality, Non-Divergence and Non-Resonant Contribution
R.Colom, *et al* ,Phys Rev. B, **98** , 085418, (2018).

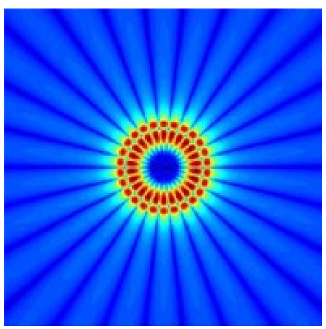
`Leaky' cavities : open resonators

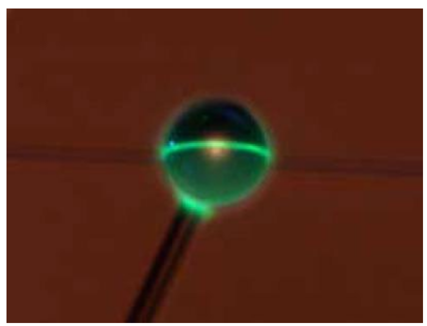
`Fox-Li' modes : lasers

A. G. Fox and T. Li, "Resonant modes in an optical maser, "Proc. IRE(Correspondence), vol. 48, pp. 1904-1905, November1960.

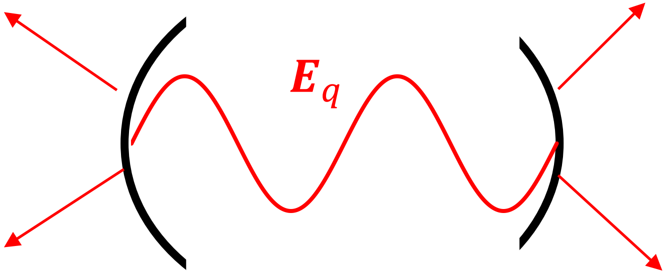


`Whispering gallery' modes





Spatial divergence is a far field effect



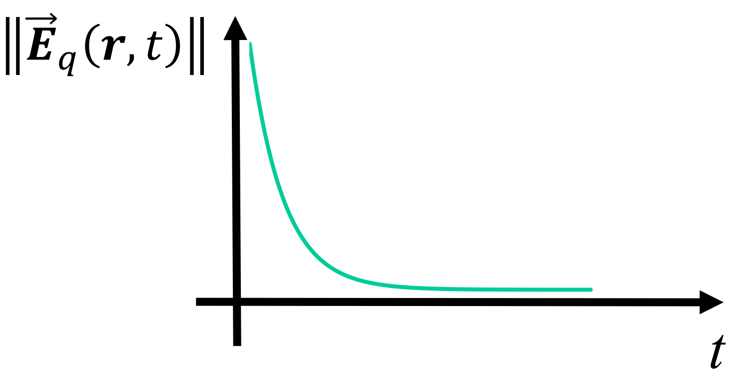
$$\omega_q = \omega_q' + i\omega_q'' \;,\; \omega_q'' < 0$$

Far field : $\Delta\psi \rightarrow \frac{1}{r}\frac{\partial^2 (r\psi)}{\partial r^2}$

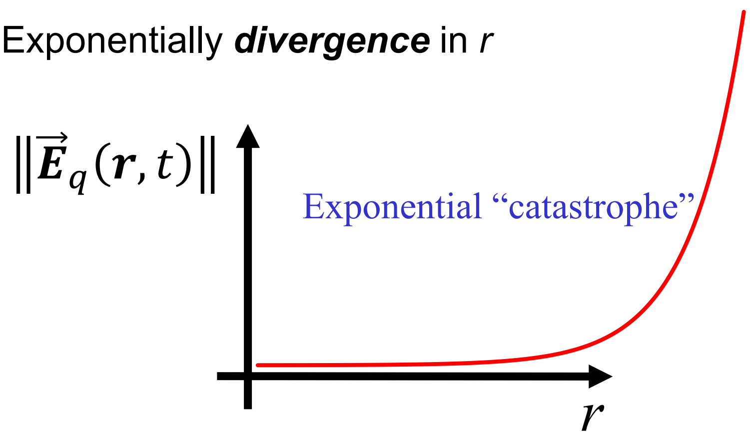
$$\frac{\partial^2}{\partial r^2} r\psi_r(r,t) = \frac{n^2}{c^2}\frac{\partial^2}{\partial t^2} r\psi_r(r,t) = -\frac{n^2}{c^2}\omega_q^2 r\psi_r(r,t)$$

$$\Rightarrow \psi_r(r,t) = A_+ \frac{e^{i\frac{\omega_q}{c}(r-ct)}}{r} + A_- \frac{e^{i\frac{\omega_q}{c}(r+ct)}}{r}$$

Exponentially ***decrease*** in time → Exponentially ***divergence*** in *r*

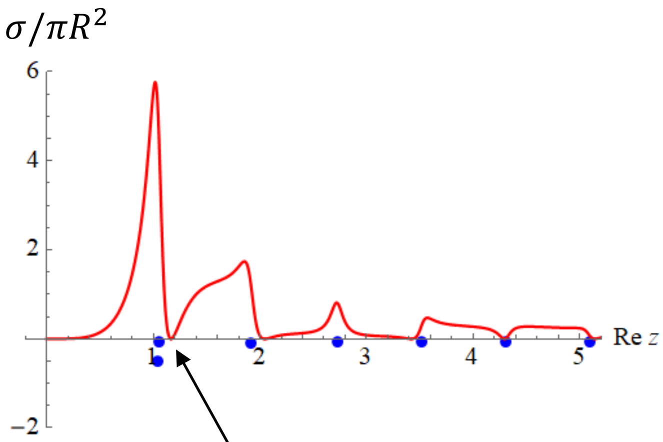


$$\boldsymbol{E}_q(\boldsymbol{r},t) = \boldsymbol{E}_n(\boldsymbol{r}) e^{-i\omega_n' t} e^{\omega_n'' t}$$

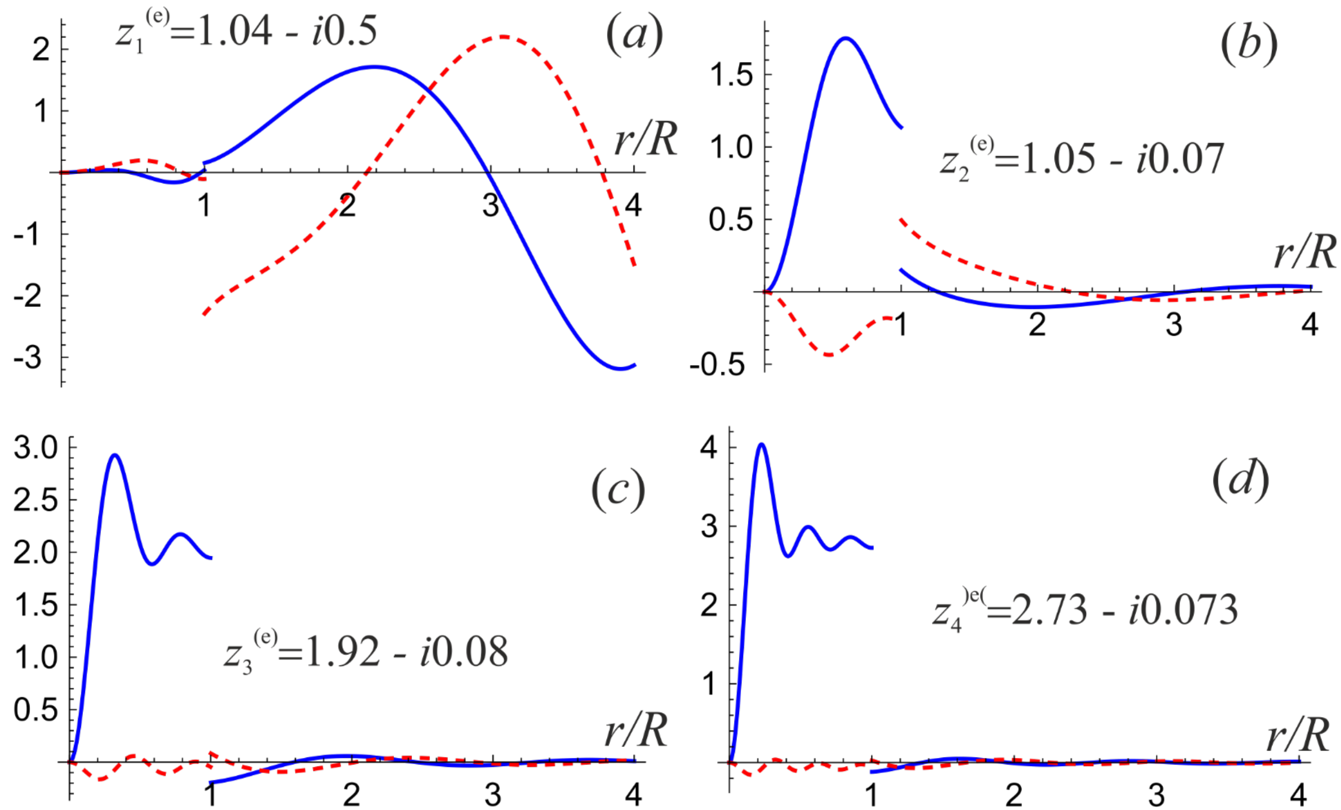


$$\boldsymbol{E}_q(\boldsymbol{r},t) = \boldsymbol{E}_n(t) e^{+i\frac{\omega_n'}{c}r} e^{-\frac{\omega_n''}{c}r}$$

Normalization of eigenstates : numerical verification



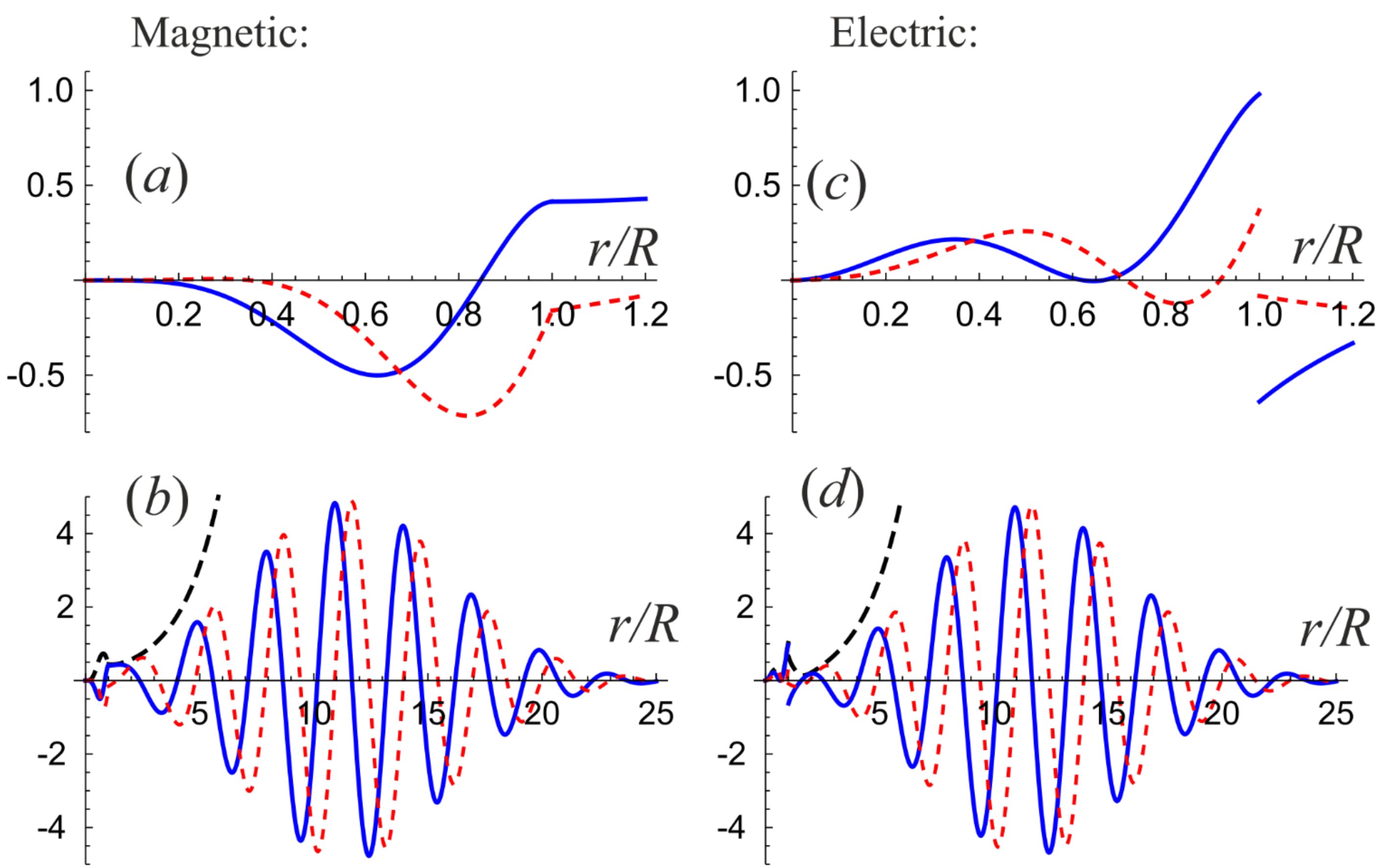
Anapole



$$\left\langle \Psi_q \left| \hat{\Gamma} \right| \Psi_q \right\rangle = \int \left[\varepsilon(\vec{\boldsymbol{r}}) \vec{\boldsymbol{e}}_q^2(\vec{\boldsymbol{r}}) - \mu(\vec{\boldsymbol{r}}) \vec{\boldsymbol{h}}_q^2(\vec{\boldsymbol{r}}) \right] d\boldsymbol{r} = z_q = \omega_q \frac{R}{c}$$

Orthogonalization of eigenstates can be verified analytically for spherical scatterers !

Resonant state: $\left|\Psi_q^{(e)}\right\rangle \equiv \begin{pmatrix} \vec{\boldsymbol{e}}_{n,m,q}(\vec{\boldsymbol{r}}) \\ \vec{\boldsymbol{h}}_{n,m,q}(\vec{\boldsymbol{r}}) \end{pmatrix} = \frac{i^n k_q^{3/2}}{\mathcal{N}_{e,n,m,q}} \begin{pmatrix} \vec{\boldsymbol{N}}_{n,m}^{(+)}(k_q \vec{\boldsymbol{r}}) \\ i^{-1} \vec{\boldsymbol{M}}_{n,m}^{(+)}(k_q \vec{\boldsymbol{r}}) \end{pmatrix}$



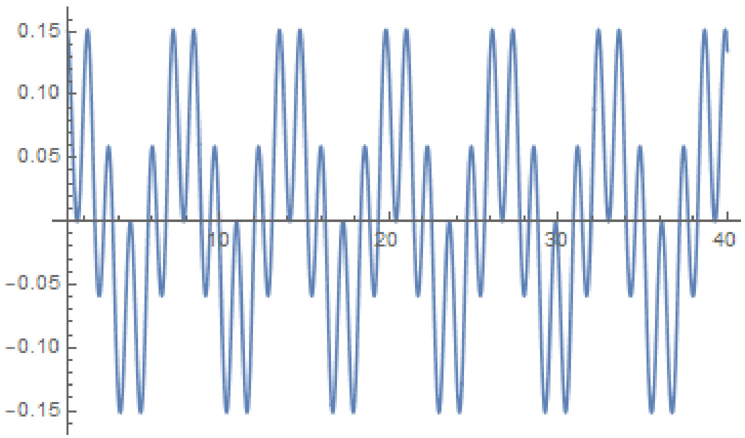
$$\left\langle \Psi_1^{(e)} \left| \hat{\Gamma} \right| \Psi_2^{(e)} \right\rangle = \int \left[\varepsilon(\vec{\boldsymbol{r}}) \vec{\boldsymbol{e}}_1^{(e)}(\vec{\boldsymbol{r}}) \vec{\boldsymbol{e}}_2^{(e)}(\vec{\boldsymbol{r}}) - \mu(\vec{\boldsymbol{r}}) \vec{\boldsymbol{h}}_1^{(e)}(\vec{\boldsymbol{r}}) \vec{\boldsymbol{h}}_2^{(e)}(\vec{\boldsymbol{r}}) \right] d\boldsymbol{r} = 0$$

Extending the regular rules of integration
Distribution theory !

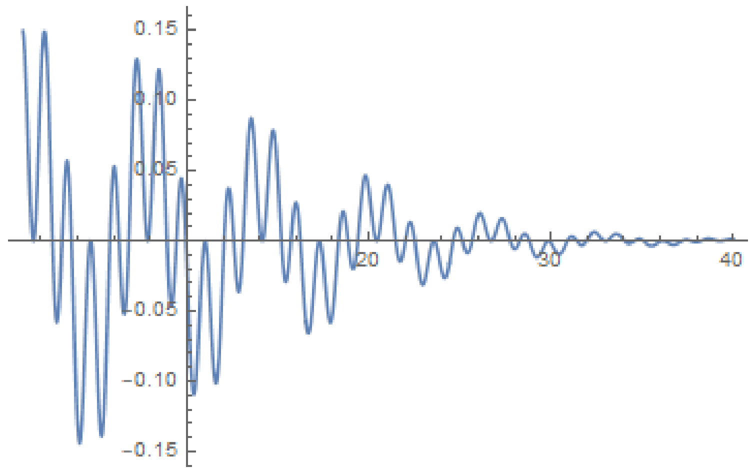
$$\lim_{\eta\to 0}\int_0^\infty r^2 e^{-\eta r^2} j_n(Kr) y_n(kr) dr = -\frac{K^n}{k^{n+1}(K^2-k^2)}$$

$$\lim_{\eta\to 0}\int_0^\infty r^2 e^{-\eta r^2} j_0(Kr) y_0(kr) dr = \lim_{\eta\to 0}\int_0^\infty e^{-\eta r^2}\sin(Kr)\cos(kr) dr = -\frac{K}{(K^2-k^2)}$$

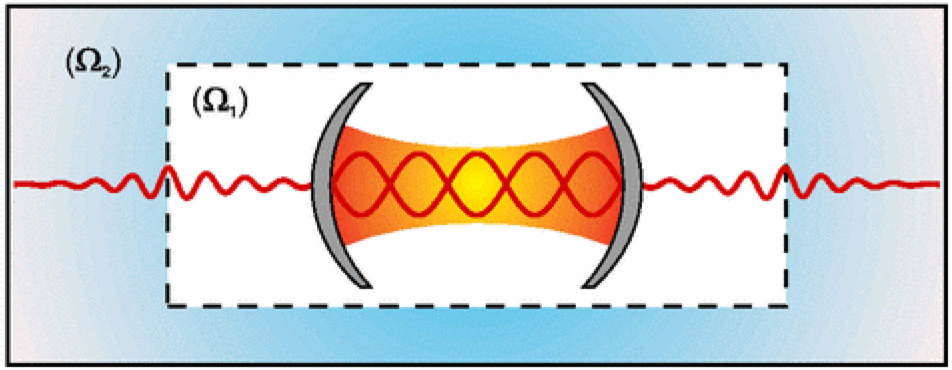
$K = 2\,, k = 3, \eta = 0$



$K = 2\,, k = 3, \eta = 0.003$



Other techniques like PMLs offer efficient numerical regularization of RS integrals

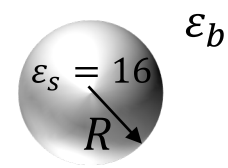


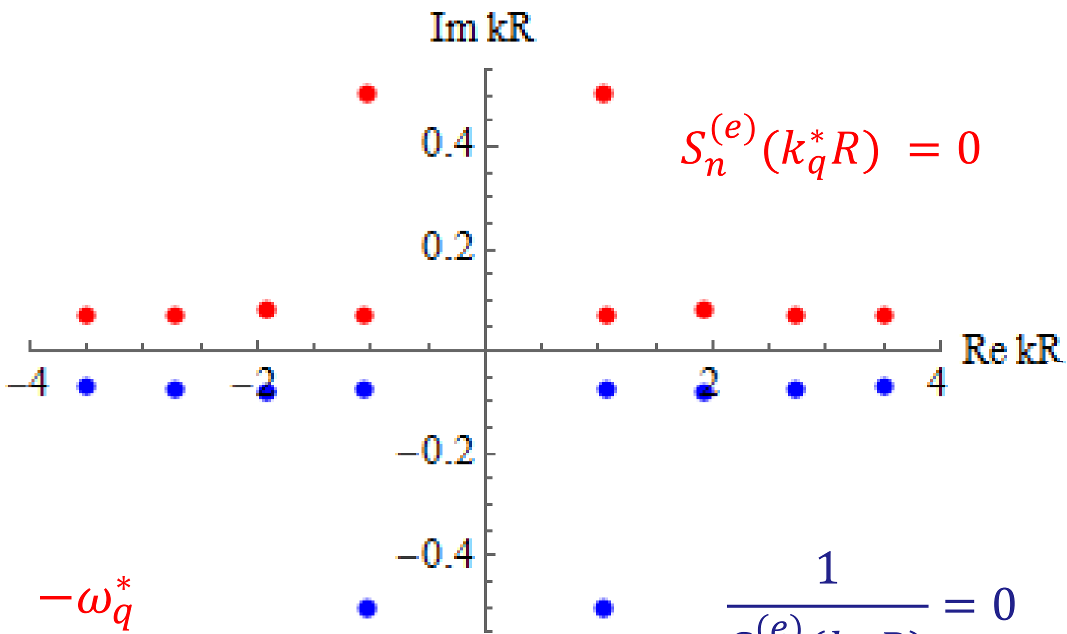
The PML technique puts a perfectly matched layer that damps the exponential catastrophe inside the medium Ω_2.

$$\left\langle \Psi_q \left| \frac{d}{d\omega}\left(\omega \hat{\Gamma}(\vec{\boldsymbol{r}},\omega)\right)\right|_{\omega=\omega_q} \Psi_q \right\rangle = \int \left[\left.\frac{d[\omega\varepsilon(\vec{\boldsymbol{r}},\omega)]}{d\omega}\right|_{\omega_q} \vec{\boldsymbol{e}}_q^{\,2}(\vec{\boldsymbol{r}}) - \left.\frac{d[\omega\mu(\vec{\boldsymbol{r}},\omega)]}{d\omega}\right|_{\omega_q} \vec{\boldsymbol{h}}_q^{\,2}(\vec{\boldsymbol{r}}) \right] d\boldsymbol{r} = 1$$

Symmetries of the *S*-matrix coefficients

$$z \equiv kR = \frac{\omega}{c} R$$





$$S_n^{(e)}(k_q^* R) = 0$$

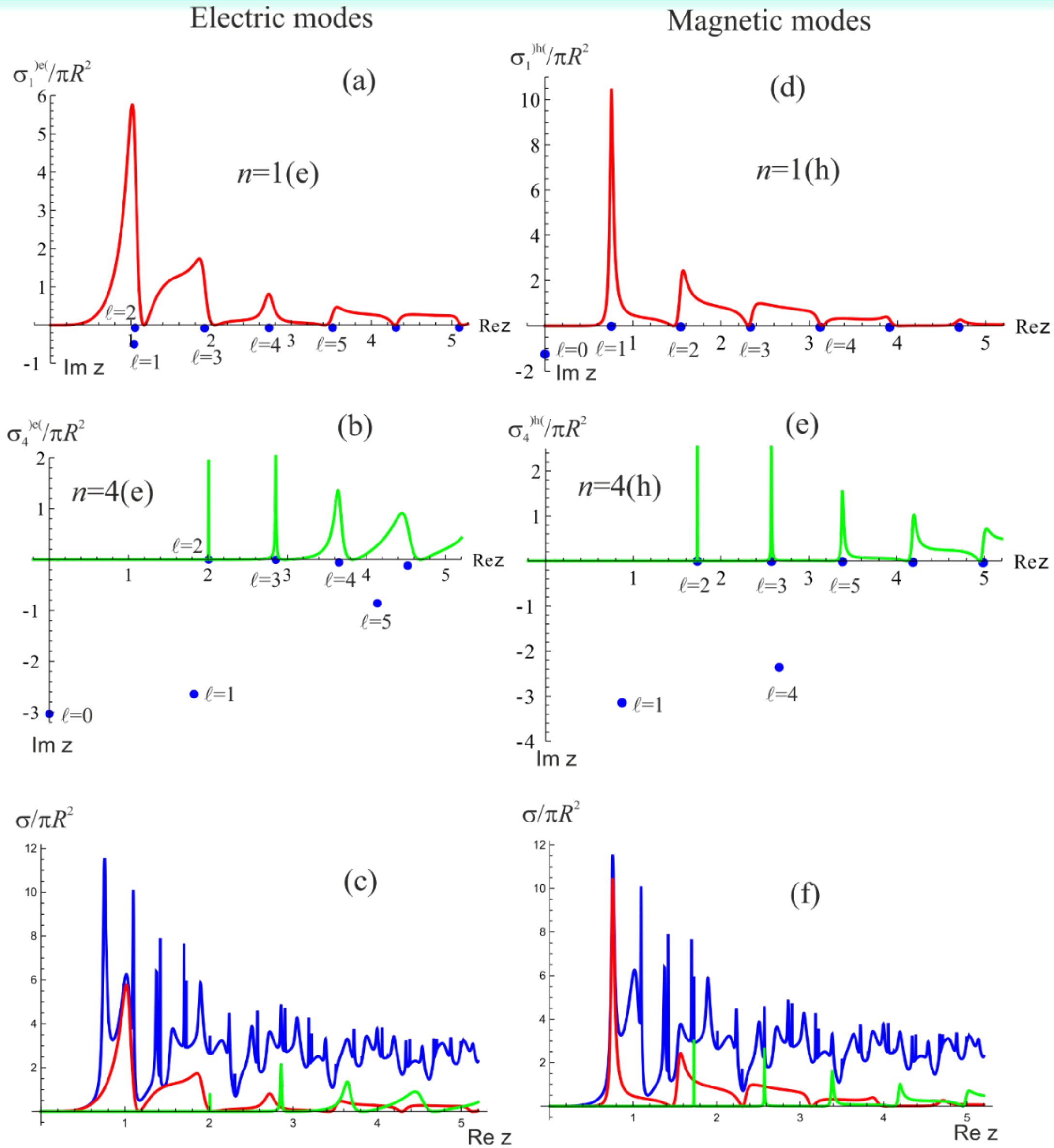
$-\omega_q^*$

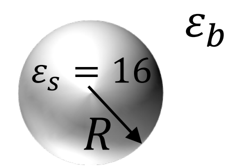
$$\frac{1}{S_n^{(e)}(k_q R)} = 0$$

Energy conservation

Time reversal symmetry

The above formulas exactly reconstruct the analytic Mie scattering results to arbitrary precision!





$$z \equiv kR = \frac{\omega}{c} R$$

Resonant States (Quasi-Normal Modes)

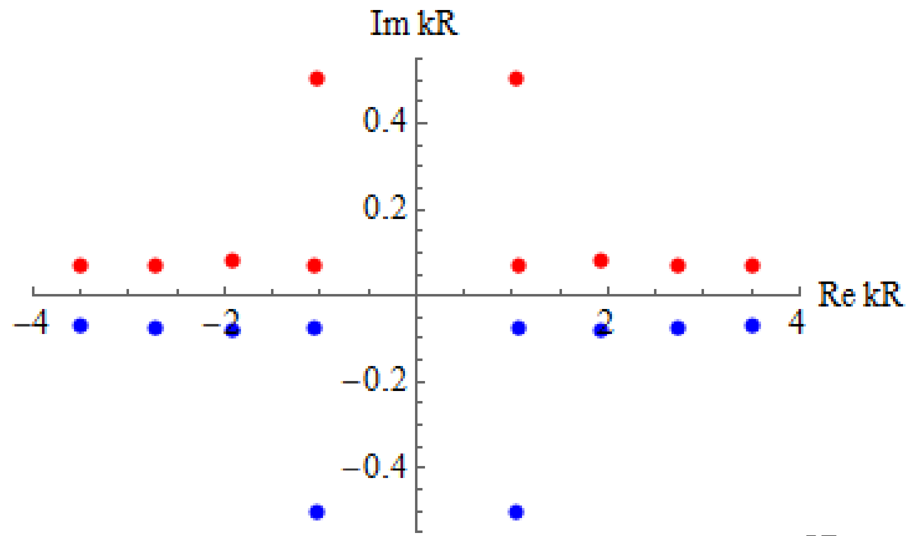
Complex eigenstates of the time independent Maxwell equation

$$\left[\omega_\alpha \begin{pmatrix} \overleftrightarrow{\varepsilon}(\vec{\boldsymbol{r}}, \omega_\alpha) & 0 \\ 0 & -\overleftrightarrow{\mu}(\vec{\boldsymbol{r}}, \omega_\alpha) \end{pmatrix} - ic \begin{pmatrix} 0 & \boldsymbol{\nabla}\times \\ \boldsymbol{\nabla}\times & 0 \end{pmatrix}\right] \begin{pmatrix} \vec{\boldsymbol{e}}_\alpha \\ \vec{\boldsymbol{h}}_\alpha \end{pmatrix} = 0$$

$$\omega_\alpha \hat{\Gamma}_{\omega_\alpha} |\Psi_\alpha\rangle - \hat{\mathbb{L}} |\Psi_\alpha\rangle = 0$$

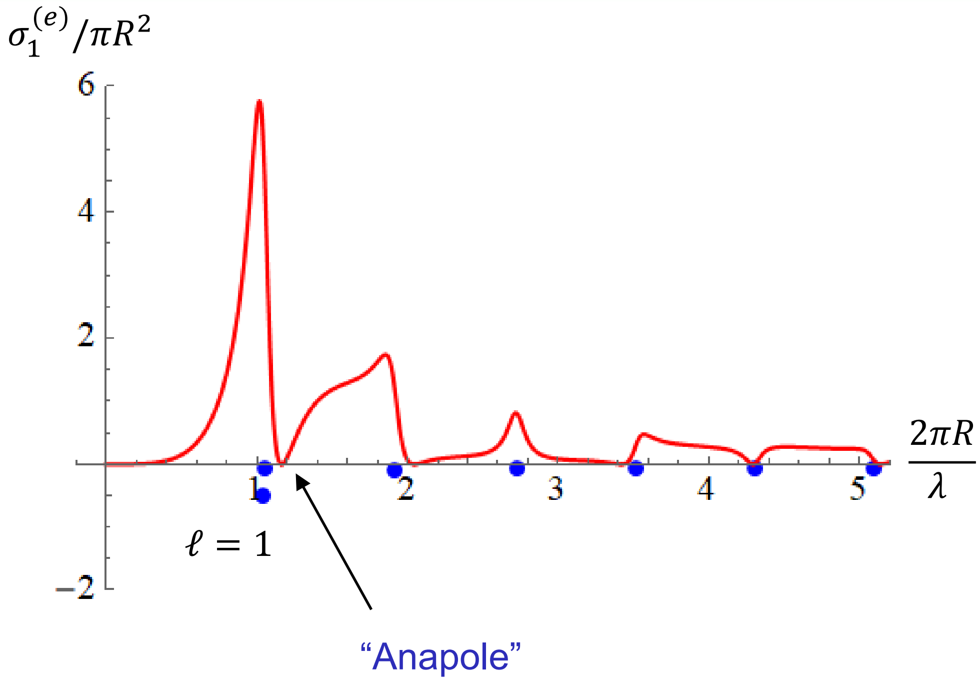
RS/QNM are eigenstates with ***outgoing boundary conditions!***

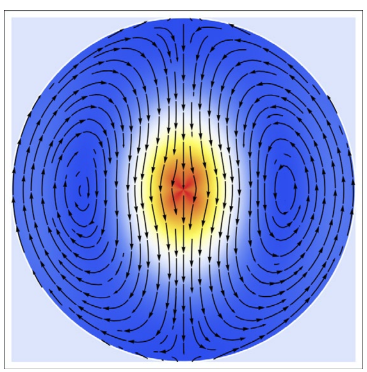
complex frequency plane



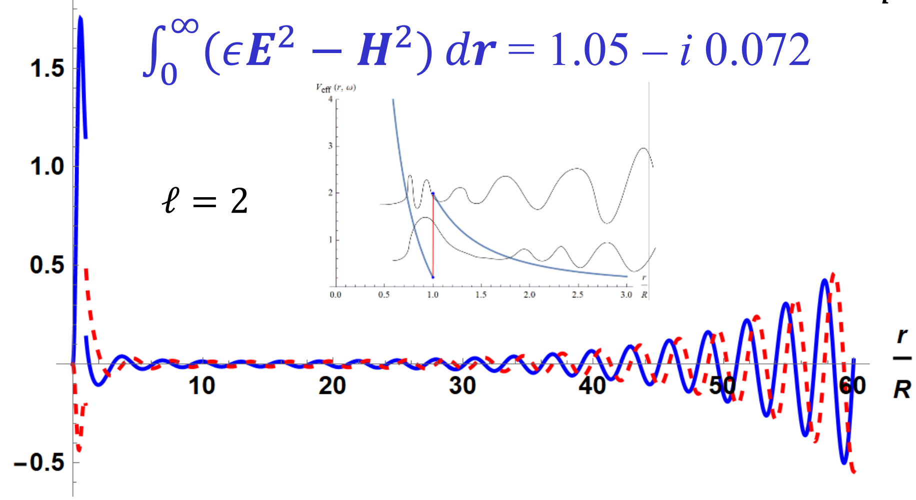
Electric dipole RSs frequencies satisfying outgoing boundary conditions, $\omega_q R/c$, are the blue dots in the complex plane for a lossless high index sphere while eigenvalues satisfying incoming boundary solutions are red dots

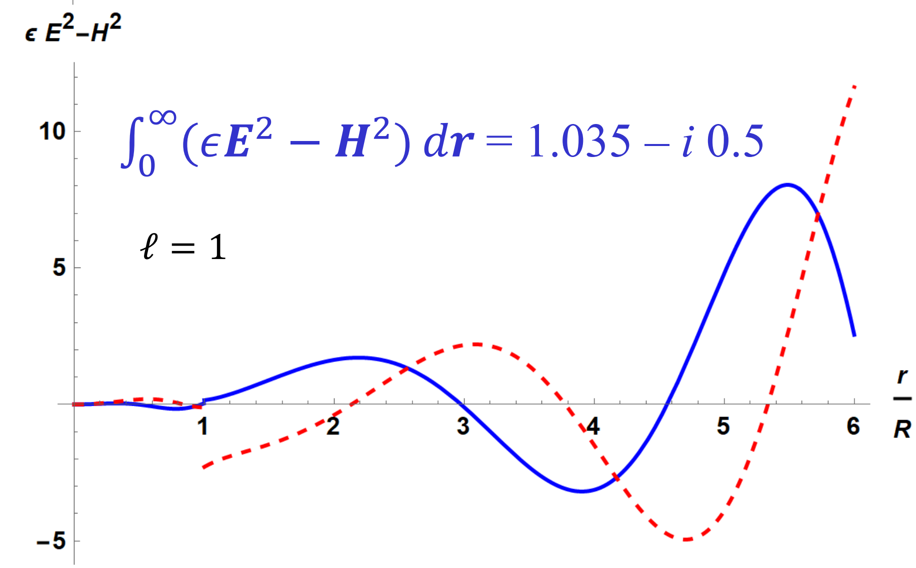
Explain physical phenomena using RS (QNMs) with well-defined normalizations





$$\langle \Psi_q | \hat{\Gamma} | \Psi_q \rangle = z_q = \omega_q \frac{R}{c} = \frac{2\pi R}{\lambda_q}$$





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Stout et al, EPL **119**(4), 44002(7), (2017).

Maxwell equations can be written in a single equation 1st order equation

$$|\Psi(\vec{\boldsymbol{r}},t)\rangle = \int_{-\infty}^{\infty} d\omega \begin{pmatrix} \vec{\boldsymbol{e}}(\vec{\boldsymbol{r}},\omega) \\ \vec{\boldsymbol{h}}(\vec{\boldsymbol{r}},\omega) \end{pmatrix} e^{-i\omega t} = \int_{-\infty}^{\infty} d\omega\, |\Psi(\omega)\rangle e^{-i\omega t} \Rightarrow$$

$$\vec{\boldsymbol{e}}(\vec{\boldsymbol{r}},-\omega^*) = \vec{\boldsymbol{e}}^*(\vec{\boldsymbol{r}},\omega)$$

$$\vec{\boldsymbol{h}}(\vec{\boldsymbol{r}},-\omega^*) = \vec{\boldsymbol{h}}^*(\vec{\boldsymbol{r}},\omega)$$

$$\vec{\boldsymbol{j}}(\vec{\boldsymbol{r}},-\omega^*) = \vec{\boldsymbol{j}}^*(\vec{\boldsymbol{r}},\omega)$$

$$\underbrace{\omega \begin{pmatrix} \overleftrightarrow{\varepsilon}(\vec{\boldsymbol{r}},\omega) & 0 \\ 0 & -\overleftrightarrow{\mu}(\vec{\boldsymbol{r}},\omega) \end{pmatrix}}_{\Gamma(\omega)} \underbrace{\begin{pmatrix} \vec{\boldsymbol{e}}(\vec{\boldsymbol{r}},\omega) \\ \vec{\boldsymbol{h}}(\vec{\boldsymbol{r}},\omega) \end{pmatrix}}_{|\Psi_\omega\rangle} - ic \underbrace{\begin{pmatrix} 0 & \boldsymbol{\nabla}\times \\ \boldsymbol{\nabla}\times & 0 \end{pmatrix}}_{\mathbb{L}} \underbrace{\begin{pmatrix} \vec{\boldsymbol{e}}(\vec{\boldsymbol{r}},\omega) \\ \vec{\boldsymbol{h}}(\vec{\boldsymbol{r}},\omega) \end{pmatrix}}_{|\Psi_\omega\rangle} = \underbrace{\begin{pmatrix} \vec{\boldsymbol{j}}(\vec{\boldsymbol{r}},\omega)/i\epsilon_0 \\ \vec{\boldsymbol{0}} \end{pmatrix}}_{|j_\omega\rangle}$$

Time harmonic Maxwell equation !

$$\omega\Gamma(\omega)|\Psi_\omega\rangle - \mathbb{L}|\Psi_\omega\rangle = |j_\omega\rangle$$

$$\hat{\Gamma}_{-\omega^*} = \hat{\Gamma}_\omega^\dagger$$

Spectral expansion of response functions

Time-harmonic equation of motion : $\omega\hat{\Gamma}_\omega|\Psi_\omega\rangle - \hat{\mathbb{L}}|\Psi_\omega\rangle = i|j_\omega\rangle$

$$\omega_\alpha\hat{\Gamma}_{\omega_\alpha}|\Psi_\alpha\rangle - \hat{\mathbb{L}}|\Psi_\alpha\rangle = 0 \qquad\qquad |\Psi_\omega\rangle \equiv \mathbb{G}(\omega)|j_\omega\rangle$$

Spectral expansion of the Green's function :

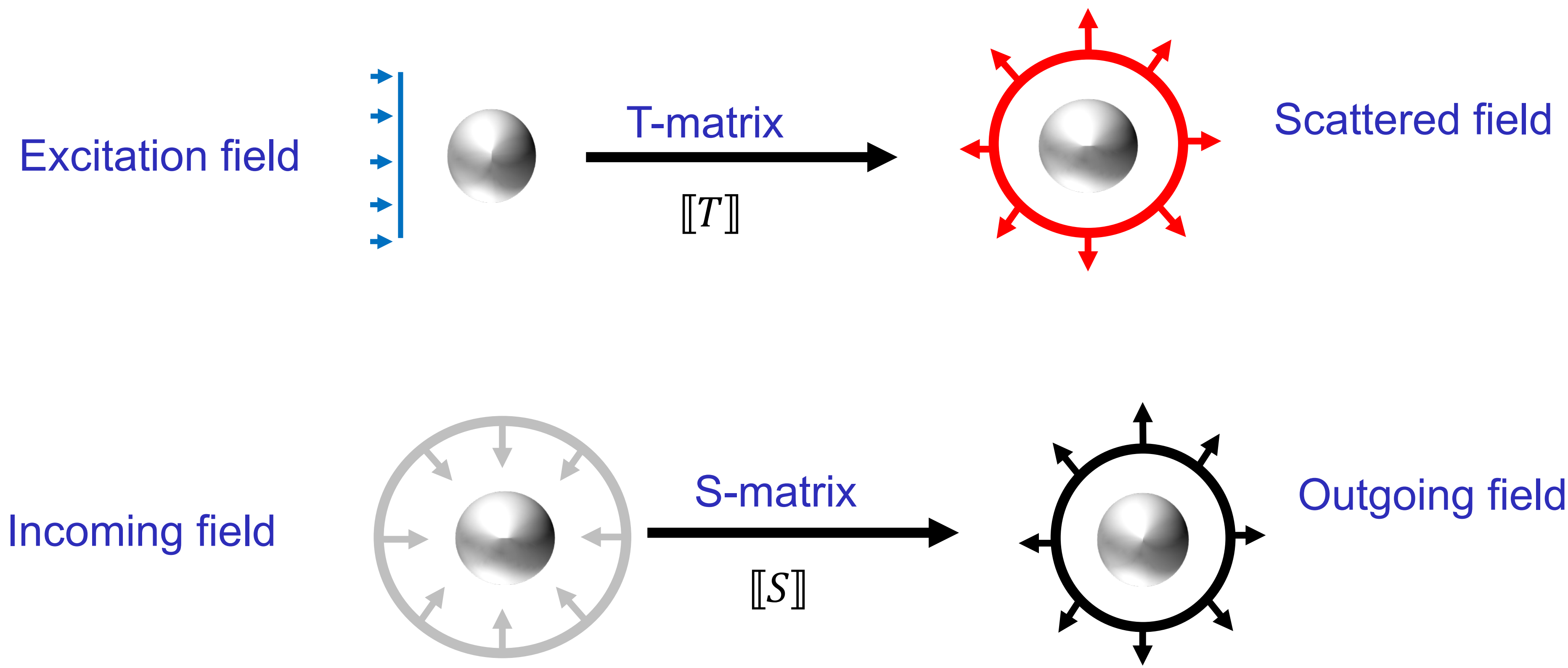
$$\left(\omega\hat{\Gamma}_\omega - \hat{\mathbb{L}}\right)\mathbb{G}(\omega) = i\mathbb{I}^{(+)} = i\sum_{\boldsymbol{\alpha}}|\Psi_\alpha\rangle\langle\Gamma_\alpha\Psi_\alpha|$$

$$\mathbb{G}(\omega) = i\sum_{\boldsymbol{\alpha}}\frac{1}{\left\langle\Psi_\alpha\right|\frac{d}{d\omega}[\omega\Gamma(\omega)]_{\omega_\alpha}\left|\Psi_\alpha\right\rangle}\frac{|\Psi_\alpha\rangle\langle\Gamma_\alpha\Psi_\alpha|}{\omega-\omega_\alpha} + \mathbb{G}_{\text{n.r.}}(\omega)$$

Resonant states correspond to S and T- matrix poles:

$$T_n(\omega_q) \to \infty \qquad S_n(\omega_q) \to \infty$$

$$\mathbb{G} = \mathbb{G}_0 + \mathbb{G}_0 \mathbb{T} \mathbb{G}_0$$



$$[\![S]\!] = 2[\![T]\!] + [\![I]\!]$$

Orthogonalization and normalization relations

Regularization insures that the symmetric operator : $\hat{\mathbb{L}} = ic\begin{pmatrix} 0 & \boldsymbol{\nabla}\times \\ \boldsymbol{\nabla}\times & 0 \end{pmatrix}$

Operates in a symmetric manner on the RS states : $\langle \hat{\mathbb{L}}\Psi_{\alpha'} | \Psi_\alpha \rangle = \langle \Psi_{\alpha'} | \hat{\mathbb{L}}\Psi_\alpha \rangle$

Given the RS equation one obtains the following “orthogonality relation” for resonant states :

$$\langle \Psi_{\alpha'}(\boldsymbol{r}')| \left[k_{\alpha'}\hat{\Gamma}_{\omega_{\alpha'}} - k_\alpha \hat{\Gamma}_{\omega_q} \right] |\Psi_\alpha\rangle = 0$$

RS normalization for a dispersive medium particles :

$$\left\langle \Psi_\alpha \left| \frac{d}{d\omega}\left(\omega\hat{\Gamma}(\vec{\boldsymbol{r}},\omega)\right)\right|_{\omega=\omega_q} \Psi_\alpha \right\rangle = \int \left[\left.\frac{d[\omega\varepsilon(\vec{\boldsymbol{r}},\omega)]}{d\omega}\right|_{\omega_\alpha} \vec{\boldsymbol{e}}_q^2(\vec{\boldsymbol{r}}) - \left.\frac{d[\omega\mu(\vec{\boldsymbol{r}},\omega)]}{d\omega}\right|_{\omega_\alpha} \vec{\boldsymbol{h}}_q^2(\vec{\boldsymbol{r}}) \right] d\boldsymbol{r} = \omega_\alpha R/\mathrm{c}$$

Regularization of the inner product

Regularization renders inner products, $\langle \Psi_{\alpha'} | \Psi_\alpha \rangle$ well defined :

Bra : $\langle \Psi_{\alpha'}| = \begin{pmatrix} \vec{\boldsymbol{e}}_{\alpha'} & \vec{\boldsymbol{h}}_{\alpha'} \end{pmatrix}$ Ket : $|\Psi_\alpha(\boldsymbol{r})\rangle = \begin{pmatrix} \vec{\boldsymbol{e}}_\alpha \\ \vec{\boldsymbol{h}}_\alpha \end{pmatrix}$

Inner product : $\langle \Psi_{\alpha'} | \Psi_\alpha \rangle = \int d\vec{\boldsymbol{r}} \begin{pmatrix} \vec{\boldsymbol{e}}_{\alpha'}(\vec{\boldsymbol{r}}) & \vec{\boldsymbol{h}}_{\alpha'}(\vec{\boldsymbol{r}}) \end{pmatrix} \cdot \begin{pmatrix} \vec{\boldsymbol{e}}_\alpha(\vec{\boldsymbol{r}}) \\ \vec{\boldsymbol{h}}_\alpha(\vec{\boldsymbol{r}}) \end{pmatrix}$

Developing the field on a multipole basis the Gaussian regularization can be reduced to regularizing integrals of spherical Hankel functions that integrated to infinity. We obtain analytical integrals of the form :

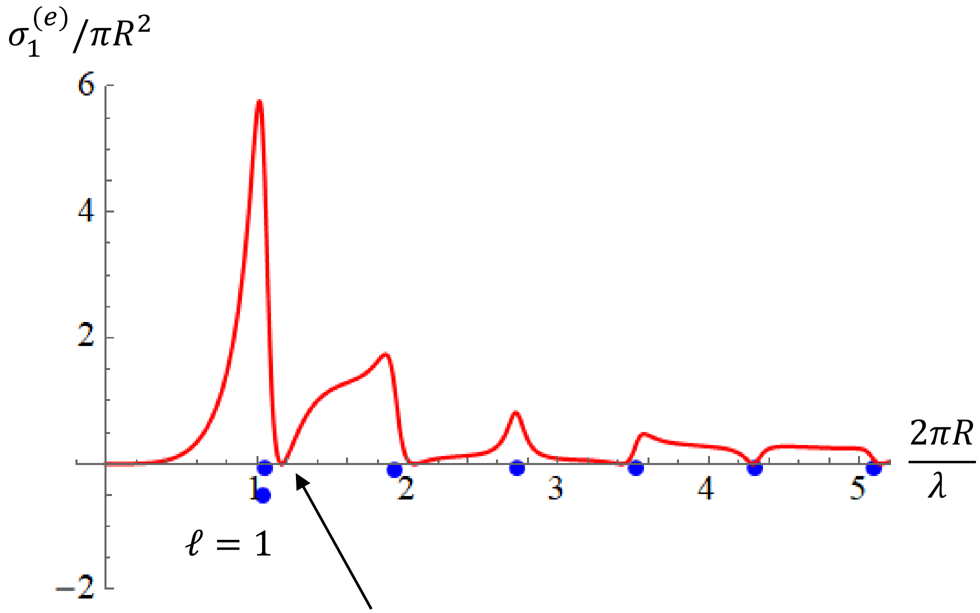
$$\lim_{\eta \to 0} \int_1^\infty r^2 e^{-\eta r^2} \left[h_n^{(+)}(z_\alpha r) \right] dr = -\frac{1}{2} z_q \frac{[\xi_n'(z_\alpha)]^2 + \xi_n^2(z_\alpha) - n(n+1) h_n^2(z_\alpha) - h_n(z_\alpha) \xi_n'(z_\alpha)}{k_{z_\alpha}^3}$$

Outgoing spherical Hankel functions :

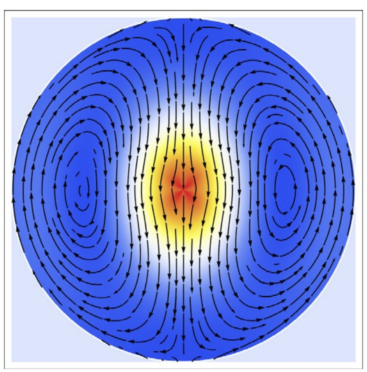
$$h_n(z) = h_n^{(+)}(z) \equiv j_n(z) + i y_n(z)$$
$$\xi_n(z) \equiv z h_n^{(+)}(z)$$

$$h_0^{(+)}(z) = -\frac{i}{z} e^{iz}$$
$$h_1^{(+)}(z) = -e^{iz} \left(\frac{1}{z} + \frac{i}{z^2} \right)$$
$$\vdots$$

Explain physical phenomena using RS (QNMs) with well-defined normalizations

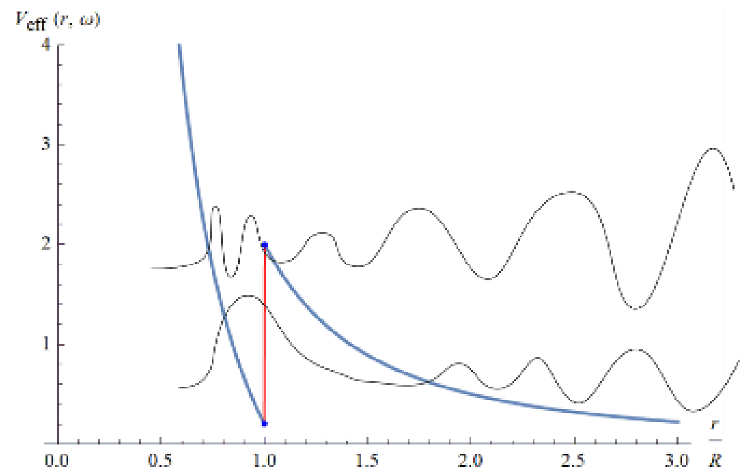


"Anapole"



$$a_1 = \frac{\frac{\varepsilon_s}{\varepsilon_b} j_1(k_s R)\psi'_1(kR) - \psi'_1(k_s R) j_1(kR)}{\frac{\varepsilon_s}{\varepsilon_b} j_1(k_s R)\xi'_1(kR) - \psi'_1(k_s R) h_1(kR)}$$

$$\sigma_1^{(e)} = \frac{6\pi}{k^2}|a_1|^2$$



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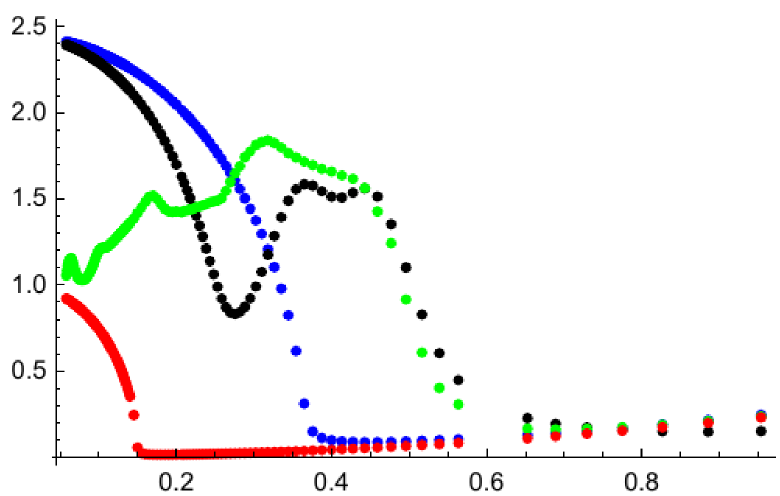
Disperson models for real metals (Gold)

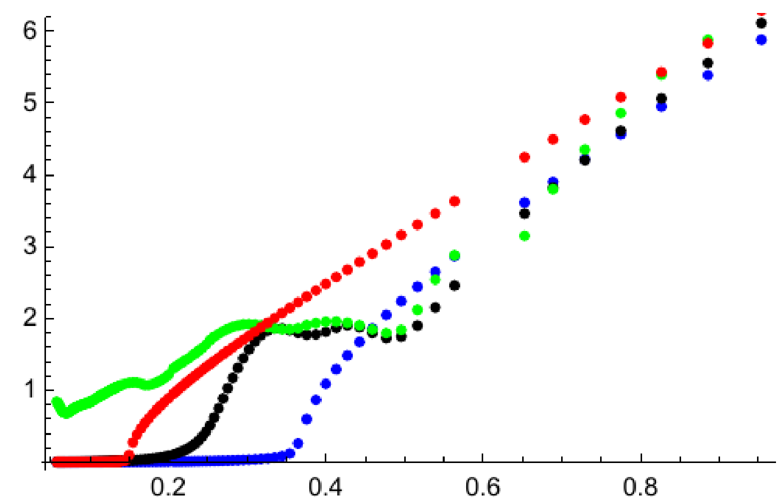
Drude model

$$\varepsilon(\omega) = \varepsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\omega\Gamma_D}$$

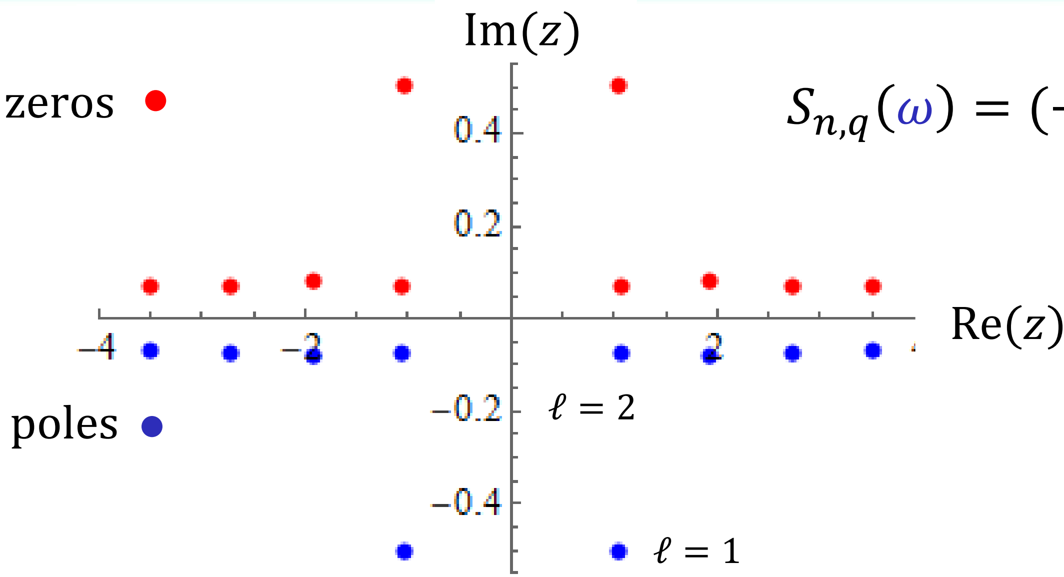
Drude-Lorenz model

$$\varepsilon(\omega) = \varepsilon_\infty - \frac{\omega_{pD}^2}{\omega^2 + i\omega\Gamma_D} - s_1 \frac{\omega_{p1,L}^2}{\omega^2 - \omega_{p1,L}^2 + i\Gamma_{1,L}\omega} - s_2 \frac{\omega_{p2,L}^2}{\omega^2 - \omega_{p2,L}^2 + i\Gamma_{2,L}\omega}$$



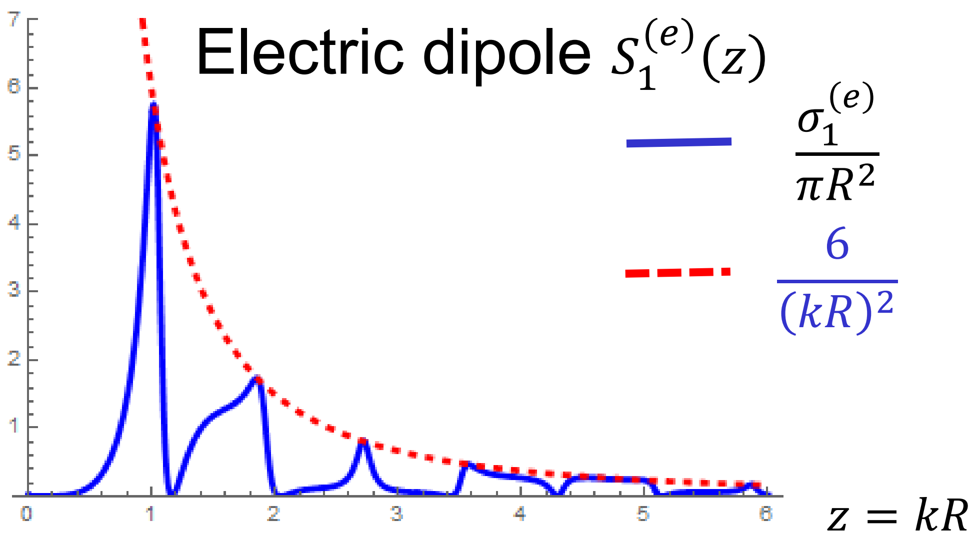


Spectral expansions of the $S_{n,q}(\omega)$ and $T_{n,q}(\omega)$ functions for spherical scatterers



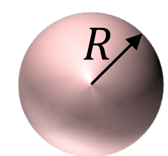
$$S_{n,q}(\omega) = (-1)^{n+q} e^{-2iz} + e^{-2iz}(-1)^{n+q} \sum_{\ell=-\infty}^{\infty} \frac{2r_\alpha}{z - z_\alpha}$$

$$q = 0 \quad (h)$$
$$q = 1 \quad (e)$$



$$z = \omega \frac{R}{c} = kR$$

$$z_\alpha = \omega_\alpha \frac{R}{c}$$

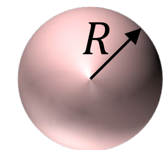


T-matrix (Mie) residues are determined by RS normalization !

$$r_\alpha = \frac{i e^{2iz_\alpha}}{\mathcal{N}_\alpha^2}$$

$$z = \omega \frac{R}{c}$$

$$z_\alpha = \omega_\alpha \frac{R}{c}$$



$$T_{n,q}(\omega) = \underbrace{\frac{(-1)^{n+q} e^{-2iz} - 1}{2}}_{\text{Non-resonant term !}} + \underbrace{e^{-2iz} \sum_{\ell=-\infty}^{\infty} \frac{r_\alpha}{z - z_\alpha}}_{\text{resonant state spectral expansion}}$$

$q = 0 \quad (h)$
$q = 1 \quad (e)$