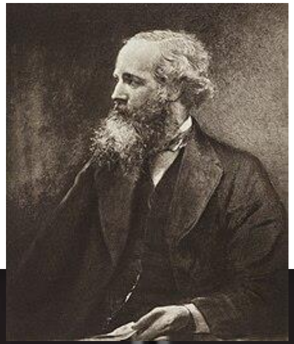
Mie Theory in Ocean Optics

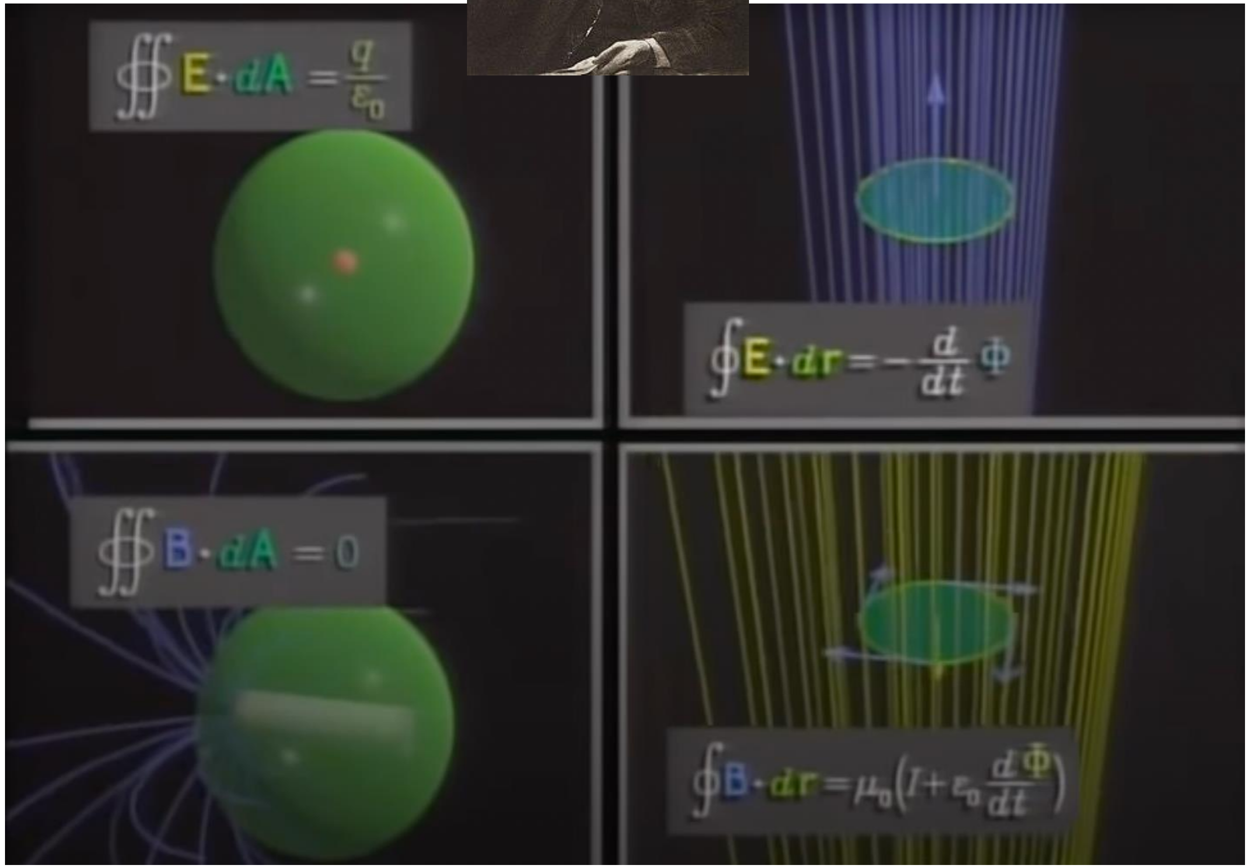
Patrick Gray

with much inspiration from Curt Mobley and Emmanuel Boss

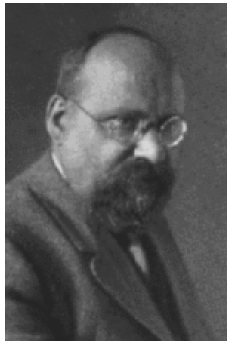
<u>If not referenced all figures are from Mobley 2022</u>

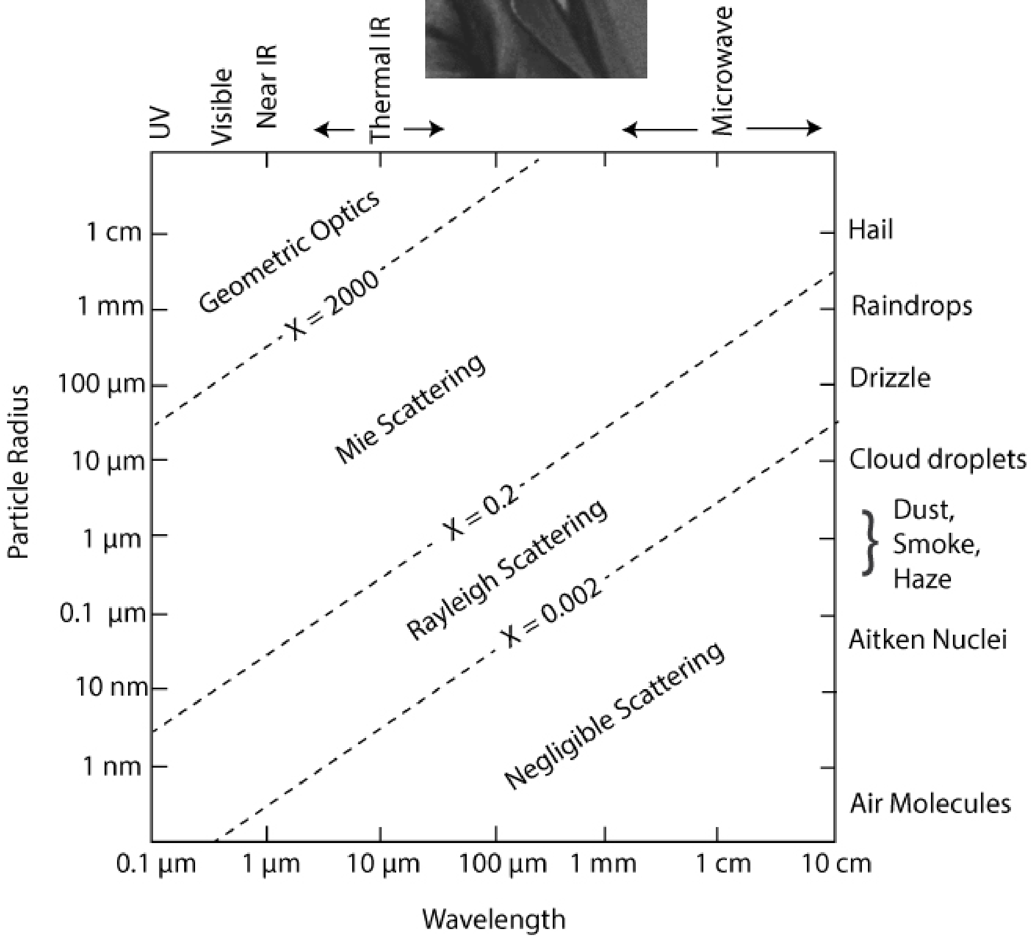
Thanks James and Gustav!





Caltech *Mechanical Universe and Beyond*
Maxwell's Equations https://www.youtube.com/watch?v=SS4tcajTsW8





X = (pi*diam*n)/ lambda

Some review

- “fundamentally, elastic scattering occurs when there is a change in the real part of the index of refraction from one spatial location to another.” – Mobley
- What is the refractive index?

$$n = \frac{c}{v}$$

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$$n = \frac{c}{v} = \sqrt{\frac{\mu\epsilon}{\mu_o\epsilon_o}}$$

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- What is the refractive index?

$$\underbrace{n}_{\text{ref index}} = \frac{\overbrace{c}^{\text{speed of light in vacuum}}}{\underbrace{v}_{\text{speed of light in the medium}}} = \sqrt{\frac{\mu\epsilon}{\mu_0\epsilon_0}}$$

magnetic permeability: μ

electric permittivity: ϵ

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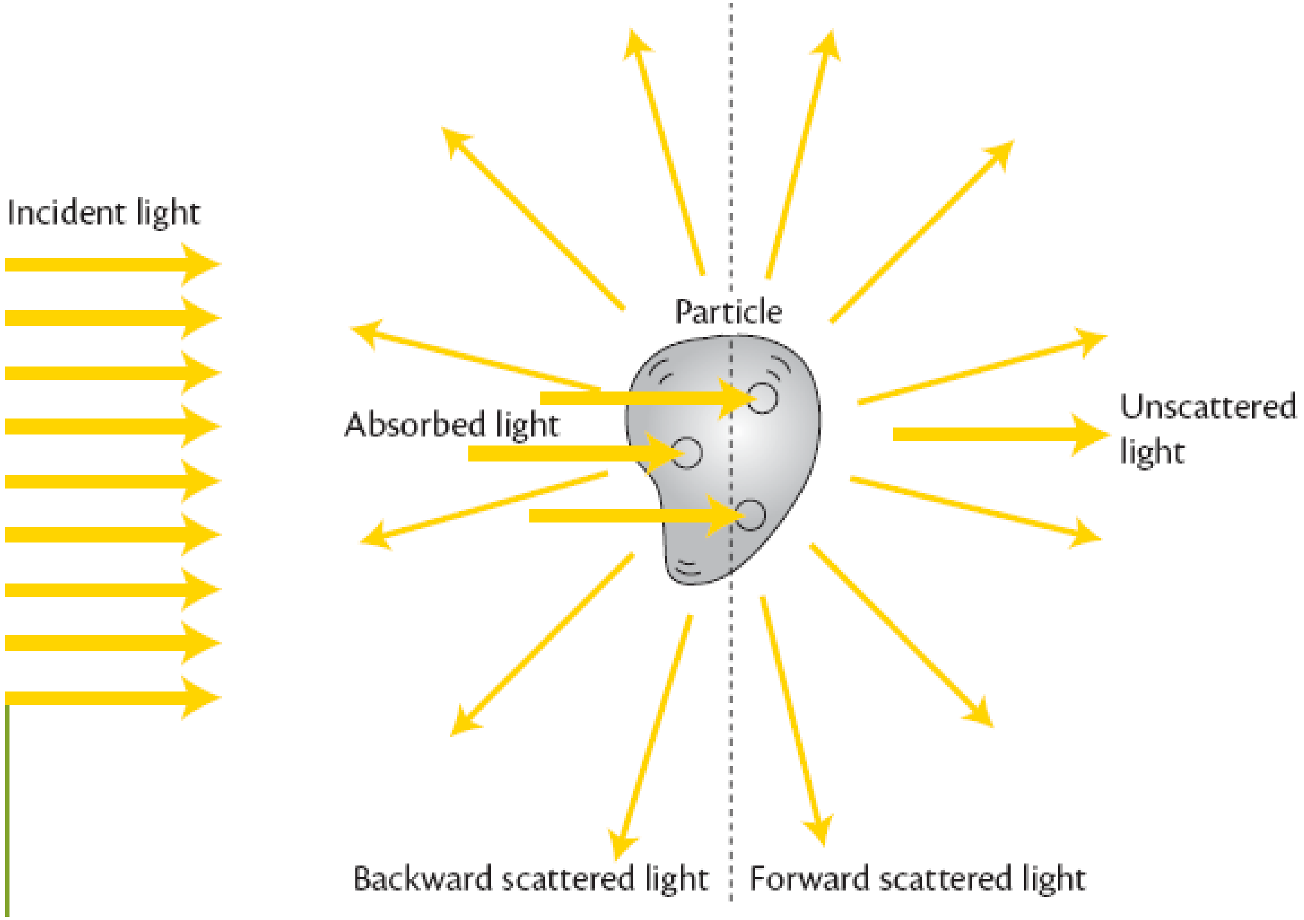
- **Embed particles!**

Mie?



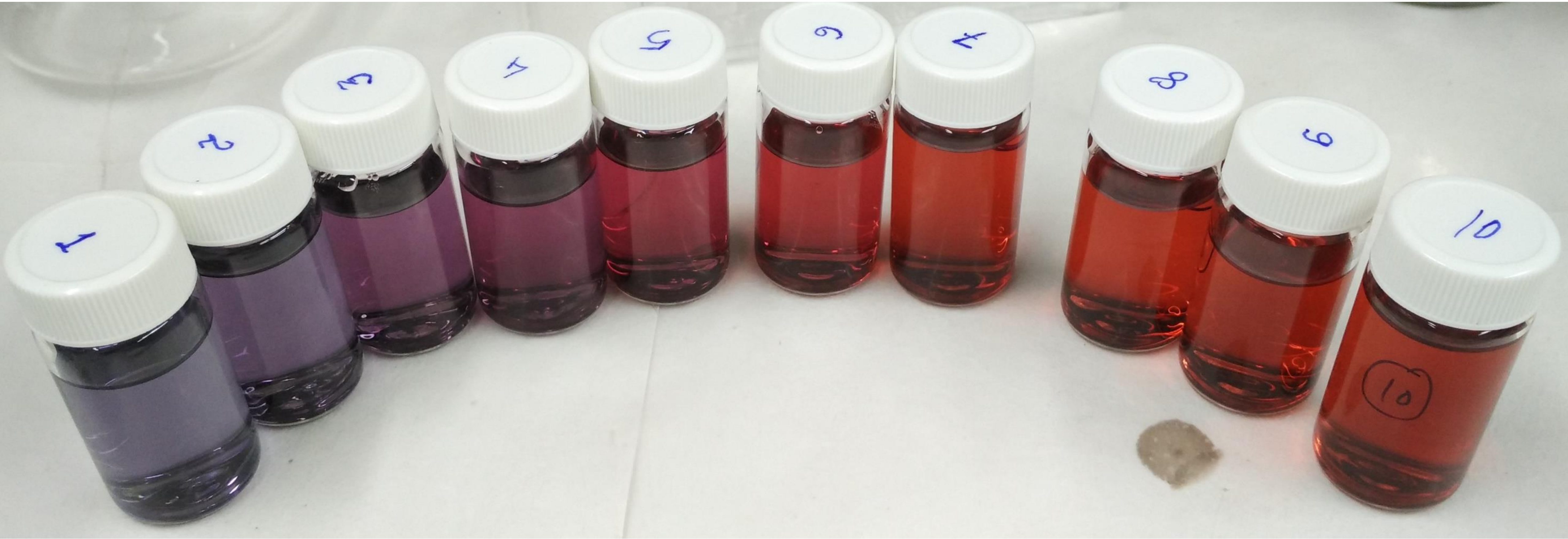
Given a particle of a specified size, shape and refractive index that is illuminated by an arbitrarily polarized monochromatic wave, determine the EM field at all points in the particles and at all points of the homogeneous medium in which it is embedded.

Why do we care?

For a given population of particles, we can develop hypotheses and expectations.

Because we can make nearly perfect spherical particles of known size and refractive index and these solutions provide a calibration to our sensors (LISST, bbs, flow-cytometers).

Origins of Gustav’s Curiosity?



Setting up the problem:

- A single homogenous sphere of radius ρ with a complex index of refraction:

$$m_s = n_s + ik_s$$

- k_s is related to the absorption coefficient via:

$$a_s(\lambda) = 4\pi k_s(\lambda)/\lambda$$

- This sphere is embedded in a homogenous non-absorbing medium:

$$m_m = n_m$$

Gustav's goal, and now our goal → find how the incident light is absorbed and scattered including the angular distribution of scattered light and its state of polarization

$$
\left\{
\begin{aligned}
&K_1(-x) = -\frac{i}{x}\cdot e^{-ix}.(1+ix),\\
&K_2(-x) = -\frac{3}{x^2}\cdot e^{-ix}.\left(\left(1-\frac{1}{3}x^2\right)+i.x\right),\\
&K_3(-x) = +\frac{15.i}{x^3}\cdot e^{-ix}.\left(\left(1-\frac{2}{5}x^2\right)+i.x.\left(1-\frac{1}{15}x^2\right)\right),\\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\
&K_\nu(-x) = (-i)^\nu\,\frac{1.3..(2\nu-1)}{x^\nu}\cdot e^{-ix}\\
&\quad\cdot\left\{\left(1+\sum_{1}^{\frac{\nu(-1)}{2}}{}_{\sigma}\,\frac{(\nu-\sigma)_\sigma(-1)^\sigma}{(2\nu-1)(2\nu-3)..(2\nu-2\sigma+1)}\cdot\frac{x^{2\sigma}}{1.3..(2\sigma-1)}\right)\right.\\
&\quad\left.+ix.\left(1+\sum_{1}^{\frac{\nu(+1)}{2}-1}{}_{\sigma}\,\frac{(\nu-\sigma-1)_\sigma(-1)^\sigma}{(2\nu-1)(2\nu-3)..(2\nu-2\sigma+1)}\cdot\frac{x^{2\sigma}}{1.3..(2\sigma+1)}\right)\right\}.
\end{aligned}
\right.
\tag{27}
$$

$$
\left\{
\begin{aligned}
&K_1'(-x) = +\frac{i}{x^2}\cdot e^{-ix}.\left((1-x^2)+ix\right),\\
&K_2'(-x) = +\frac{6}{x^3}\cdot e^{-ix}.\left(\left(1-\frac{1}{2}x^2\right)+ix.\left(1-\frac{1}{6}x^2\right)\right),\\
&K_3'(-x) = -\frac{45.i}{x^4}\cdot e^{-ix}.\left(\left(1-\frac{7}{15}x^2+\frac{1}{45}x^4\right)+ix.\left(1-\frac{2}{15}\cdot x^2\right)\right),\\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\
&K_\nu'(-x) = -(-i)^\nu.\nu\cdot\frac{1.3..(2\nu-1)}{x^{\nu+1}}\cdot e^{-ix}\\
&\quad\cdot\left\{\left(1+\sum_{1}^{\frac{\nu(+1)}{2}}{}_{\sigma}(-1)^\sigma\,\frac{(\nu-\sigma)_\sigma+\frac{2\sigma-1}{\nu}\cdot(\nu-\sigma)_{\sigma-1}}{(2\nu-1)(2\nu-3)..(2\nu-2\sigma+1)}\cdot\frac{x^{2\sigma}}{1.3..(2\sigma-1)}\right)\right.\\
&\quad\left.+i.x.\left(1+\sum_{1}^{\frac{\nu(-1)}{2}}{}_{\sigma}(-1)^\sigma\,\frac{(\nu-\sigma-1)_\sigma+\frac{2\sigma+1}{\nu}\cdot(\nu-\sigma-1)_{\sigma-1}}{(2\nu-1)(2\nu-3)...(2\nu-2\sigma+1)}\cdot\frac{x^{2\sigma}}{1.3..(2\sigma+1)}\right)\right\}.
\end{aligned}
\right.
\tag{28}
$$

$$
\left\{
\begin{aligned}
&I_1(x) = \frac{x^2}{3}\cdot\left(1-\frac{3}{5}\cdot\frac{x^2}{3!}+\frac{3}{7}\cdot\frac{x^4}{5!}-\frac{3}{9}\cdot\frac{x^6}{7!}+\ldots\right),\\
&I_2(x) = \frac{x^3}{15}\cdot\left(1-\frac{3}{7}\cdot\frac{x^2}{3!}+\frac{3.5}{7.9}\cdot\frac{x^4}{5!}-\frac{3.5}{9.11}\cdot\frac{x^6}{7!}+\ldots\right),\\
&I_3(x) = \frac{x^4}{105}\cdot\left(1-\frac{3}{9}\cdot\frac{x^2}{3!}+\frac{3.5}{9.11}\cdot\frac{x^4}{5!}-\frac{3.5.7}{9.11.13}\cdot\frac{x^6}{7!}+\ldots\right),\\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\
&I_\nu(x) = \frac{x^{\nu+1}}{1.3..(2\nu+1)}\cdot\left(1-\frac{3}{2\nu+3}\cdot\frac{x^2}{3!}+\frac{3.5}{(2\nu+3)(2\nu+5)}\cdot\frac{x^4}{5!}\right.\\
&\qquad\left.-\frac{3.5.7}{(2\nu+3)(2\nu+5)(2\nu+7)}\cdot\frac{x^6}{7!}+\ldots\right).
\end{aligned}
\right.
\tag{29}
$$

$$
\left\{
\begin{aligned}
&I_1'(x) = \frac{2.x}{3}\cdot\left(1-2\cdot\frac{3}{5}\cdot\frac{x^2}{3!}+3\cdot\frac{3}{7}\cdot\frac{x^4}{5!}-4\cdot\frac{3}{9}\cdot\frac{x^6}{7!}+\ldots\right),\\
&I_2'(x) = \frac{3.x^2}{15}\cdot\left(1-\frac{5}{7}\cdot\frac{x^2}{3!}+\frac{5}{9}\cdot\frac{x^4}{5!}-\frac{5}{11}\cdot\frac{x^6}{7!}+\ldots\right),\\
&I_3'(x) = \frac{4.x^3}{104}\cdot\left(1-\frac{3}{2}\cdot\frac{3}{9}\cdot\frac{x^2}{3!}+\frac{4}{2}\cdot\frac{3.5}{9.11}\cdot\frac{x^4}{5!}\right.\\
&\qquad\left.-\frac{5}{2}\cdot\frac{3.5.7}{9.11.13}\cdot\frac{x^6}{7!}+\ldots\right),\\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\
&I_\nu'(x) = \frac{(\nu+1).x^\nu}{1.3..(2\nu+1)}\cdot\left(1-\frac{\nu+3}{\nu+1}\cdot\frac{3}{2\nu+3}\cdot\frac{x^2}{3!}\right.\\
&\qquad\left.+\frac{\nu+5}{\nu+1}\cdot\frac{3.5}{(2\nu+1)(2\nu+5)}\cdot\frac{x^4}{5!}-\ldots\right).
\end{aligned}
\right.
\tag{30}
$$

Diese Reihen sind für Zahlenrechnungen meistens weit bequemer als die endlichen Ausdrücke, die man nach (24) für I_ν und I_ν' bekommt. Für andere Zwecke muß man aber auch diese kennen:

$$
\left\{
\begin{aligned}
&I_1(x) = -\cos x+\frac{\sin x}{x},\\
&I_2(x) = -\sin x-\frac{3.\cos x}{x}+\frac{3.\sin x}{x^2},\\
&I_3(x) = +\cos x-\frac{6.\sin x}{x}-\frac{15.\cos x}{x^2}+\frac{15.\sin x}{x^3},\\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\
&I_\nu(x) = \sin\left(x-\frac{\nu\pi}{2}\right)+\sum_{1}^{\nu}{}_{r}\sin\left(x-\frac{(\nu-r)\pi}{2}\right)\\
&\qquad\cdot\frac{(\nu+r)!}{(\nu-r)!\,r!}\cdot\frac{1}{2^r.x^r}.
\end{aligned}
\right.
\tag{29a}
$$

$$
\left\{
\begin{aligned}
&I_1'(x) = +\sin x+\frac{\cos x}{x}-\frac{\sin x}{x^2},\\
&I_2'(x) = -\cos x+\frac{3.\sin x}{x}+\frac{6.\cos x}{x^2}-\frac{6.\sin x}{x^3},\\
&I_3'(x) = -\sin x-\frac{6.\cos x}{x}+\frac{21.\sin x}{x^2}+\frac{45.\cos x}{x^3}-\frac{45.\sin x}{x^4},\\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\
&I_\nu'(x) = \cos\left(x-\frac{\nu.\pi}{2}\right)+\sum_{1}^{\nu+1}{}_{r}\cos\left(x-\frac{(\nu-r)\pi}{2}\right)\\
&\qquad\cdot\frac{(\nu+r-1)!}{(\nu-r+1)!\,r!}\cdot\frac{\left(\nu(\nu+1)+r(r-1)\right)}{2^r.x^r}.
\end{aligned}
\right.
\tag{30a}
$$

Approaching the solution

- “Readers of Mie (1908) will have acquired virtue through suffering”

  – B&H 1983

- Recommended versions of the details:
  - van de Hulst (1957)
  - Bohren and Huffman (1983)
  - Mobley (2022)

Amplitude scattering matrix

- For any particle we can describe the scattered wave as:

$$\begin{bmatrix} E_{\|\mathrm{s}} \\ E_{\perp\mathrm{s}} \end{bmatrix} = \frac{e^{ik(r-z)}}{-ikr} \begin{bmatrix} S_2 & S_3 \\ S_4 & S_1 \end{bmatrix} \begin{bmatrix} E_{\|\mathrm{i}} \\ E_{\perp\mathrm{i}} \end{bmatrix} .$$

Amplitude scattering matrix

- For any *spherical* particle we can describe the scattered wave as:

$$\begin{bmatrix} E_{\|\mathrm{s}} \\ E_{\perp\mathrm{s}} \end{bmatrix} = \frac{e^{ik(r-z)}}{-ikr} \begin{bmatrix} S_2 & \cancel{S_3} \\ \cancel{S_4} & S_1 \end{bmatrix} \begin{bmatrix} E_{\|\mathrm{i}} \\ E_{\perp\mathrm{i}} \end{bmatrix} .$$

Mie Inputs

Size parameter →

$$x = \frac{2\pi\rho}{\lambda_{\mathrm{m}}} = \frac{2\pi\,\rho\,n_{\mathrm{m}}}{\lambda}$$

Refractive index relative to the medium →

$$m = \frac{n_{\mathrm{s}}}{n_{\mathrm{m}}} + i\,\frac{k_{\mathrm{s}}}{n_{\mathrm{m}}}$$

Mie Inputs

Size parameter →

radius

ref index of medium

$$x = \frac{2\pi\rho}{\lambda_{\mathrm{m}}} = \frac{2\pi\,\rho\,n_{\mathrm{m}}}{\lambda}$$

wavelength in medium

wavelength in vacuum

Refractive index relative to the medium →

real part of ref index

imaginary part of ref index (related to absorption)

$$m = \frac{n_{\mathrm{s}}}{n_{\mathrm{m}}} + i\,\frac{k_{\mathrm{s}}}{n_{\mathrm{m}}}$$

real part of ref index of the medium

real part of ref index of the medium

Solution

"Mie's solution is in the form of infinite series of very complicated mathematical functions." - Mobley

$$S_1 = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} (a_n \pi_n + b_n \tau_n)$$

$$S_2 = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} (a_n \tau_n + b_n \pi_n)$$

"You eventually get down to something normal people can understand, likes sines and cosines." - Curt

$$a_n = \frac{m\,\psi_n(mx)\,\psi_n'(x) - \psi_n(x)\,\psi_n'(mx)}{m\,\psi_n(mx)\,\xi_n'(x) - \xi_n(x)\,\psi_n'(mx)}$$

$$b_n = \frac{\psi_n(mx)\,\psi_n'(x) - m\,\psi_n(x)\,\psi_n'(mx)}{\psi_n(mx)\,\xi_n'(x) - m\,\xi_n(x)\,\psi_n'(mx)}$$

Spherical Bessel functions

Riccati-Bessel functions

Solution

What happens when *m* = 1 + *i*0? i.e. the refractive index is the same as the medium?

$$S_1 = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} \left(a_n \pi_n + b_n \tau_n\right)$$

$$S_2 = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} \left(a_n \tau_n + b_n \pi_n\right)$$

$$a_n = \frac{m\,\psi_n(mx)\,\psi_n'(x) - \psi_n(x)\,\psi_n'(mx)}{m\,\psi_n(mx)\,\xi_n'(x) - \xi_n(x)\,\psi_n'(mx)}$$

$$b_n = \frac{\psi_n(mx)\,\psi_n'(x) - m\,\psi_n(x)\,\psi_n'(mx)}{\psi_n(mx)\,\xi_n'(x) - m\,\xi_n(x)\,\psi_n'(mx)}$$

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$$b_n = \xcancel{\frac{\psi_n(mx)\,\psi_n'(x) - m\,\psi_n(x)\,\psi_n'(mx)}{\psi_n(mx)\,\xi_n'(x) - m\,\xi_n(x)\,\psi_n'(mx)}}$$

From scattering amplitudes to Mueller Matrix

- Most Mie codes output S1 and S2 “the scattering amplitudes”

$$\begin{pmatrix} I_s \\ Q_s \\ U_s \\ V_s \end{pmatrix} = \frac{1}{k^2 r^2} \begin{pmatrix} S_{11} & S_{12} & S_{13} & S_{14} \\ S_{21} & S_{22} & S_{23} & S_{24} \\ S_{31} & S_{32} & S_{33} & S_{34} \\ S_{41} & S_{42} & S_{43} & S_{44} \end{pmatrix} \begin{pmatrix} I_i \\ Q_i \\ U_i \\ V_i \end{pmatrix}$$

$$S_{11} = \tfrac{1}{2}\left(|S_1|^2 + |S_2|^2 + |S_3|^2 + |S_4|^2\right),$$

$$S_{12} = \tfrac{1}{2}\left(|S_2|^2 - |S_1|^2 + |S_4|^2 - |S_3|^2\right),$$

Bohren and Huffman, pg 62

More practically…

- Most Mie codes output S1 and S2 “the scattering amplitudes”
- The VSF we know and love can be easily calculated as:

$$\tilde{\beta} = \frac{1}{2}\left(|S_1|^2 + |S_2|^2\right) = \frac{1}{2}\left(S_1 S_1^* + S_2 S_2^*\right)$$

- The other outputs are typically absorption and scattering efficiencies:
  - Q_a → fraction of incident radiant energy absorbed by the sphere
  - Q_b → fraction of incident radiant energy scattered by the sphere

“incident” defined as the energy that hits the sphere’s cross-sectional area

More practically…

- You may also see absorption or scattering cross sections:

$$\sigma_{\mathrm{a}} = Q_{\mathrm{a}} A_{\mathrm{s}} = Q_{\mathrm{a}} \pi \rho^2 \qquad (\mathrm{m}^2)$$

How does this depart from what we measure?

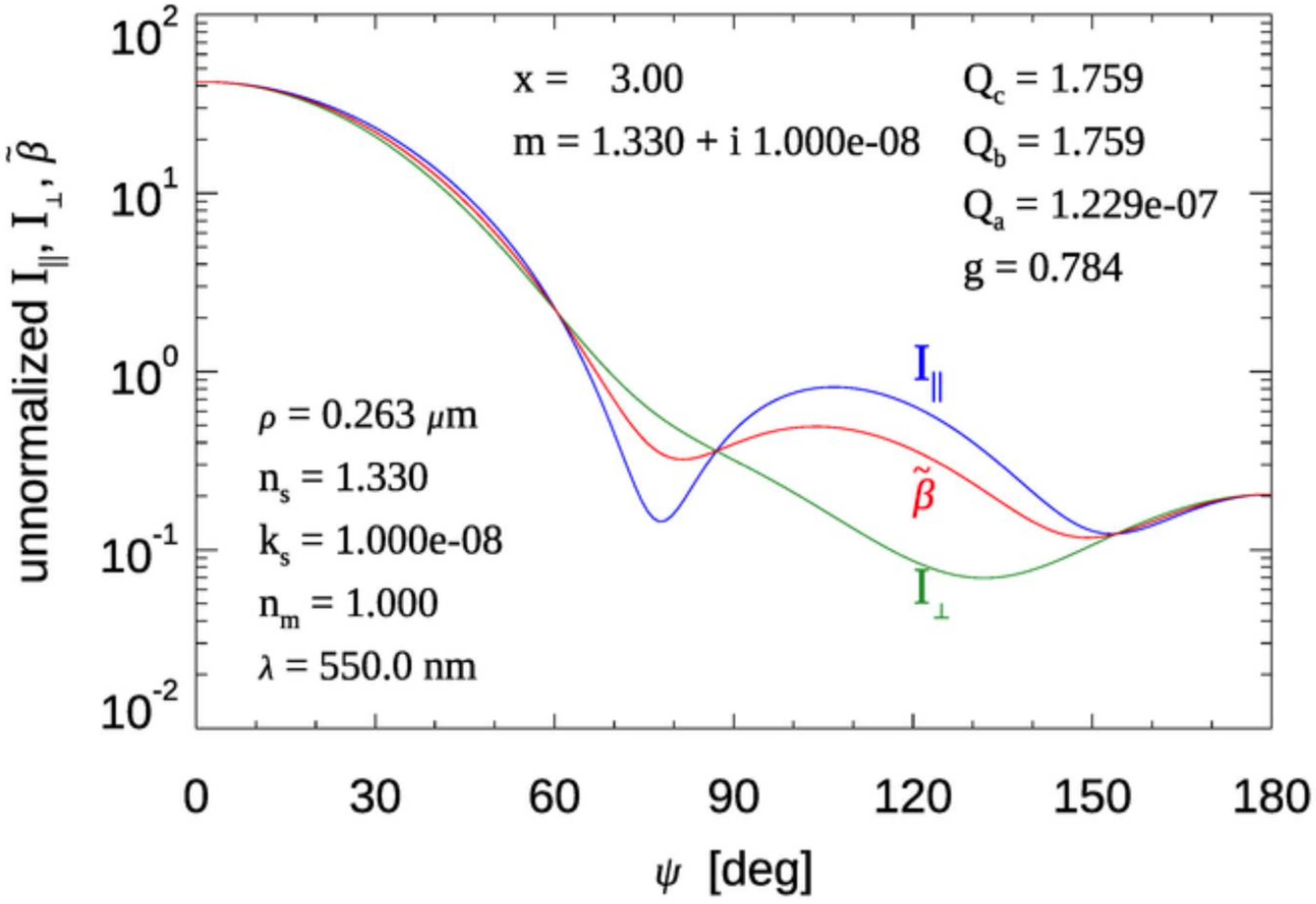
$$b(\rho) = \mathcal{N}(\rho)\, \sigma_{\mathrm{b}}(\rho) \qquad (\mathrm{m}^{-1})$$

N is per m^3

$$b(\text{all sizes}) = \int_0^{\infty} \sigma_{\mathrm{b}}(\rho)\, PSD(\rho)\ d\rho$$

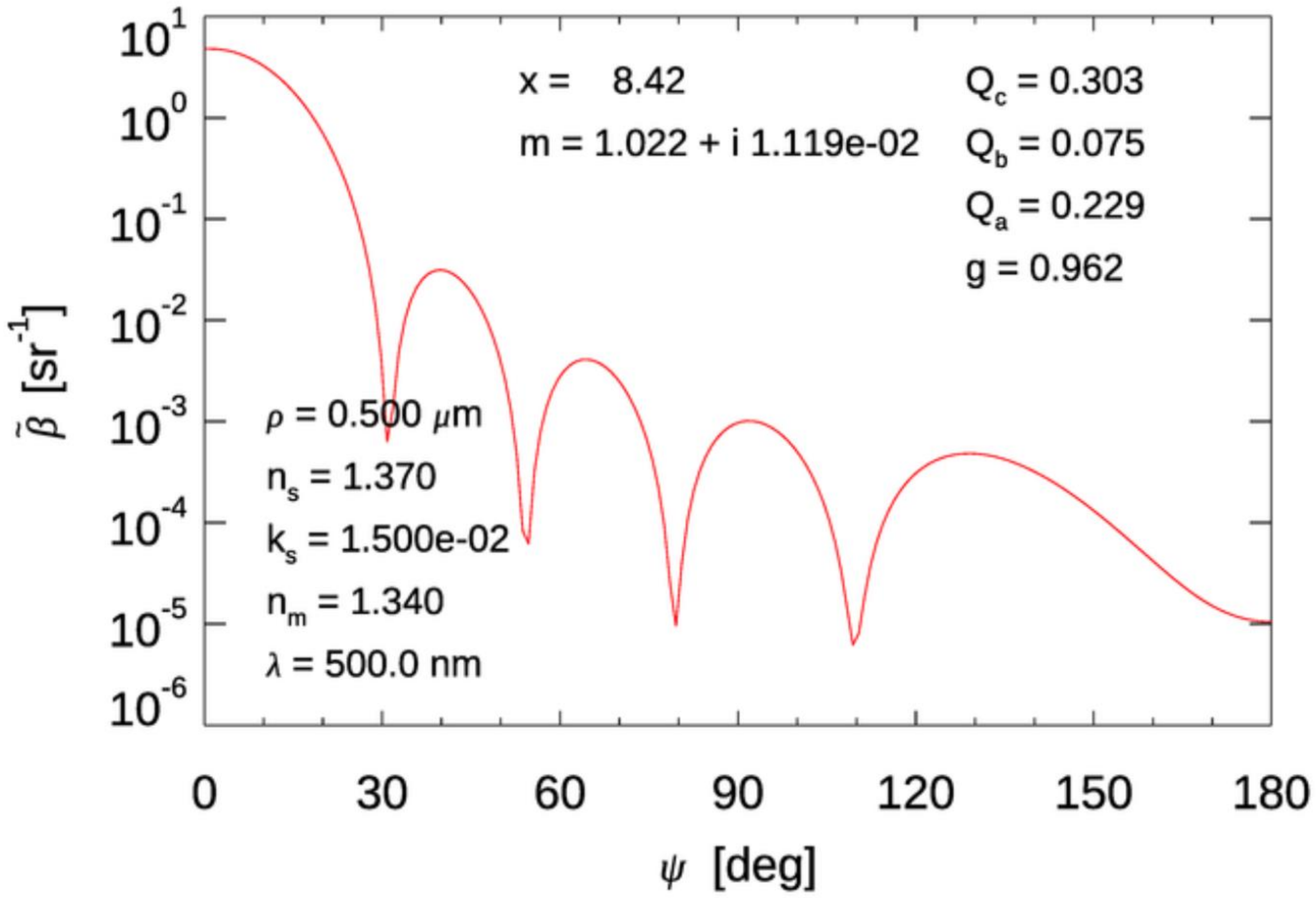
$$b(\text{all sizes, all types}) = \sum_{i=1}^{M} \sum_{j=\rho_{\min}}^{\rho_{\max}} \sigma_{\mathrm{b}}(\rho_j, i)\, PSD(\rho_j, i)\ \Delta\rho_j$$

So what does this look like for particles we care about?



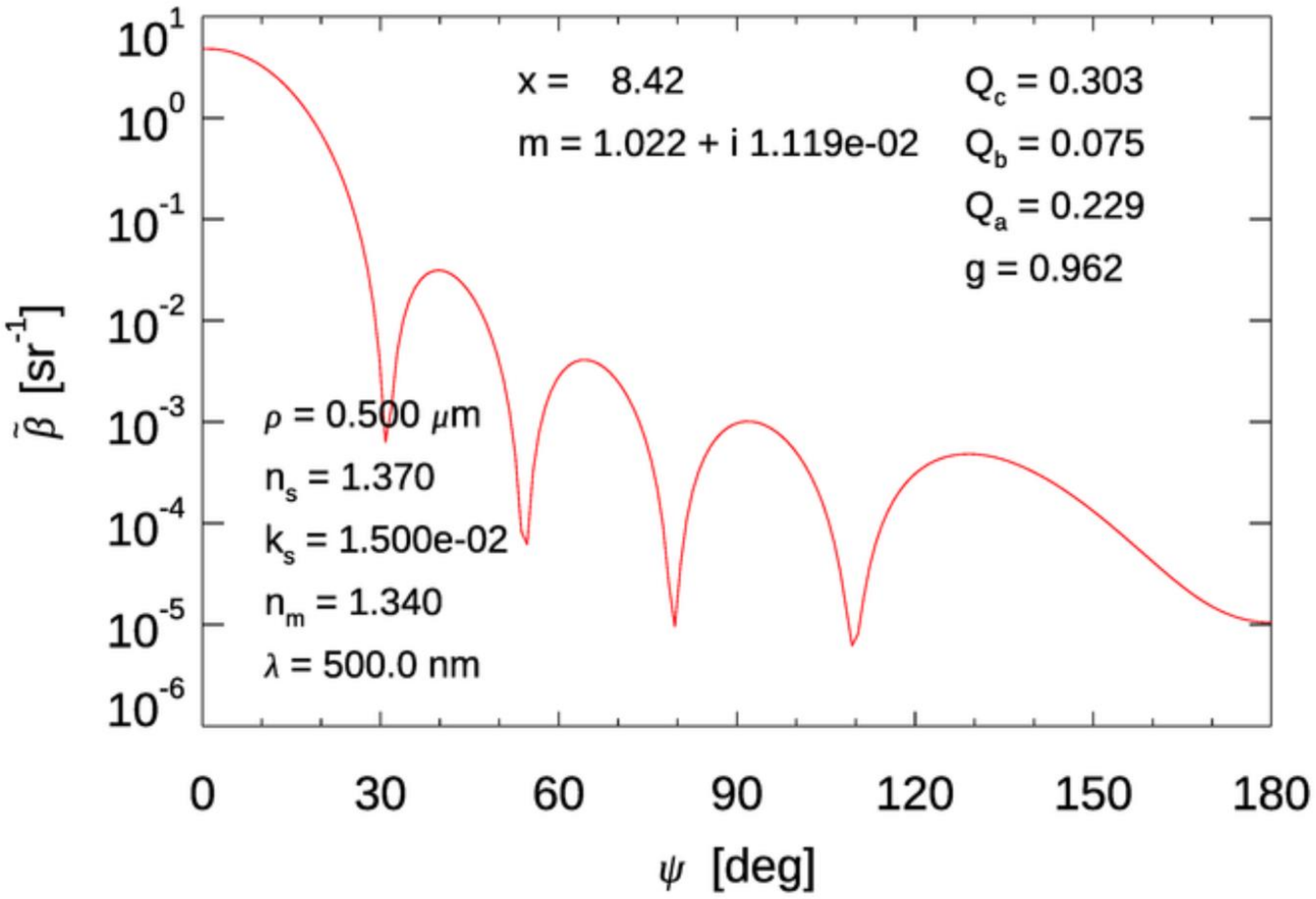
B&H, modified by Mobley

Something more like a phyto?



Something more like a phyto?

What does this pattern make you think of?



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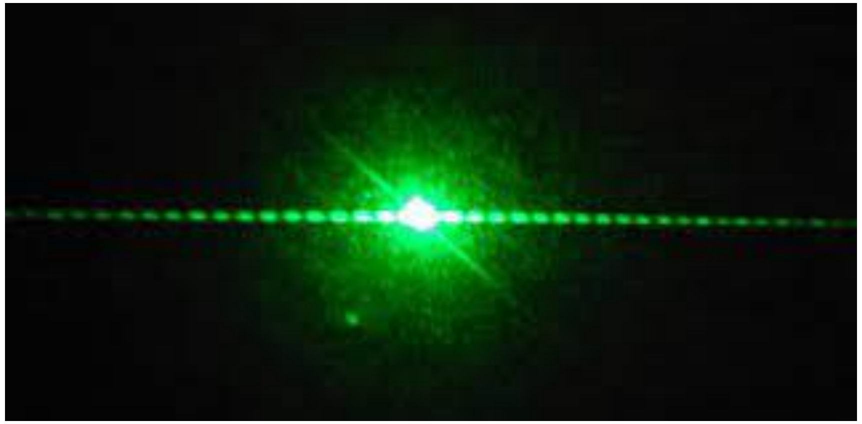
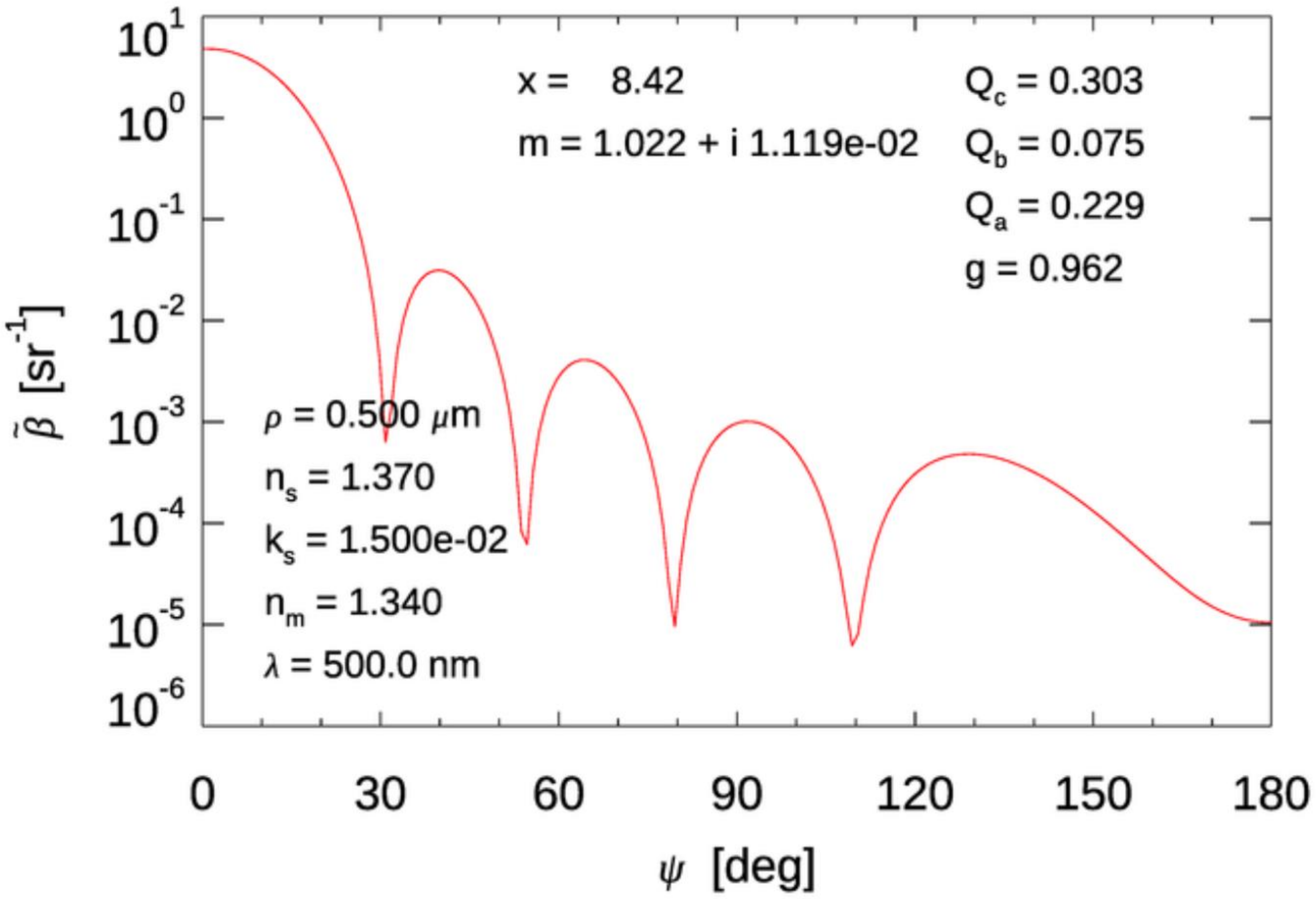
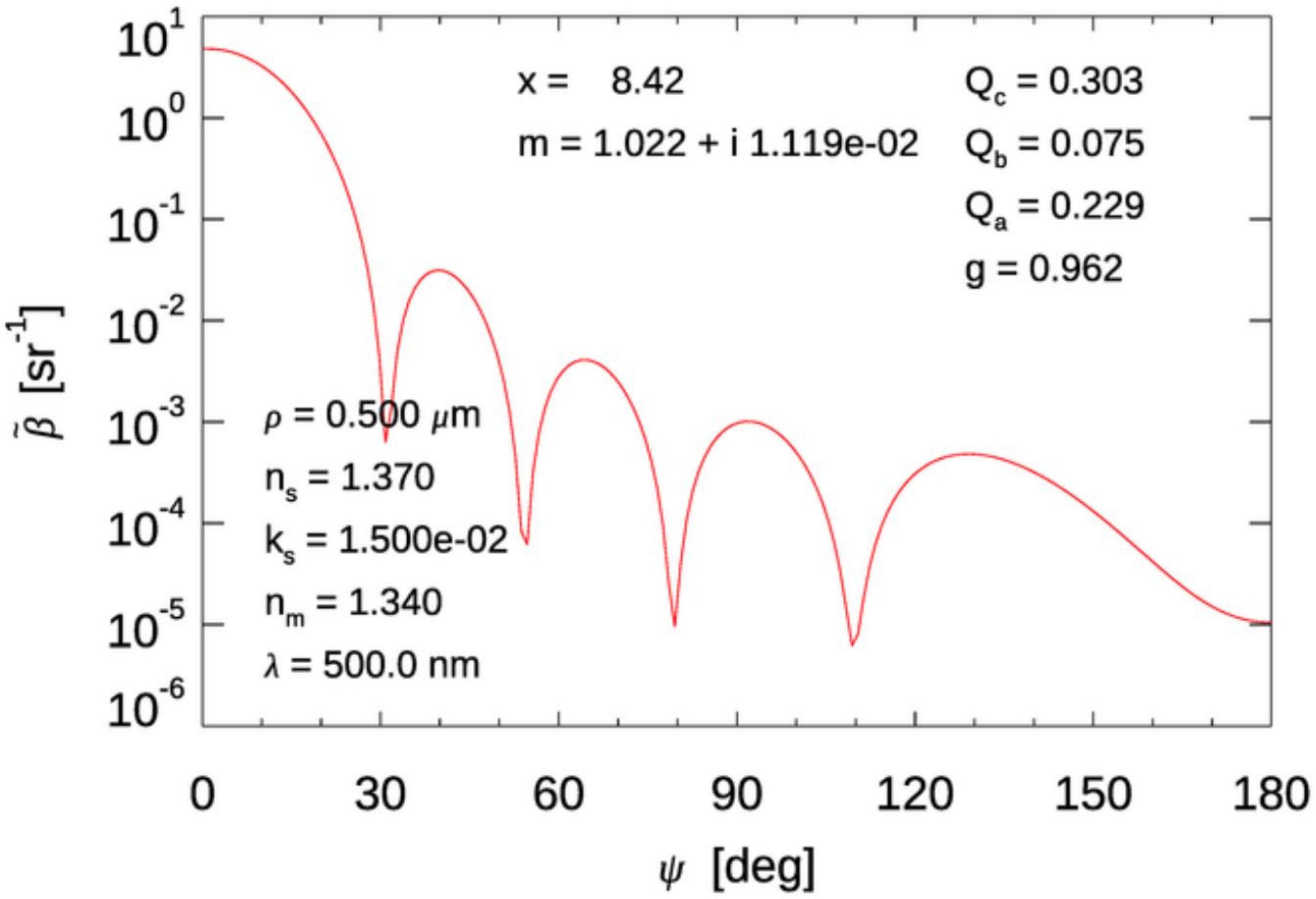




Something more like a phyto?

Does this look like what we measure?



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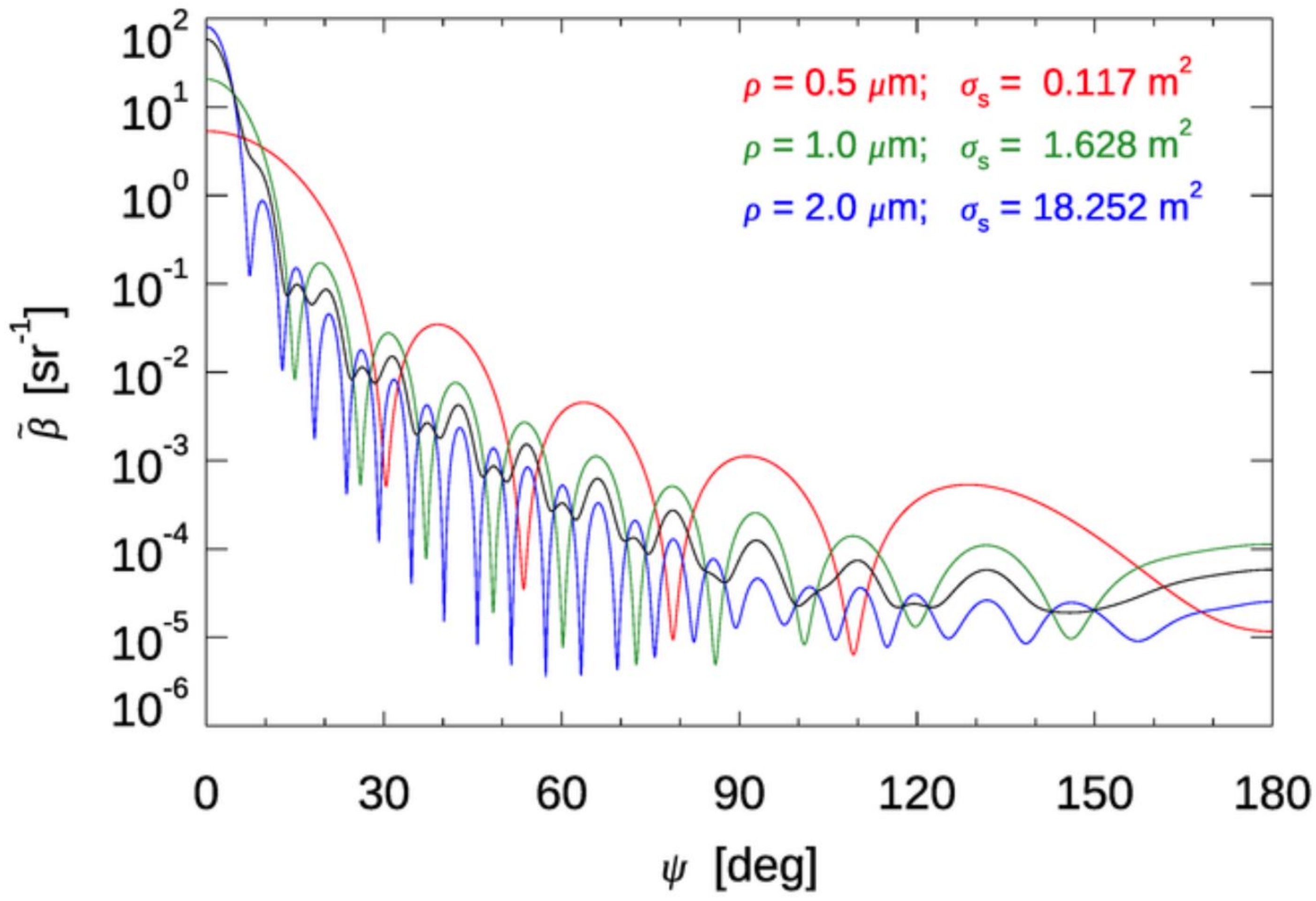
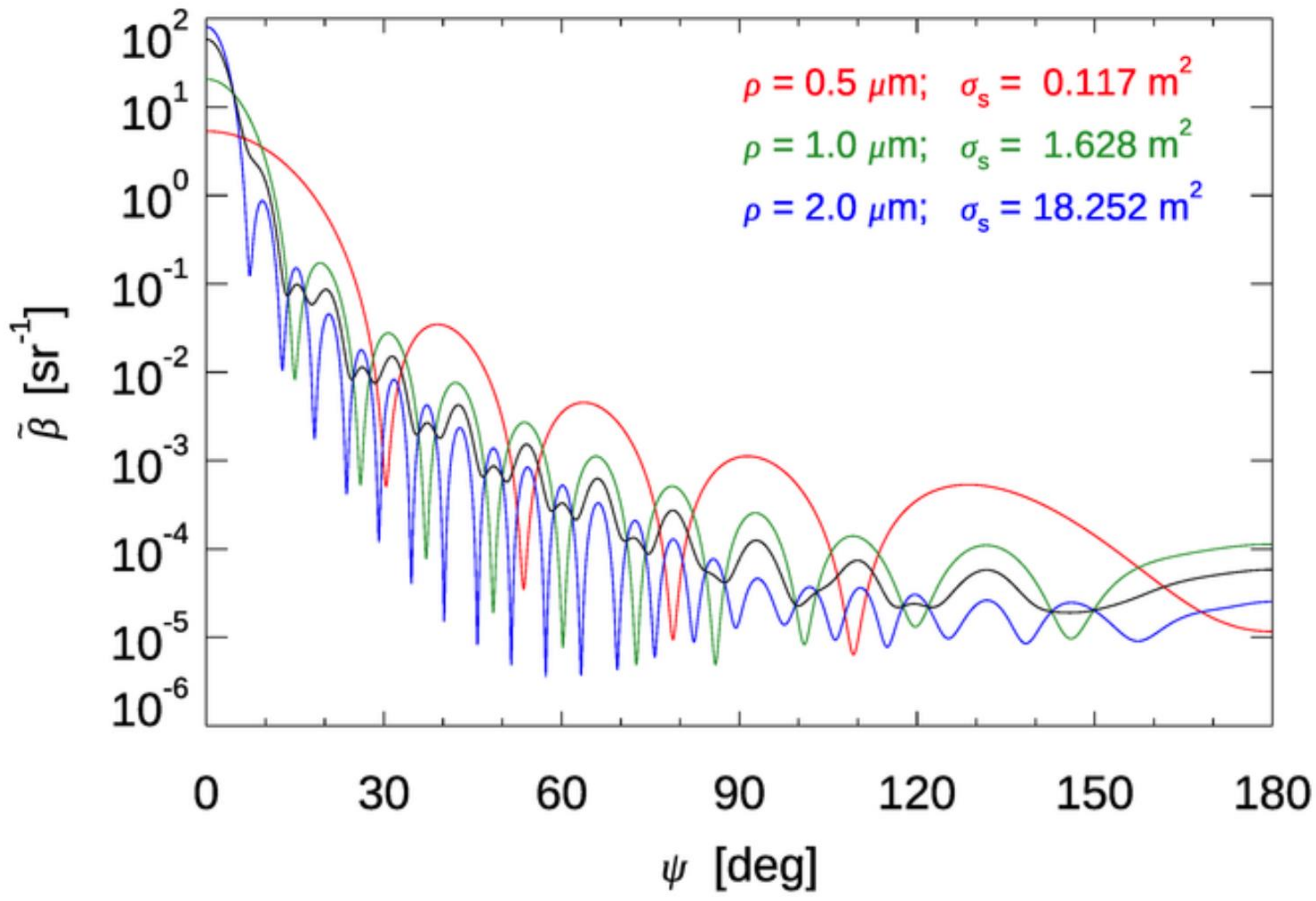


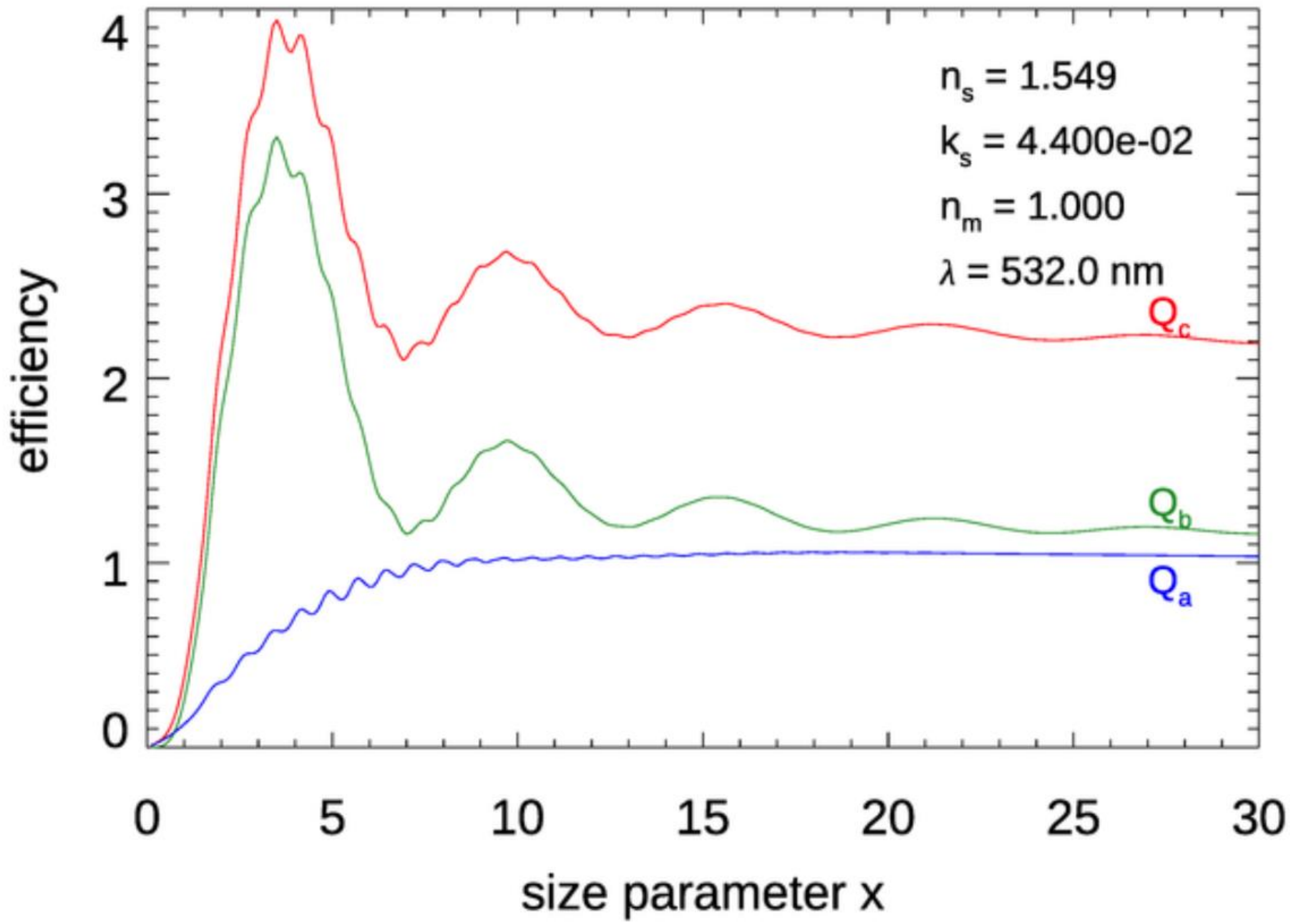
Something more like a phyto?

Does this look like what we measure?

The peaks and valleys flatten out for polydisperse particle size distributions.

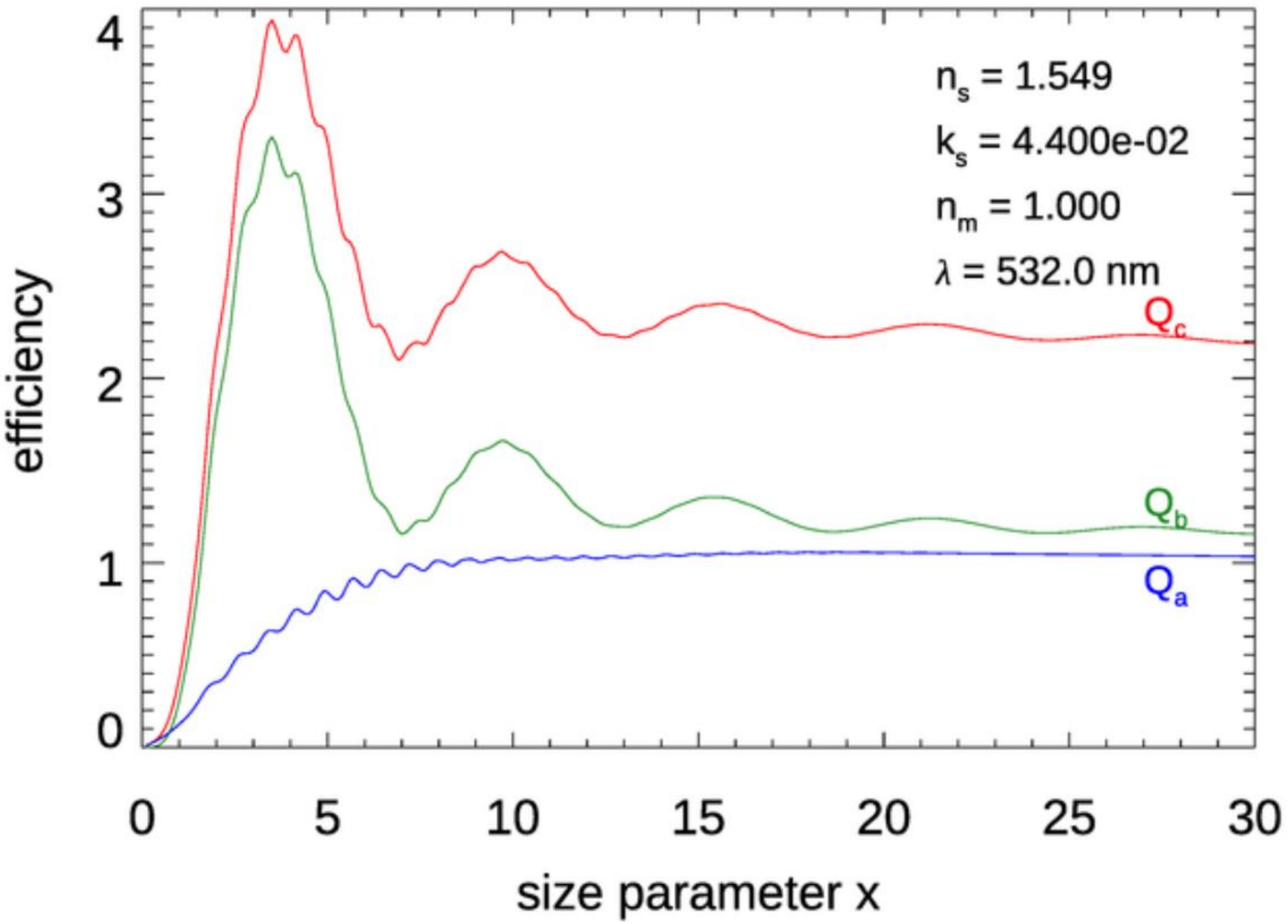


What do you notice here?



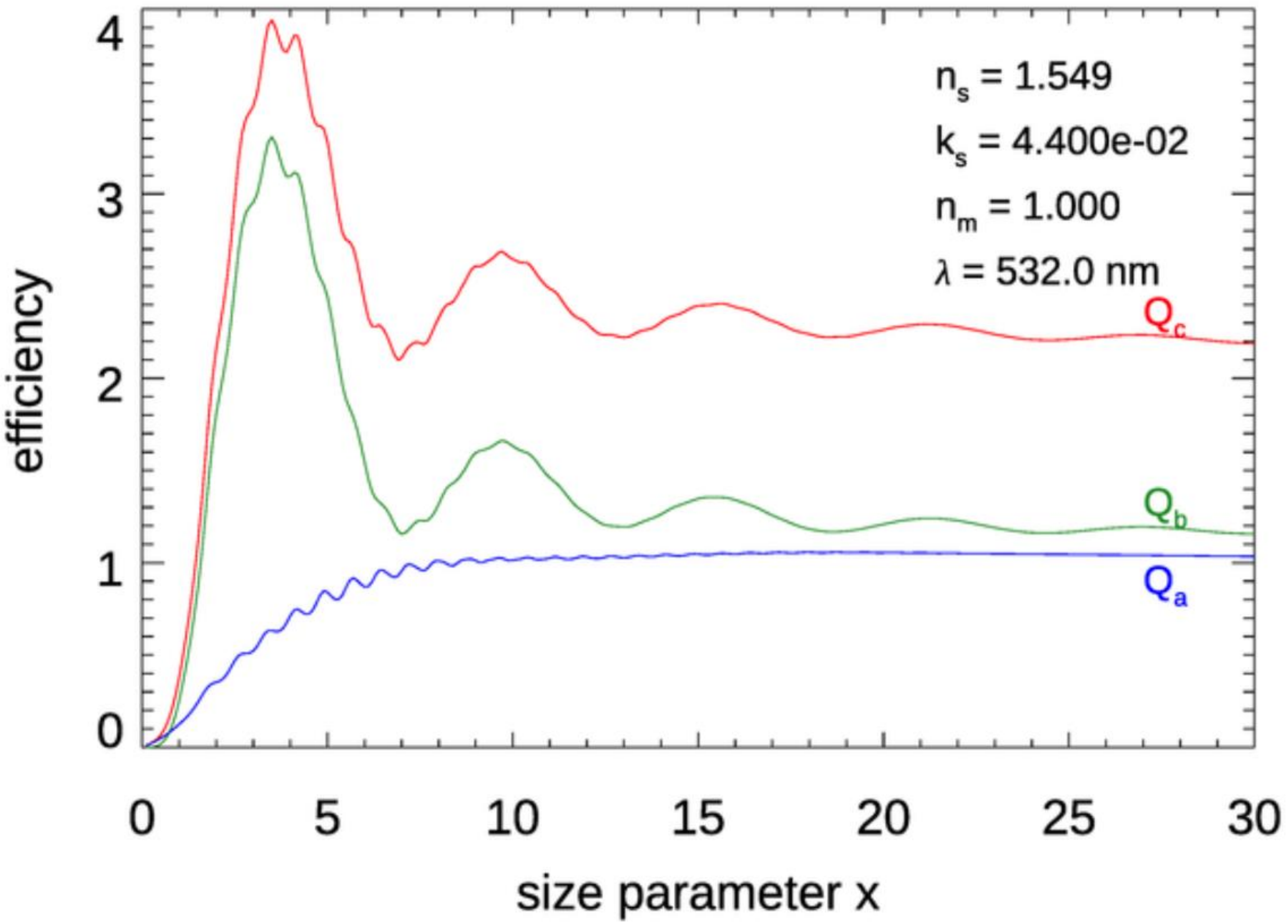
What do you notice

- Oscillations in efficiency
- “Extinction Paradox”

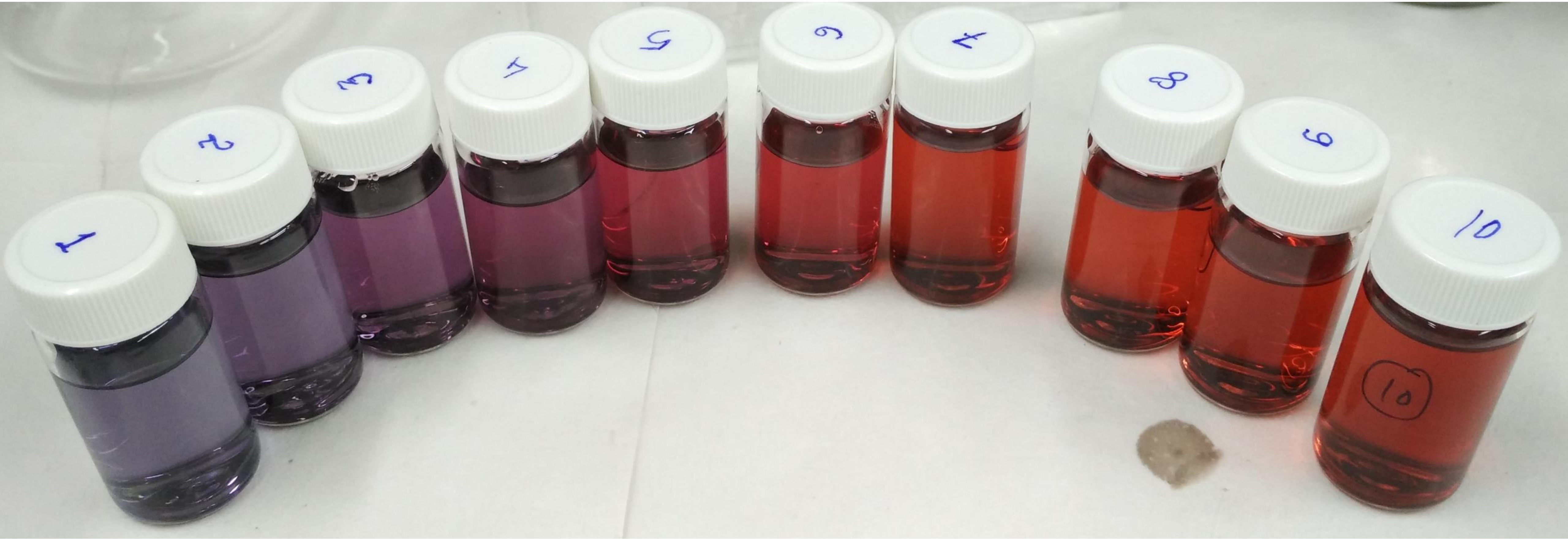


What do you notice

- Oscillations in efficiency
  - constructive+destructive interference
- "Extinction Paradox"
  - Extra scattering mostly due to diffraction
  - Still under investigation!



Can you explain this example?



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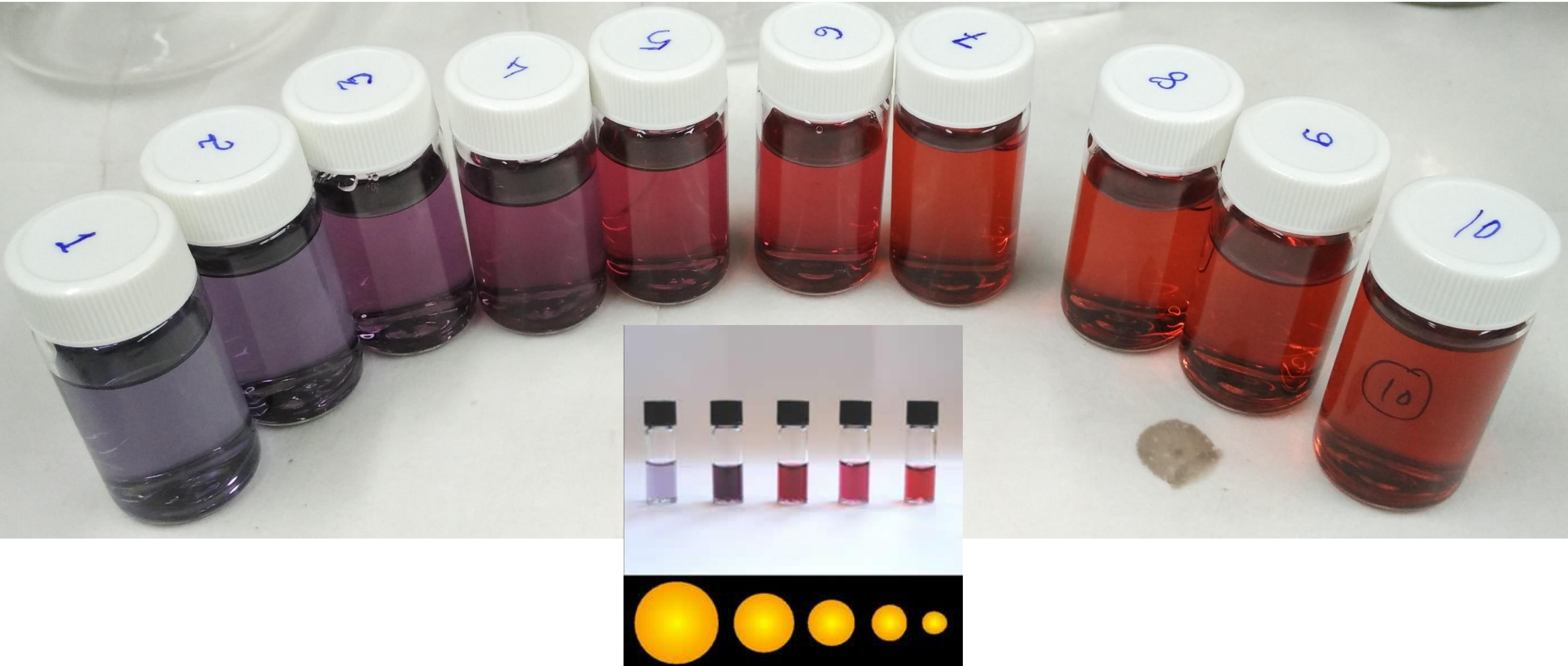
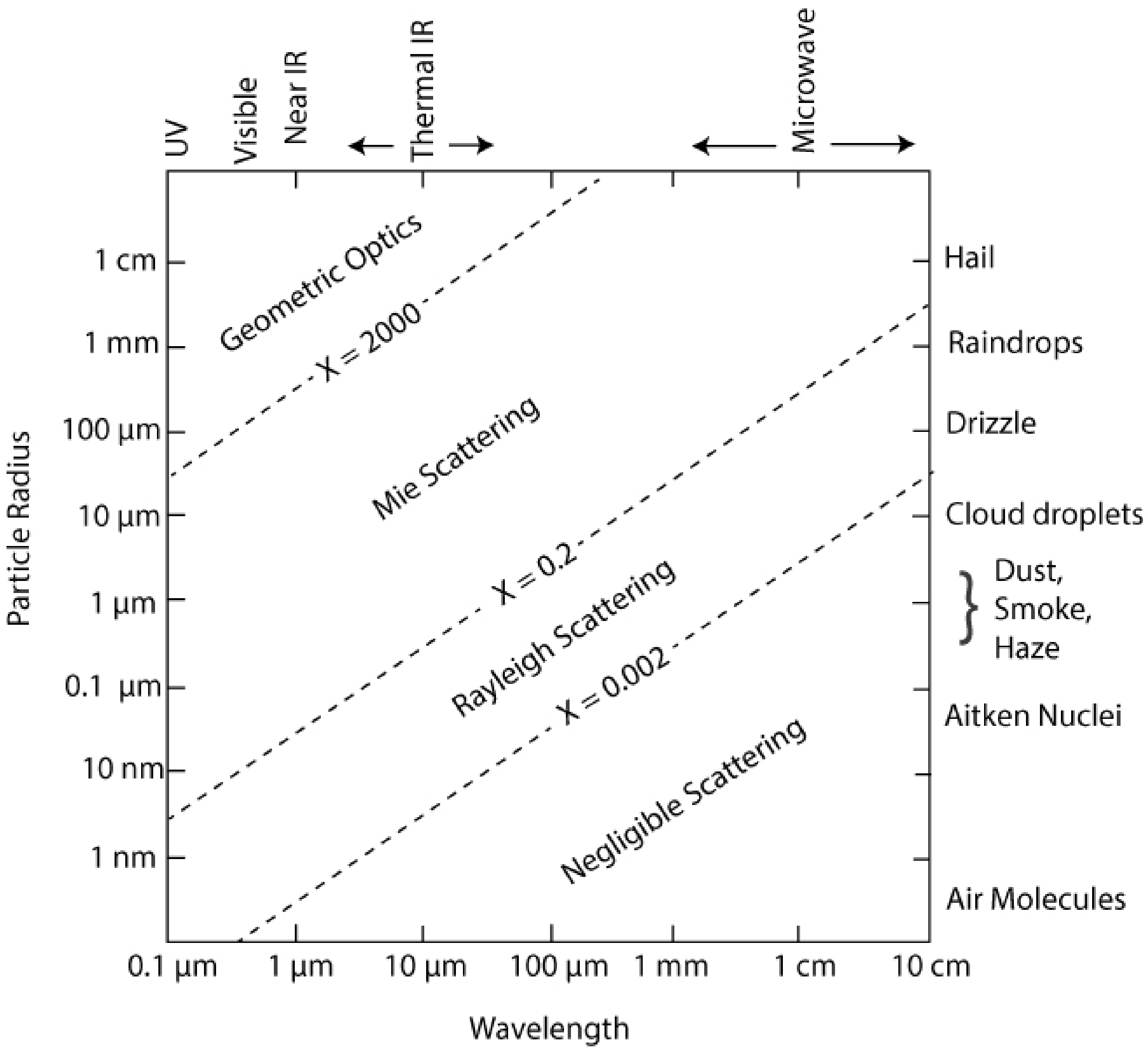


Reminders

Note: Mie's solution is exact and valid for all sizes of homogenous spheres, indices of refraction, and wavelengths.

Rayleigh is a useful *approximation*. We will discuss other approximations in the lab.

All scattering (e.g. diffraction, reflection) is from a change in refractive index.



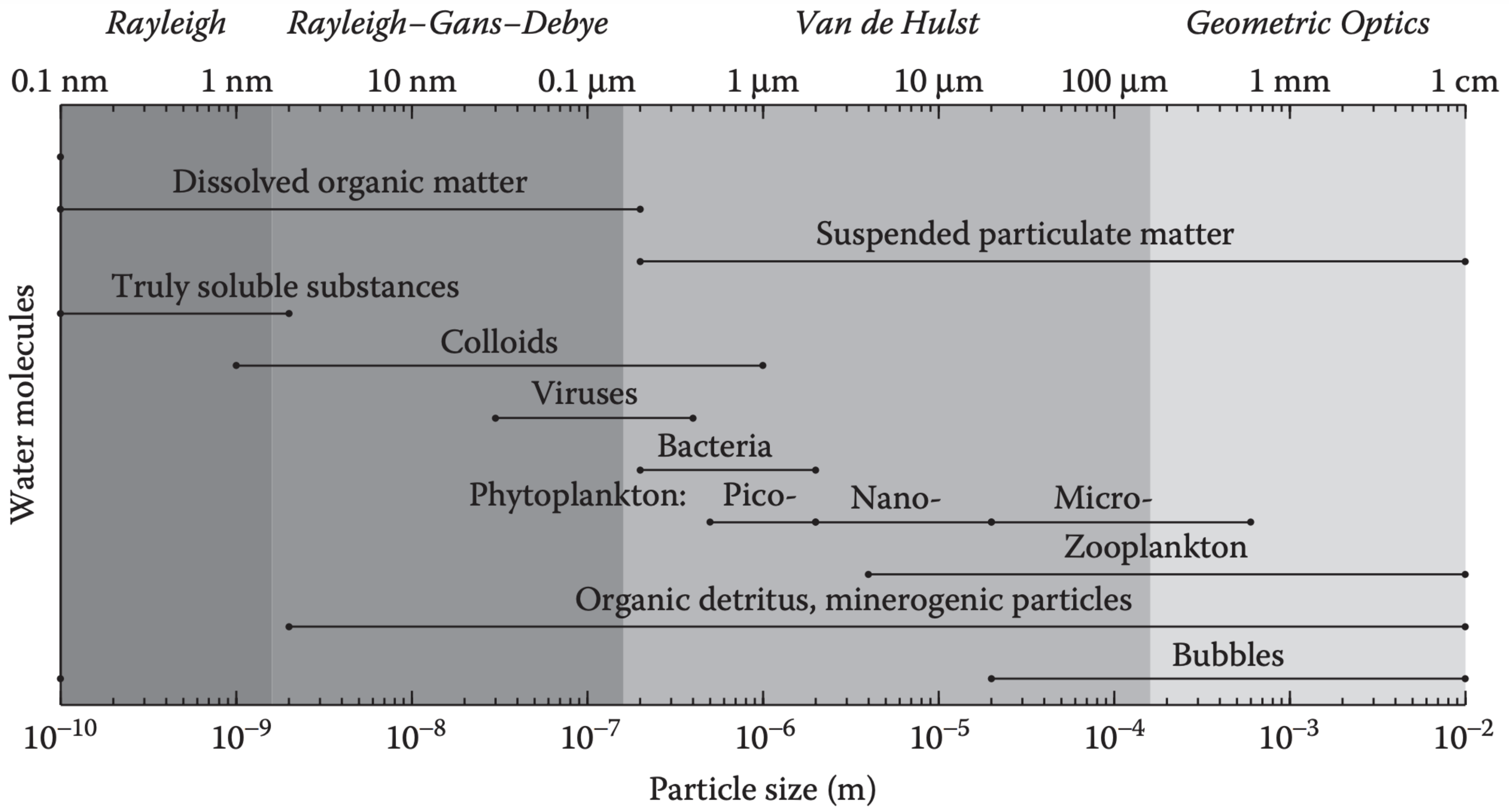
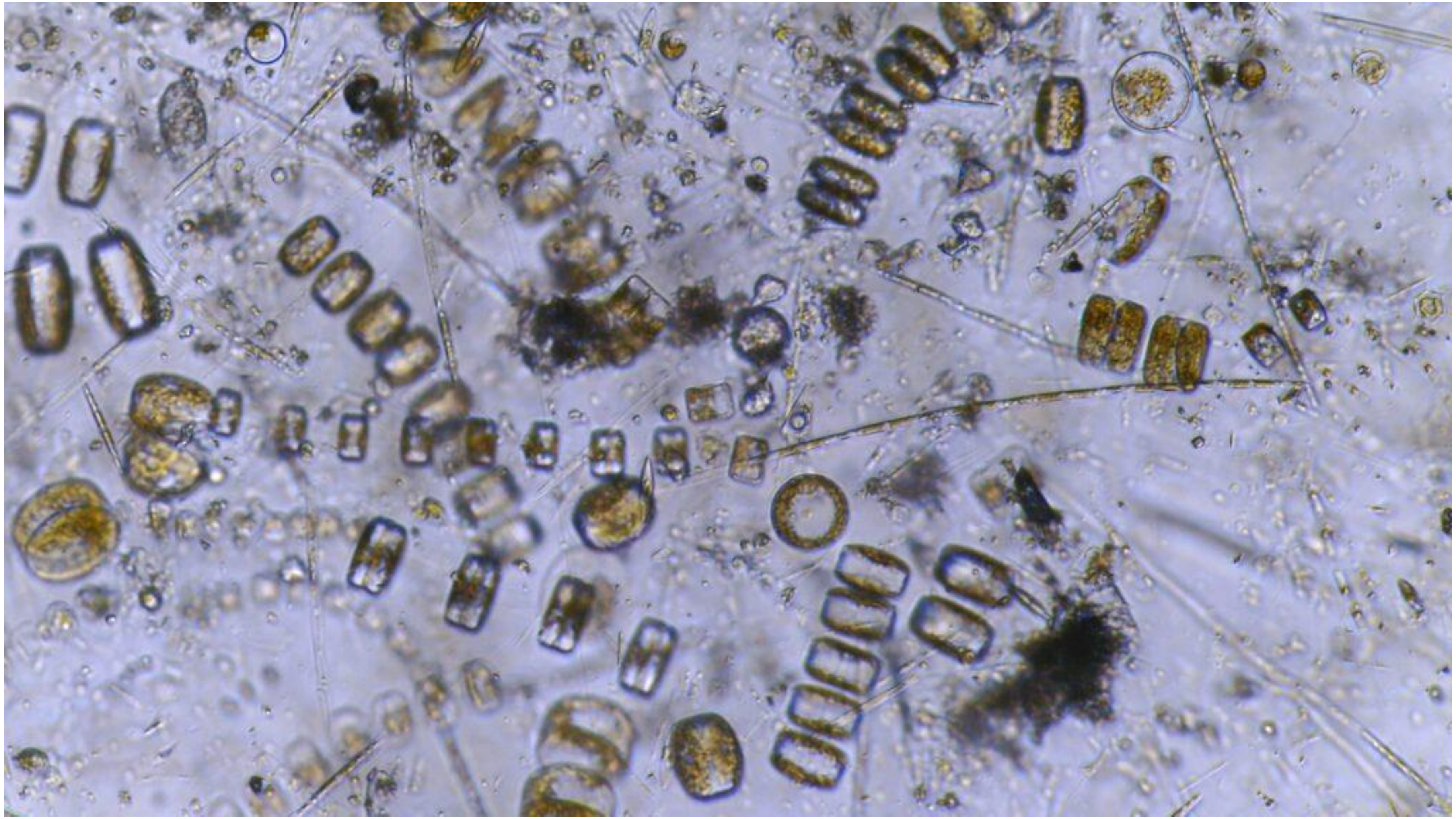


Figure 2 Representative sizes of different constituents in sea-water, after Stramski et al (2004). Optical regions referred to in the text are denoted at the top axis (shading represents approximate boundaries between these regions). These boundaries vary with refractive index for a given particle size.

Some caveats?

Some caveats?



Some caveats?

- For particles much smaller than the wavelength of light the IOPs of non-spherical particles are similar to those of spheres with a similar volume
- For randomly oriented convex particles much larger than the wavelength of light IOPs are similar to those of spheres with a similar cross-sectional area
- The only safe thing to say for non-spherical particles is that the IOPs, and particularly the phase function, is *probably* within a factor of 10

References

- Oceanic Optics (2022)
- QED by Feynman (1984)
- A Student’s Guide to Maxwell’s Equations by Fleisch (2008)
- Scattering and Absorption by Small Particles by Bohren and Huffman (1983)

- A potential path to getting your head around this:
  - I recommend a full 8 hour day with a large coffee and reading the chapters on *Elastic Scattering (*chp 6) and *Mie Theory* (chp 12) in Mobley’s *Oceanic Optics*
  - From there if you’re still interested you can go much more in depth with Bohren and Huffman
  - If you just want to explore the fundamental weirdness, read QED by Feynman
  - If you want a slow and approachable refresher on Maxwell’s Eqns as a starting point I highly recommend Fleish

Optics Class Shirts!!

- Student organized and designed
- We recommend you try to order them and get them sent here while we’re all still together
- Get a good quality shirt! (spend the extra $5)

Lab Format

- Playing together
  - https://colab.research.google.com/drive/19dgfGM2o0uCGdS1f0Zw5uy2me6UJbmZK#scrollTo=p05gKZ7vLCDp
- Then working on the handout as you go about your afternoon