Dust Models and Optical Properties

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Since the scattering and infrared emission properties of cometary dust were discussed by D.H. Wooden (and H.U. Keller), and the dynamic properties of dust in circumstellar disks and comets will be discussed by M.C. Wyatt, I will therefore pay more attention to interstellar dust – after all interstellar grains are the building blocks of young stars, comets and other planetary systems. Since this is a "school", I will first present the underlying basic physics for scattering and optical properties of dust.

- Part I: Optics of Dust;
- Part II: Interstellar Dust;
- Part III: Models for Interstellar Dust, Cometary Dust, and Dust Disks;

Dust Models and Optical Properties: Part I. Optics of Dust

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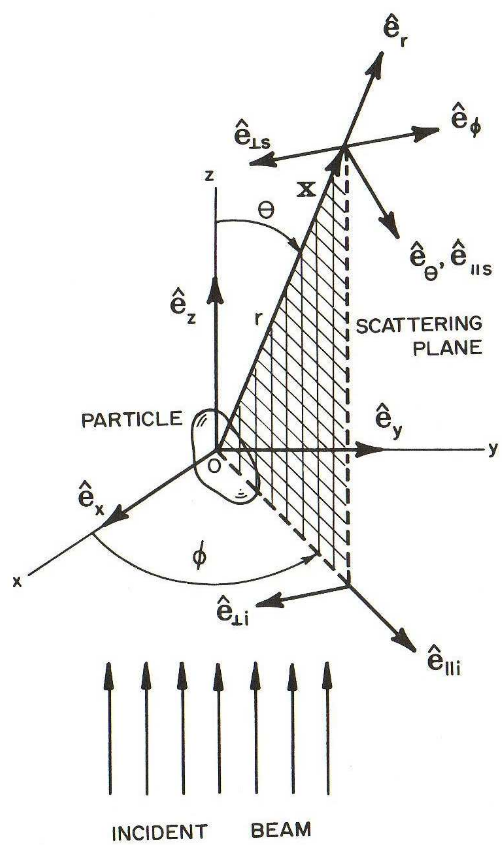
Optical Properties of Dust: Why Do We Care? — Our knowledge about interstellar, circumstellar and cometary dust is mainly derived from its interaction with electromagnetic radiation: extinction (scattering, absorption), polarization (differential extinction), and emission.

- Definitions for Light Scattering;
- Physical Basis for Scattering and Absorption;
- Physical Basis for Optical Properties of Materials (dielectric function/index of refraction);
- Calculational Techniques
  - Mie Theory ⟶ spheres, infinite cylinders;
  - Rayleigh Approximation ⟶ spheres, spheroids;
  - T-matrix Method ⟶ spheroids, finite cylinders;
  - Separation of Variables/Series Expansion ⟶ spheroids;
  - Discrete Dipole Approximation ⟶ irregular grains;
  - Effective Medium Theory → "average" dielectric functions;
  - Kramers-Kronig Relations;

Definitions for Scattering and Absorption of Light by Small Particles

When light impinges on a particle it is either scattered or absorbed.

- I_0 — intensity of incident light;
- $I(\theta, \phi)$ – intensity of light scattered into an angle θ ("scattering angle" from the incident direction), and ϕ (azimuthal angle);
- $I = I_0 \frac{F(\theta,\phi)}{k^2 r^2}$ (if $kr \gg 1$ – "far-field" region), $F(\theta, \phi)$ — angular scattering distribution, $k = 2\pi/\lambda$;



- $C_{\rm sca} = k^{-2} \int F(\theta, \phi) d\omega$ – total scattering cross-section (integral of scattering function $F(\theta, \phi)$ over all solid angles);

- $C_{\rm abs}$ — total absorption cross-section, $C_{\rm ext}$ — total extinction cross-section $\longrightarrow$

$$C_{\rm ext} = C_{\rm sca} + C_{\rm abs} = \frac{\text{total radiant energy scattered and absorbed per unit time}}{\text{incident radiant energy per unit area per unit time}} \quad (1)$$

- $C_{\rm ext}$ – dimensionally an area – "effective" blocking area to radiation;

- Define "extinction efficiency" $Q_{\rm ext} \equiv C_{\rm ext}/C_{\rm geo}$, $C_{\rm geo}$ – geometrical cross section (for spheres $C_{\rm geo} = \pi a^2$). $Q_{\rm ext} \rightarrow 2$ for $a/\lambda \rightarrow \infty$; $Q_{\rm ext} \rightarrow 0$ for $a/\lambda \rightarrow 0$;

- $Q_{\rm abs} \equiv C_{\rm abs}/C_{\rm geo}$ – absorption efficiency, $Q_{\rm sca} \equiv C_{\rm abs}/C_{\rm geo}$ – scattering efficiency;

- albedo — $\alpha \equiv C_{\rm sca}/C_{\rm ext}$; $\alpha \rightarrow 0$ for grains much smaller than wavelength ($2\pi a/\lambda \ll 1$);

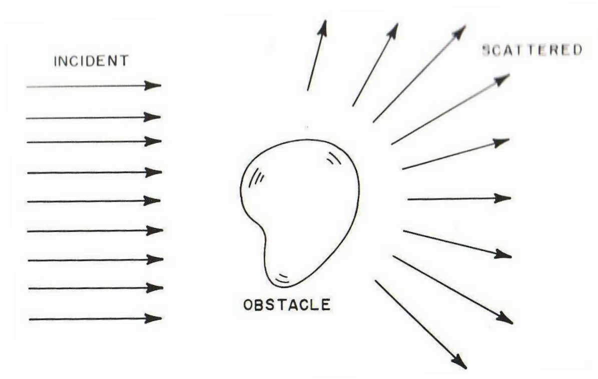
- asymmetry factor — $g \equiv \langle \cos(\theta) \rangle = \frac{1}{k^2 C_{\rm sca}} \int F(\theta, \phi) \cos(\theta) d\omega$ — degree of scattering in the forward direction; if dust scatters light isotropically $\rightarrow g = 0$; if dust scatters more light toward the forward direction $\theta = 0^{\rm o} \rightarrow g > 0$; if dust scatters more light toward the back direction $\theta = 180^{\rm o} \rightarrow g < 0$;

- radiation pressure cross section — $C_{\rm pr} = C_{\rm abs} + (1-g)\, C_{\rm sca} \leftarrow$ light carries momentum $\rightarrow$ photons absorbed by a grain transfer all their momentum to the grain in the direction of propagation; for scattering, the net-rate of momentum transfer in the direction of propagation $\propto (1-g)\, C_{\rm sca}$.

Physical Basis for Scattering of Light

Matter is composed of discrete electric charges (electrons and protons).

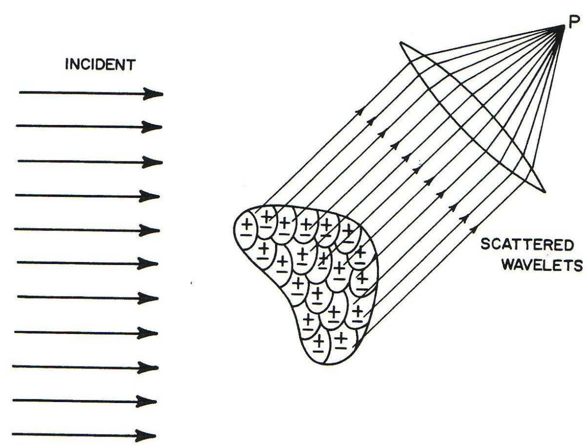
- Illuminated by an electromagnetic wave, electric charges in a grain are set into oscillatory motion by the electric field of the incident wave.
- Accelerated electric charges radiate electromagnetic energy in all directions ("secondary radiation") $\longrightarrow$ scattering;
- The excited elementary charges may transform part of the incident electromagnetic energy into other forms (e.g. thermal energy) $\longrightarrow$ absorption;



Consider an arbitrary grain, conceptually subdivided into many small regions.

- An incident electromagnetic wave induces a dipole moment in each region.
- The amplitude and phase of the induced dipole moment (for a given frequency) depend on the grain material $\longrightarrow$ grain optical properties matter!

- These dipoles oscillate at the frequency of the applied field → scatter secondary radiation in all directions.
- In a particular direction, the total scattered field is obtained by superposing the scattered wavelets, with their phase differences taken.
- These phase relations change for a different scattering direction → The scattered field varies with scattering direction.
- If $a \ll \lambda$ → all the secondary wavelets are approximately in phase → scattering does not vary much with direction.
- If $a \uparrow$ → more mutual enhancement and cancellation of the scattered wavelets → for larger particles, more peaks and valleys in the scattering pattern.
- Shape also affects the phase relations.



⟶ The scattering and absorption of light are affected by grain size, shape, and optical properties (dielectric function, index of refraction/optical constants).

Physical Basis for Dielectric Function $\epsilon = \epsilon' + i\,\epsilon''$

Classical Lorentz harmonic oscillator model — the electrons and ions of matter are treated as simple harmonic oscillators subject to the driving force of applied electromagnetic fields. The applied field distorts the charge distribution and therefore produces an induced dipole moment.

- Consider polarizable matter as a collection of identical, independent, isotropic harmonic oscillators with mass m and charge q; each oscillator is acted upon by 3 forces —
  - restoring force $K\vec{\mathbf{x}}$ (K – spring constant/stiffness, $\vec{\mathbf{x}}$ – displacement from equilibrium);
  - damping force $b\dot{\vec{\mathbf{x}}}$ (b: damping constant);
  - driving force $q\vec{\mathbf{E}}$ (produced by the local electric field $\vec{\mathbf{E}}$).
- $\rightarrow$ Equation of motion of oscillators

$$m\ddot{\vec{\mathbf{x}}} + b\dot{\vec{\mathbf{x}}} + K\vec{\mathbf{x}} = q\vec{\mathbf{E}} \tag{2}$$

- For time harmonic electric field (with frequency ω) $\vec{\mathbf{E}} \propto e^{-i\omega t} \rightarrow$

$$\vec{\mathbf{x}} = \frac{(q/m)\,\vec{\mathbf{E}}}{{\omega_{\rm o}}^2 - \omega^2 - i\gamma\omega}\ ,\ {\omega_{\rm o}}^2 = K/m\ ,\ \gamma = b/m\ . \tag{3}$$

- The induced dipole moment $\vec{\mathbf{p}}$ of an oscillator is $\vec{\mathbf{p}} = q\vec{\mathbf{x}}$; Let N be the number of oscillators per unit volume. $\rightarrow$ polarization $\equiv$ dipole moment per unit volume: $\vec{\mathbf{P}} = N\vec{\mathbf{p}} = N\,q\vec{\mathbf{x}}$.

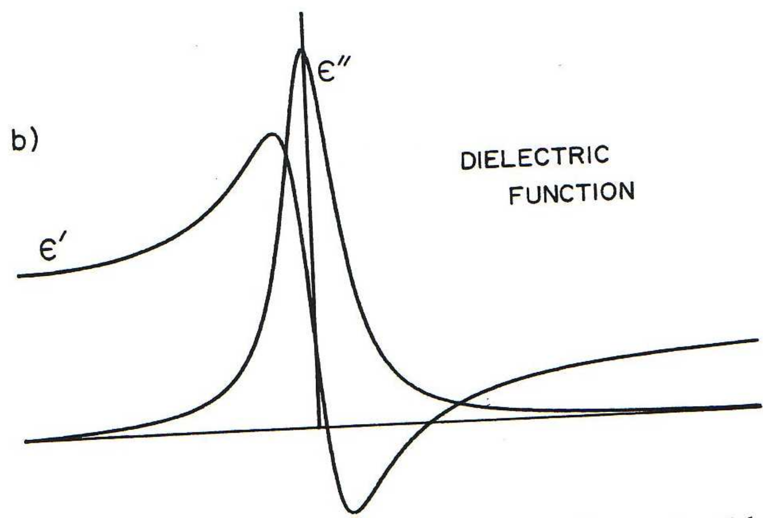
$$\vec{\mathbf{P}} = \frac{{\omega_{\rm p}}^2}{{\omega_{\rm o}}^2 - \omega^2 - i\gamma\omega}\epsilon_{\rm o}\vec{\mathbf{E}}\ \ ,\ \ {\omega_{\rm p}}^2 = Nq^2/m\epsilon_{\rm o}\ :\ \text{plasma frequency.} \tag{4}$$

- Since $\vec{\mathbf{P}} = \epsilon_\mathrm{o}\chi\vec{\mathbf{E}}$ (χ: susceptibility) $\longrightarrow$ the dielectric function for a simple harmonic oscillator is

$$\epsilon = 1 + \chi = 1 + \frac{{\omega_\mathrm{p}}^2}{{\omega_\mathrm{o}}^2 - \omega^2 - i\gamma\omega} \tag{5}$$

$$\epsilon' = 1 + \chi' = 1 + \frac{{\omega_\mathrm{p}}^2\left({\omega_\mathrm{o}}^2 - \omega^2\right)}{\left({\omega_\mathrm{o}}^2 - \omega^2\right)^2 + \gamma^2\omega^2} \tag{6}$$

$$\epsilon'' = 1 + \chi'' = \frac{{\omega_\mathrm{p}}^2\gamma\omega}{\left({\omega_\mathrm{o}}^2 - \omega^2\right)^2 + \gamma^2\omega^2} \ , \quad \text{For } \omega \rightarrow 0 : \epsilon'' \propto \omega \ ! \tag{7}$$



- refractive index $m = m' + i\,m''$: $\epsilon = m^2 \rightarrow$

$$m' = \sqrt{\frac{\sqrt{\epsilon'^2 + \epsilon''^2} + \epsilon'}{2}} \ , \ m'' = \sqrt{\frac{\sqrt{\epsilon'^2 + \epsilon''^2} - \epsilon'}{2}} \ , \tag{8}$$

$$\epsilon' = m'^2 - m''^2 \ , \ \epsilon'' = 2m'm'' \tag{9}$$

Free Electron Contribution to $\epsilon = \epsilon' + i\,\epsilon''$

- Lorentz harmonic oscillator model: for the dielectric response of the bound charges (electrons and nucleus within an atom): they undergo a finite displacement $\rightarrow$ individual atoms/molecules acquire an electric dipole moment (Draine 2003).

- Free charges respond to the applied electric field in the form of an electric current density $\vec{\mathbf{J}} = \sigma\vec{\mathbf{E}}$, contributing to ϵ with an amount of $4\pi i\sigma(\omega)/\omega$,
  - Consider a material with a density n_e of free electrons subject to drag force

$$m_e\ddot{\vec{\mathbf{x}}} = e\vec{\mathbf{E}} - m_e\dot{\vec{\mathbf{x}}}/\tau_e \quad , \quad \tau_e \ : \ \text{electron collision time} \ . \tag{10}$$

  - $\rightarrow$ For $\vec{\mathbf{E}} \propto e^{-i\omega t}$, $\sigma(\omega) \equiv n_e e\dot{\vec{\mathbf{x}}}/E$ is

$$\sigma(\omega) = \frac{\sigma_{\rm o}}{1 - i\,\omega\tau_e} \quad , \quad \sigma_{\rm o} = \frac{n_e e^2\tau_e}{m_e} \ : \ \text{d.c. conductivity} \ . \tag{11}$$

  - $\epsilon = 4\pi i\sigma(\omega)/\omega \rightarrow$

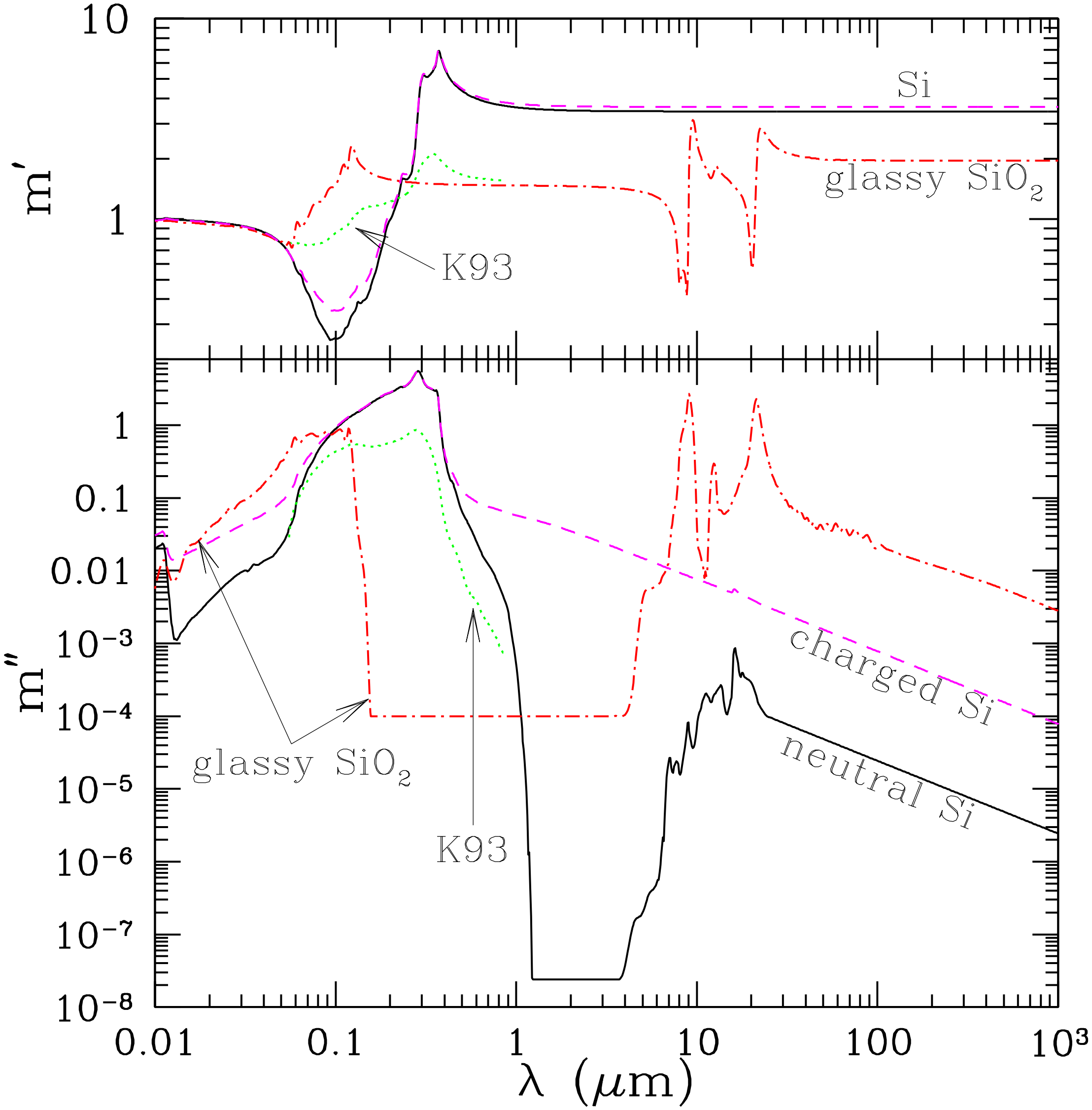
$$\epsilon = -\frac{4\pi\sigma_{\rm o}\tau_e}{1 - \omega^2\tau_e^2} + i\frac{4\pi\sigma_{\rm o}}{\omega\,(1 - \omega^2\tau_e^2)} \tag{12}$$

  - For $\omega \rightarrow 0$

$$\epsilon' \rightarrow -4\pi\sigma_{\rm o}\tau_e \ = \ \text{constant} \ , \ \epsilon'' \rightarrow \frac{4\pi\sigma_{\rm o}}{\omega} \ \propto \frac{1}{\omega} \ ! \tag{13}$$

Index of Refraction of Silicon and SiO_2

(Li & Draine 2002, ApJ, 564, 803; silicon: 10 Å)



Techniques for Calculating $C_{\rm abs}$ and $C_{\rm sca}$

- Spheres: Mie theory (Mie 1908; Debye 1909) for homogeneous or (multi-)layered spheres of isotropic material;
- Infinite Cylinders: Mie theory;
- Spheroids
  - Series expansion (Asano & Yamamoto 1975; Asano & Sato 1980) — for grain size comparable to λ;
  - Separation of variables (Voshchinnikov & Farafonov 1993) — for grain size comparable to λ;
  - Separation of variables (Farafonov, Voshchinnikov & Somsikov 1996) — for core-mantle spheroids;
  - Discrete Dipole Approximation (DDA) — for grain size modestly larger than λ;
  - T-matrix method (Mishchenko, Travis, & Macke 2000) — for grain size modestly larger than λ;
- Finite Cylinders — T-matrix method; DDA;
- Irregular Grains — DDA (Draine 1988);
- Cosmic grains are commonly modeled as spheres, spheroids, or irregular grains.

What Astronomers Usually Do...

- Interstellar extinction ($2\pi a/\lambda \rightarrow 20$) modeling $\leftarrow$ spheres;
- Interstellar polarization modeling $\leftarrow$ spheroids;
- Interstellar infrared emission modeling $\leftarrow$ spheres;
- Cometary dust, dust disks – porous dust:
  - IR emission modeling $\leftarrow$ spheres (Mie theory plus effective medium theory);
  - Scattered light — DDA;
  - Polarization — DDA;

- See Mann et al. 2006, *A&A Rev.*, **13**, 159 (§8): for an extensive review on light scattering of cometary and circumstellar dust.
- See Mann et al. 2004, *J. Quant. Spectr. Rad. Trans.*, **89**, 291: for a detailed comparison between DDA and T-matrix studies of cometary dust aggregates.
- See Wooden 2000, *Earth, Moon, and Planets*, **89**, 247: for a review on cometary dust IR emission modeling.
- See Mukai et al. 1992, *A&A*, **262**, 315: for radiation pressure on fluffy porous dust.
- Scattering of light by cometary porous aggregates: Kozasa, Blum, & Mukai 1992, A&A, 263, 423; Kozasa, Blum, Okamoto, & Mukai 1993, A&A, 276, 278; Kimura, Kolokolova, & Mann 2003, A&A, 407, L5; Kimura, Kolokolova, & Mann 2006, A&A, 449, 1243; Levasseur-regourd et al. 2005...

Rayleigh Approximation: $2\pi a/\lambda \ll 1$ ($C_{\rm abs} \gg C_{\rm sca}$)

- For Sphere (of volume V):

$$C_{\rm abs}/V = \frac{9\omega}{c}\frac{\epsilon''}{(\epsilon'+2)^2+\epsilon''^2} \tag{14}$$

  - At long wavelength, for dielectric spheres $\epsilon' \rightarrow$ constant $\gg \epsilon''$, $\epsilon'' \propto \omega$, $\longrightarrow C_{\rm abs} \propto \omega\epsilon'' \propto \omega^2$;
  - At long wavelength, for metallic spheres $\epsilon'' \propto 1/\omega$, $\epsilon' \rightarrow$ constant $\ll \epsilon''$, $\longrightarrow C_{\rm abs} \propto \omega/\epsilon'' \propto \omega^2$;
  - $\longrightarrow$ for both dielectric and metallic dust, $C_{\rm abs} \propto \lambda^{-2}$ at long wavelength!

- For Spheroids:

$$C_{\rm abs}^{\parallel,\perp}/V = \frac{\omega}{c}{\rm Im}\left\{\frac{\epsilon-1}{(\epsilon-1)L^{\parallel,\perp}+1}\right\} \tag{15}$$

  - $L^{\parallel}/L^{\perp}$ = depolarization factors parallel/perpendicular to grain symmetry axis;
  - $L^{\parallel}+2L^{\perp}=1$ (for spheres $L^{\parallel}=L^{\perp}=1/3$).

$$L^{\parallel} = \begin{cases} \frac{1-e^2}{e^2}\left[\frac{1}{2e}\ln\left(\frac{1+e}{1-e}\right)-1\right], & \text{for prolate } (a>b) \\ \frac{1+e^2}{e^2}\left(1-\frac{1}{e}\tan^{-1}e\right), & \text{for oblate } (a<b) \end{cases} \tag{16}$$

- For CDE (Continuous Distribution of Ellipsoids) $\rightarrow$ average over a distribution of shapes. Assuming all shapes are equally probable $\rightarrow$

$$\langle C_{\rm abs}/V\rangle = \frac{\omega}{c}{\rm Im}\left\{\frac{2\epsilon}{\epsilon-1}{\rm Log}\epsilon\right\} \quad , \quad {\rm Log}\epsilon = \text{principal value of the logarithm of } \epsilon\ . \tag{17}$$

Inhomogeneous Grains: Average Dielectric Function

Use "Effective Medium Theory" to obtain "average" dielectric functions for inhomogeneous grains —

- Maxwell-Garnett mixing rule (for a two-component mixture composed of spherical inclusions of $\epsilon_{\rm i}$ embedded in homogeneous matrix of $\epsilon_{\rm m}$) —

$$\langle\epsilon\rangle = \epsilon_{\rm m}\frac{(1+2f_{\rm i})\,\epsilon_{\rm i}+2\,(1-f_{\rm i})\,\epsilon_{\rm m}}{(1-f_{\rm i})\,\epsilon_{\rm i}+(2+f_{\rm i})\,\epsilon_{\rm m}} \;\;,\;\; f_{\rm i} \;=\; \text{volume fraction of the inclusions}\;, \tag{18}$$

- Bruggeman mixing rule (for a randomly inhomogeneous mixture of N components) —

$$\sum_{j=1}^{N} f_j \frac{\epsilon_j-\langle\epsilon\rangle}{\epsilon_j+2\langle\epsilon\rangle} = 0 \;\;,\;\; f_j \;=\; \text{volume fraction of the } j_{\rm th} \text{ component}\;, \tag{19}$$

- Major differences: for Maxwell-Garnett theory, there are distinguishable inclusions embedded in a definite matrix; for Bruggeman theory, it is a completely randomly inhomogeneous medium, there are no distinguishable inclusions embedded in a definite matrix;

- For modeling the IR emission of comets and dust disks of which the dust is thought to be porous aggregates, Bruggeman theory is preferred. Not good for scattering studies! See Mann et al. 2004, Kimura et al. 2003, Kozasa et al. 1993...

Kramers-Kronig Relations

- Kramers (1927) and Kronig (1926) independently found: ϵ' and ϵ'' are not independent:

$$\epsilon'(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{x\epsilon''(x)}{x^2-\omega^2}\,dx \quad , \tag{20}$$

$$\epsilon''(\omega) = \frac{-2\omega}{\pi} P \int_0^\infty \frac{\epsilon'(x)}{x^2-\omega^2}\,dx \quad , \tag{21}$$

$$P\int_0^\infty \frac{x\epsilon''(x)}{x^2-\omega^2}\,dx = \lim_{a\to 0}\left[\int_0^{\omega-a}\frac{x\epsilon''(x)}{x^2-\omega^2}\,dx + \int_{\omega+a}^\infty \frac{x\epsilon''(x)}{x^2-\omega^2}\,dx\right] \quad , \; P \; = \; \text{Cauchy Principal value} \; . \tag{22}$$

- Kramers-Kronig relations apply to any "linear response function" (e.g. ϵ) which characterizes response (e.g. $\vec{\mathbf{P}}$) to an applied stress (e.g. $\vec{\mathbf{E}}$). Only assumptions are linearity and causality.

- m' and m'' are also connected through Kramers-Kronig relation:

$$m'(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{x m''(x)}{x^2-\omega^2}\,dx \quad , \tag{23}$$

$$m''(\omega) = \frac{-2\omega}{\pi} P \int_0^\infty \frac{m'(x)}{x^2-\omega^2}\,dx \quad . \tag{24}$$

- Purcell (1969) used Kramers-Kronig relations to relate $\int C_{\rm ext}(\lambda)\,d\lambda$ to grain volume V

$$\int_0^\infty C_{\rm ext}(\lambda)\,d\lambda = 3\pi^2 V F\,(\epsilon_0;\text{shape}) \; , \; F \equiv \text{static polarizability/polarizability of conducting sphere} \; . \tag{25}$$

$$\int_0^\infty C_{\rm ext}(\lambda)\,d\lambda = 3\pi^2 V F\,(\epsilon_0;\mathrm{shape})$$

- F is a small number unless for grains which are both conducting ($\epsilon_o \rightarrow \infty$) and extremely elongated ($F \approx 0.4$ for dielectric grains, $F < 1.5$ for modestly elongated conducting grains; Draine 2003) $\rightarrow$ $3\pi^2 V F$ is a finite number $\rightarrow$ $\int_0^\infty C_{\rm ext}(\lambda)\,d\lambda$ must be convergent! $\rightarrow$ $C_{\rm ext}$ must decline more rapidly than $1/\lambda$ $\rightarrow$ Xing & Hanner (1997)'s DDA calculations of $C_{\rm ext} \propto 1/\lambda$ for porous aggregates can only be correct for a limited range of wavelengths.

- Galactic extinction $\int_{0.1\,\mu\rm m}^{30\,\mu\rm m} \frac{\tau_{\rm ext}}{N_{\rm H}} d\lambda = 1.1 \times 10^{-25}\,{\rm cm}^3/{\rm H}$ $\rightarrow$ constraints on the minimum amount of dust (relative to H; Purcell 1969) $\rightarrow$ subsolar abundance not able to account for extinction (Li 2005)!