

Interstellar Medium (ISM)

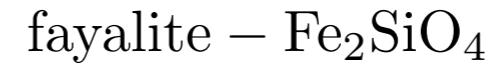
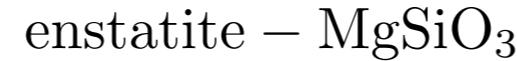
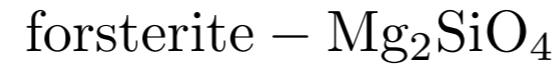
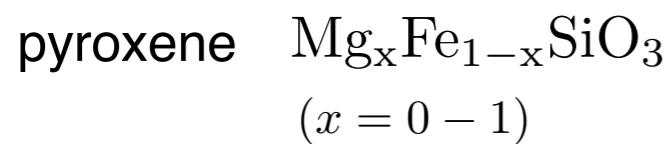
Lecture 12
May 22 (Monday), 2023

updated 05/21, 22:14

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Dust Materials

- Silicates
 - The two main types of silicates in dust are pyroxene and olivine.



[Left] Olivine is the simplest silicate structure, which is composed of isolated tetrahedra bonded to iron and/or magnesium ions. No oxygen atom is shared to two tetrahedra.

[Middle] In pyroxene, silica tetrahedra are linked together in a single chain, where one oxygen ion from each tetrahedra is shared with the adjacent tetrahedron.

[Right] Other types are possible. In amphibole structures, two oxygen ions from each tetrahedra are shared with the adjacent tetrahedra.

In mica structures, the tetrahedra are arranged in continuous sheets, where each tetrahedron shares three oxygens with adjacent tetrahedra.

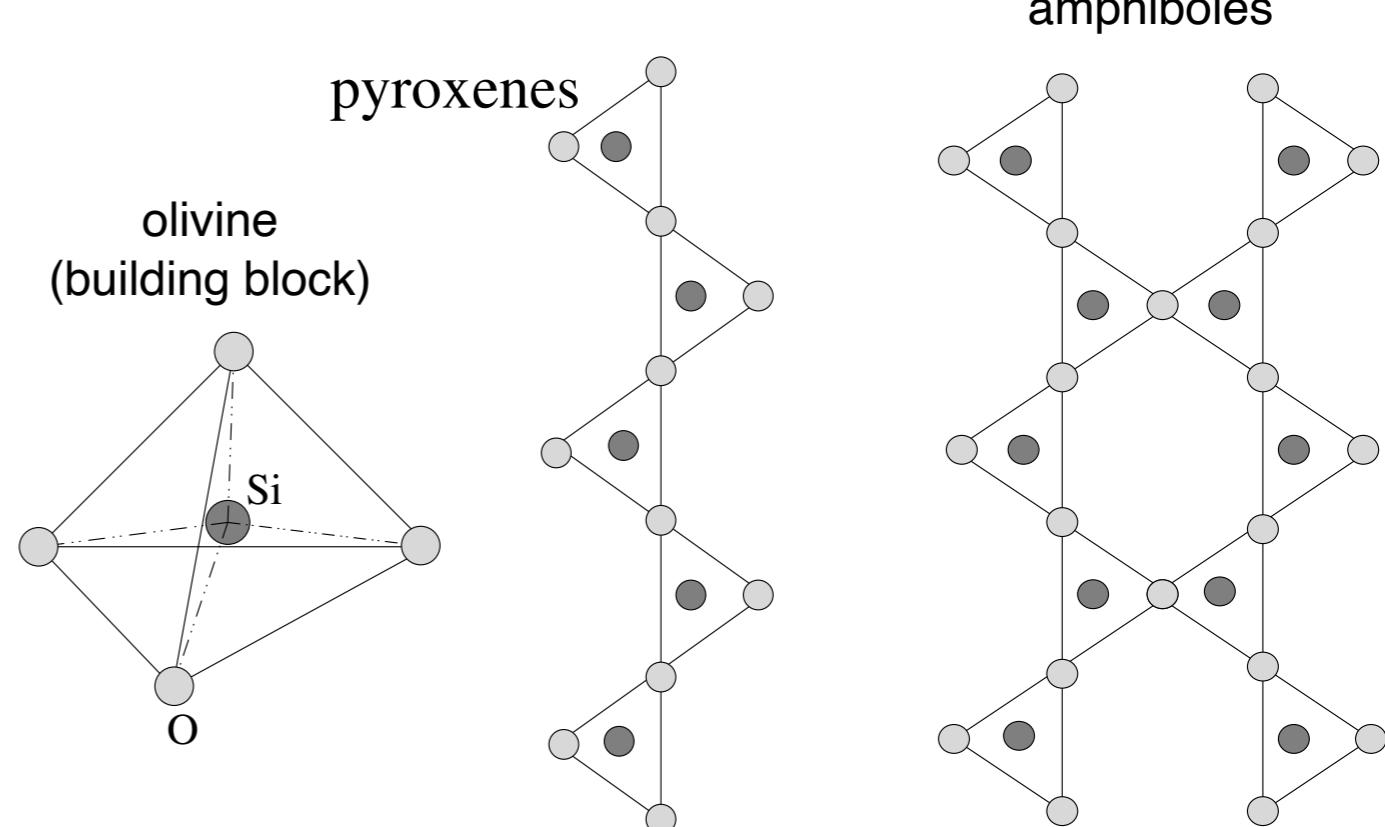
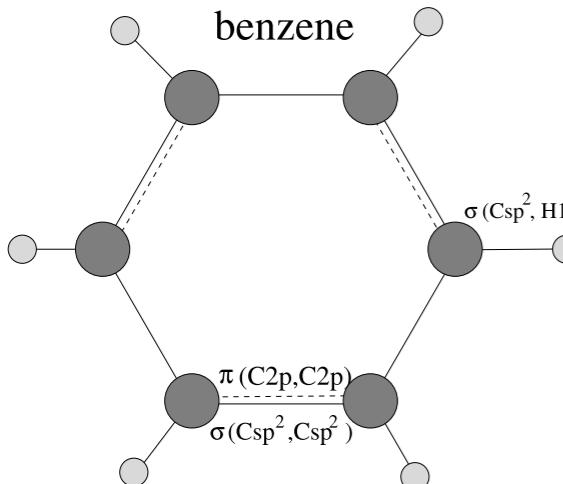


Fig 5.9 Krugel
 [An Introduction to the Physics of Interstellar Dust]

- **The observed interstellar absorption is broad and smooth, quite unlike the highly structured absorption profiles measured for crystalline silicate minerals** in the laboratory. It appears that the interstellar material is amorphous rather than crystalline.
- Upper limits can be placed on the fraction of interstellar silicates that are crystalline. Li & Draine (2001) found that not more than 5% of interstellar Si atoms could be in crystalline silicates. Kemper et al. (2005) places a tighter upper limit of 2.2%.
- However, the IR spectra of some AGB stars (de Vries et al. 2010), as well as some comets (Wooden et al. 1999; Comet Hale-Bopp) and disks around T Tauri stars (Olofsson et al. 2009) do show fine structure characteristic of crystalline silicates.

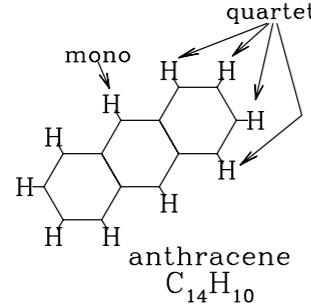
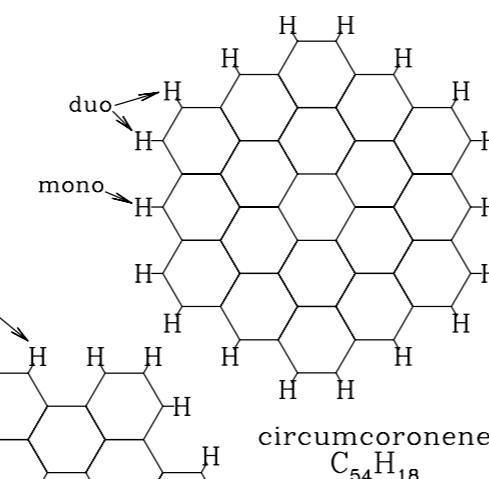
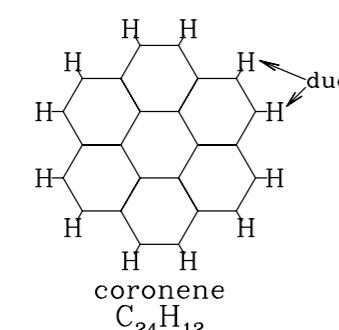
- Polycyclic Aromatic Hydrocarbons

- The IR emission spectra of spiral galaxies show emission features at **3.3, 6.2, 7.7, 8.6, 11.3, and 12.7 μm** that are attributable to vibrational transitions in polycyclic aromatic hydrocarbon (PAH) molecules.
- **PAH molecules are planar structures** consisting of carbon atoms organized into hexagonal rings, with hydrogen atoms attached at the boundary.

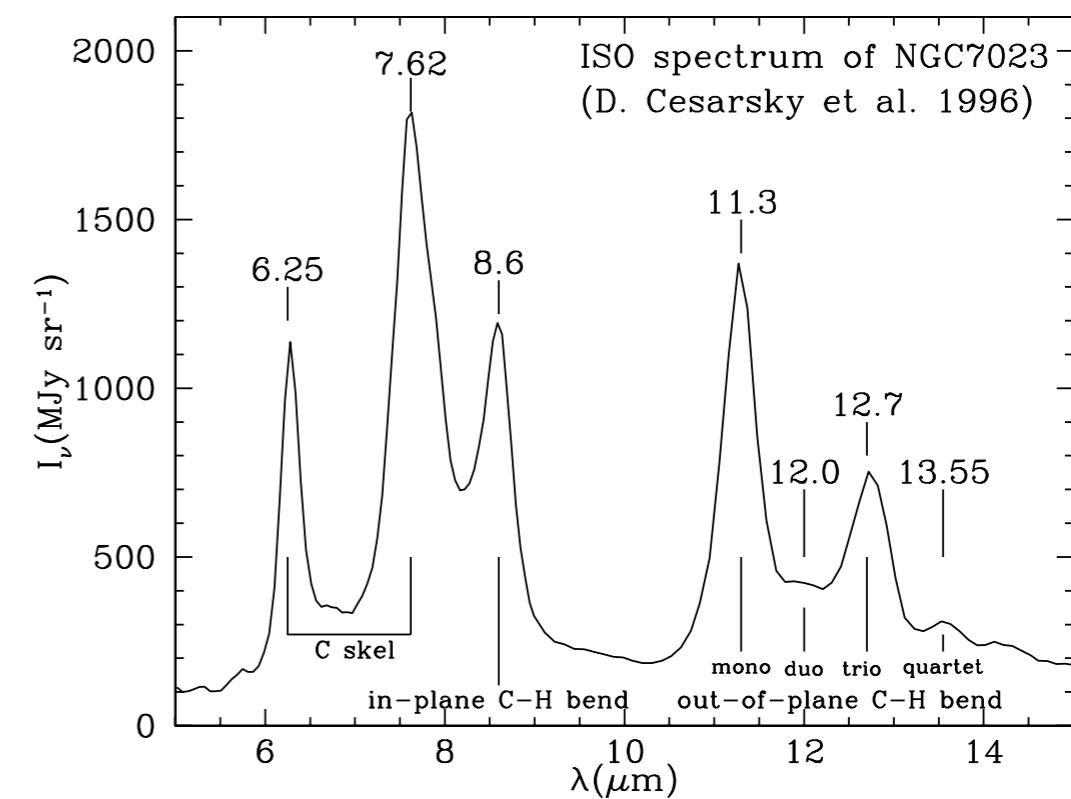


Bezene ring:
The simplest type of PAHs.

[Fig 5.6 in Krugel]



Structure of four PAHs.
[Fig 23.9 in Draine]



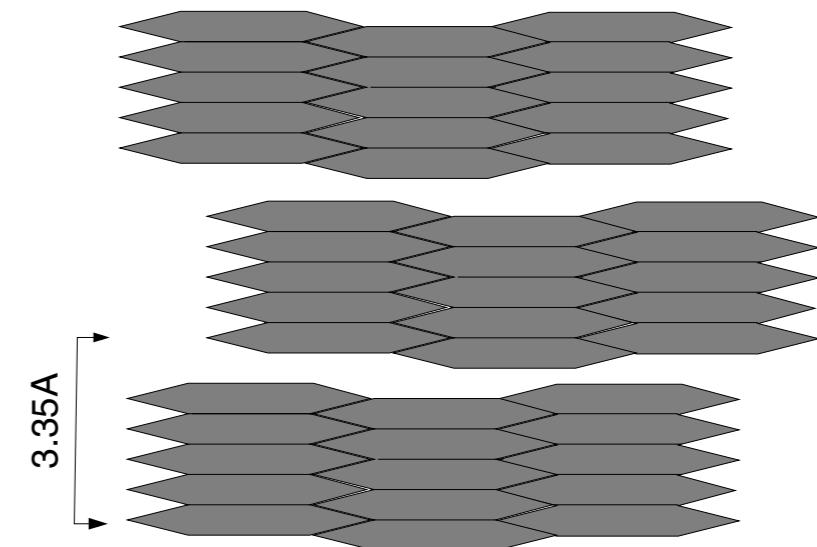
The IR spectrum of the reflection nebula NGC 7023 (Cesarsky et al. 1996)

- PAH emission features can account for as much as 20% of the total IR luminosity of a star-forming galaxy.
- Line identifications:
 - ▶ 3.3 μ m : C-H stretching mode
 - ▶ 6.2 and 7.7 μ m : vibrational modes of the carbon skeleton
 - ▶ 8.6 μ m : in-plane C-H bending modes
 - ▶ 11.3, 12.0, 12.7, and 13.55 μ m : out-of-plane C-H bending modes, of H atoms at “mono”, “duo”, “trio”, or “quartet” sites, defined by the number of adjacent H atoms.
- PAH ionization:
 - ▶ A neutral PAH can be photo ionized by the < 13.6 eV starlight in diffuse clouds, creating a PAH⁺ cation, and large PAHs can be multiply ionized.
 - ▶ Collision of a neutral PAH with a free electron can create a PAH⁻ anion.
- The matches between observations and laboratory spectra are always close, but never close enough. This has lead some researchers to suspect that the PAH features arise from complex mixtures of different carriers (mixture of neutral and charged PAHs; “damaged” or “modified” PAHs).
- The fraction of interstellar carbon that is incorporated into PAH material is uncertain. Based on the observed strength of the PAH emission features, it appears that ~ **10-15% of the interstellar carbon resides in PAHs** containing fewer than ~500 C atoms.
- *The PAH emission features are excited only in PAHs that are sufficiently small so that absorption of a single optical or UV photon can heat the grain to $T > 250$ K.* Additional PAH material may be incorporated into larger grains.

- Graphite
 - Graphite is the most stable form of carbon (at low pressure), consisting of infinite parallel sheets of **sp²-bonded carbon**.
 - ▶ A single (infinite) sheet of carbon hexagons is known as **graphene**. Each carbon atom in graphene has three nearest neighbors, with a nearest-neighbor distance of 1.421Å.
 - ▶ Crystalline graphite consists of regularly stacked graphene sheets, with an interlayer separation of 3.354Å and a density of 2.26 g cm⁻³.
 - ▶ The sheets are weakly bound to one another by **van der Waals forces**.
 - **Graphite is a semimetal**, with nonzero electrical conductivity even at low temperatures. It is a strongly anisotropic material; the response to applied electric field depends on the orientation of the electric field relative to the “basal plane”.
 - Stecher & Donn (1965) noted that **small, randomly oriented graphite spheres would be expected to produce strong UV absorption with a profile very similar to the UV bump near 2175Å**. This absorption is due to π - π* transitions in the graphite.
 - The electron orbitals of the C atoms in the interior of a large PAH molecule are very similar to the electron orbitals in graphite. PAHs therefore also have strong absorption near 2175Å.
 - Given the abundance of PAHs required to account for the observed IR emission features, **it now seems possible that the observed 2175Å extinction feature may be produced primarily by absorption in PAH molecules, or clusters of PAHs, rather than particles of graphite**.

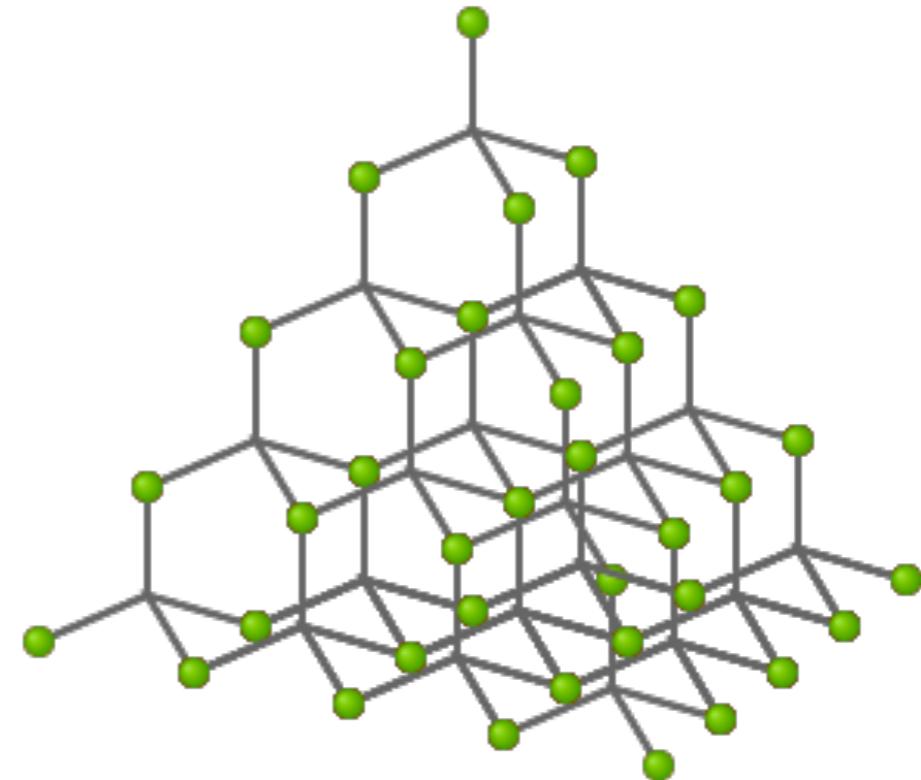


graphite sheets



Graphite structure
[Fig 5.7 in Krugel]

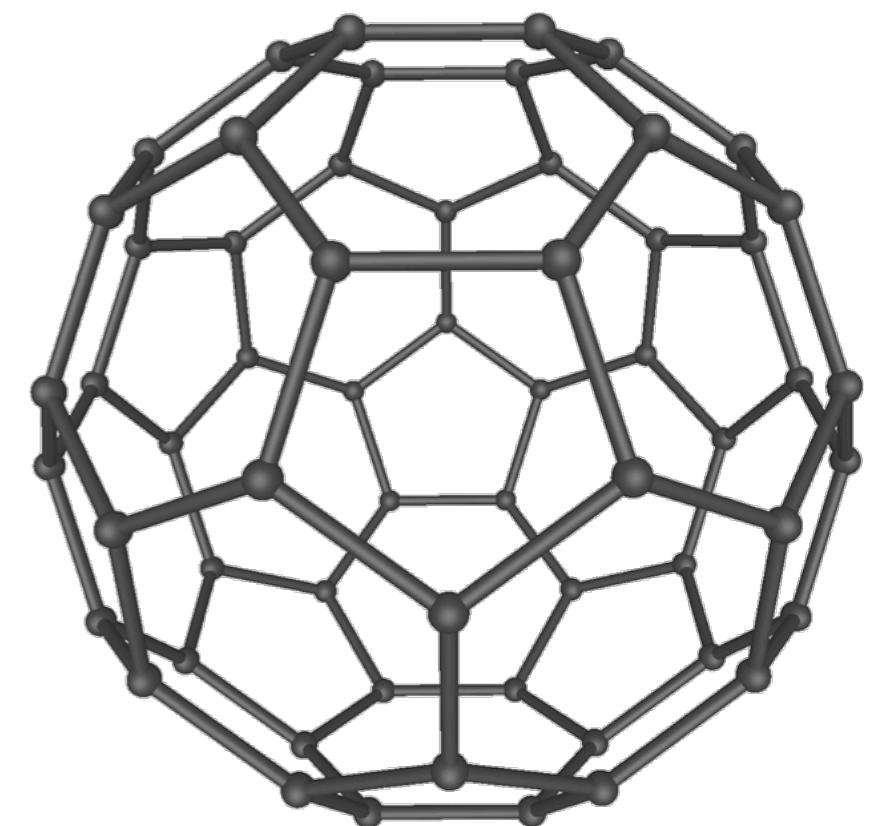
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- Nanodiamond
 - Diamond consists of **sp³-bonded carbon** atoms, with each carbon bonded to four equidistant nearest neighbors (enclosed angles are 109.47°).
 - Diamond nanoparticles are relatively abundant in primitive meteorites. Based on isotopic anomalies associated with them, we know that **some fraction of the nanodiamond was of presolar origin.**
 - But, its abundance in the ISM is not known.



Structure of diamond.

- Armorphous carbon
 - Armorphous carbon is **a mixture of sp₂- and sp₃-bonded carbon** - one can think of it as a jumble of micro crystallites with more-or-less random orientations. Armorphous carbon is not a well-defined material, and its properties depend on the method of preparation. Armorphous carbon is an **insulator**.
- Hydrogenated amorphous carbon (HAC)
 - HAC is a class of materials obtained when sufficient hydrogen is present, with H:C ratios ranging from 0.2:1 to 1.6:1 (Angus & Hayman 1988). As with amorphous carbon, the properties of HAC depend on the method of preparation. HAC is a **semiconductor**.
- Glassy or vitreous carbon
 - This is composed **primarily of sp₂-bonded carbon**, but without long-range order, and is another form of solid carbon that is generally considered to be distinct from amorphous carbon. Vitreous carbon is **electrically conducting**, with a conductivity similar to the conductivity of graphite for conduction in the basal plane.

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- Fullerenes
 - Fullerenes are cage-like carbon molecules, including C₆₀, C₇₀, C₇₆, and C₈₄, where the carbon is **sp²-bonded** with 3 near-coplanar nearest neighbors, but where a few of the hexagons are replaced by pentagons to allow the surface to close upon itself.
 - **C₆₀ (also known as buckminsterfullerene) is the most stable fullerene.**
 - Foing & Ehrenfreund (1994) found DIBs at 9577Å and 9632Å that are consistent with lab measurements of absorption by C₆₀⁺, but the identification remains tentative, because of failure to detect associated features expected near 9366Å and 9419Å.
 - Sellgren et al. (2010) reported observation of IR emission features at 7.04, 17.4, and 18.9um, that appear to confirm the presence of neutral C₆₀ in the reflection nebula NGC 7023.
 - Cami et al. (2010) report detection of IR bands of C₆₀ and C₇₀ in a young, carbon-rich, planetary nebula.



Buckminsterfullerene

Dust Theory: cross section and efficiency factors

- **Cross Sections:**

- A dust grain has wavelength-dependent cross sections for absorption and scattering. **Extinction is the sum of absorption and scattering processes.**

$$C_{\text{ext}}(\lambda) = C_{\text{abs}}(\lambda) + C_{\text{sca}}(\lambda)$$

- For a population of dust grains with number density n_d , the extinction cross section is related to the extinction coefficient and the dust optical depth by:

| | |
|------------------------|---|
| extinction coefficient | $\kappa_\lambda = n_d C_{\text{ext}}(\lambda)$ |
| dust optical depth | $\tau_\lambda = n_d C_{\text{ext}}(\lambda)L$ $= 1.086A_\lambda$ |

L = pathlength

- **Efficiency Factors:**

- The cross section is often expressed in terms of efficiency factors, normalized to the geometric cross section of an equal-solid-volume sphere:

$$Q_{\text{ext}}(\lambda) = \frac{C_{\text{ext}}(\lambda)}{\pi a^2}, \quad Q_{\text{abs}}(\lambda) = \frac{C_{\text{abs}}(\lambda)}{\pi a^2}, \quad Q_{\text{sca}}(\lambda) = \frac{C_{\text{sca}}(\lambda)}{\pi a^2}$$

$$V = \frac{4\pi}{3}a^3 \quad a = \text{the radius of an equal-volume sphere}$$

- Albedo and Scattering phase function

- The single scattering **albedo** is defined by

$$\omega(\lambda) = \frac{C_{\text{sca}}(\lambda)}{C_{\text{ext}}(\lambda)}$$

- Scattering is a function of the scattering angle and thus expressed in terms of the **differential scattering cross section**:

$$C_{\text{sca}}(\lambda) = \int_0^{2\pi} \int_0^\pi \frac{d\sigma_{\text{sca}}(\theta, \phi; \lambda)}{d\Omega} \sin \theta d\theta d\phi$$

$\frac{d\sigma_{\text{scatt}}}{d\Omega}$ = differential scattering cross section

- The **scattering asymmetry factor** is defined by:

$$g \equiv \langle \cos \theta \rangle = \frac{1}{\sigma_{\text{sca}}} \int_0^{2\pi} \int_0^\pi \cos \theta \frac{d\sigma_{\text{sca}}}{d\Omega} \sin \theta d\theta d\phi$$

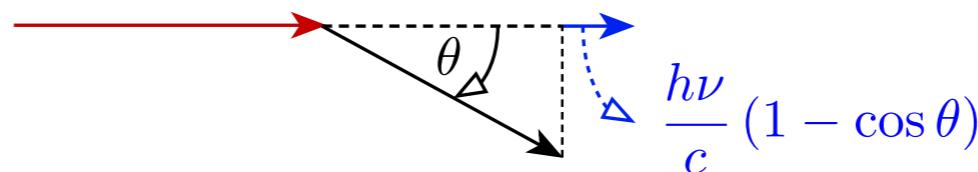
- The scattering phase function can be described by the **Rayleigh function (dipole phase function)** or **Henyey-Greenstein function**:

$$\mathcal{P}(\theta) \equiv \frac{1}{\sigma_{\text{sca}}} \int_0^\pi \frac{d\sigma_{\text{sca}}}{d\Omega} d\phi$$

$$\rightarrow \begin{aligned} \mathcal{P}_{\text{Ray}}(\theta) &= \frac{1}{2} (1 + \cos^2 \theta) && \text{for } \frac{2\pi a}{\lambda} \ll 1 \longrightarrow \langle \cos \theta \rangle = 0 \\ \mathcal{P}_{\text{HG}}(\theta) &= \frac{1}{2} \frac{1 - g^2}{(1 + g^2 - 2g \cos \theta)^{3/2}} && \text{for } \frac{2\pi a}{\lambda} \gg 1 \longrightarrow \langle \cos \theta \rangle = g \end{aligned}$$

- ▶ The Rayleigh scattering is not isotropic, even though $g = 0$.
 - ▶ **The Henyey-Greestein phase function is only introduced for computational convenience and has no physical meaning.**
- ***Radiation pressure cross section:*** Electromagnetic radiation exerts a pressure on a grain. A photon that is absorbed deposits its full momentum. $h\nu/c$. If it is scattered at an angle θ , the grain receives (in the forward direction) only the fraction $1 - \cos \theta$. Therefore, the cross section for radiation pressure can be written as:

$$\sigma_{\text{rp}} = \sigma_{\text{abs}} + (1 - \langle \cos \theta \rangle) \sigma_{\text{sca}}$$

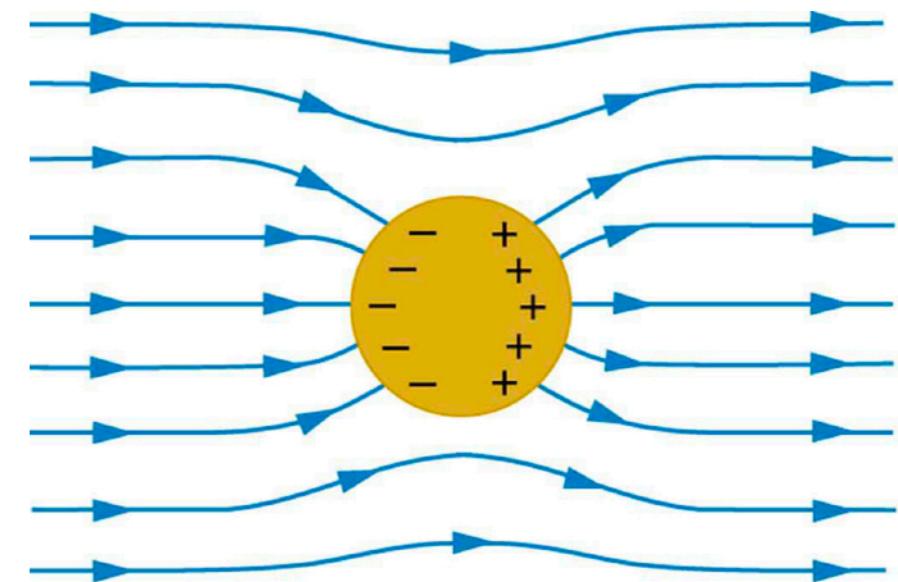
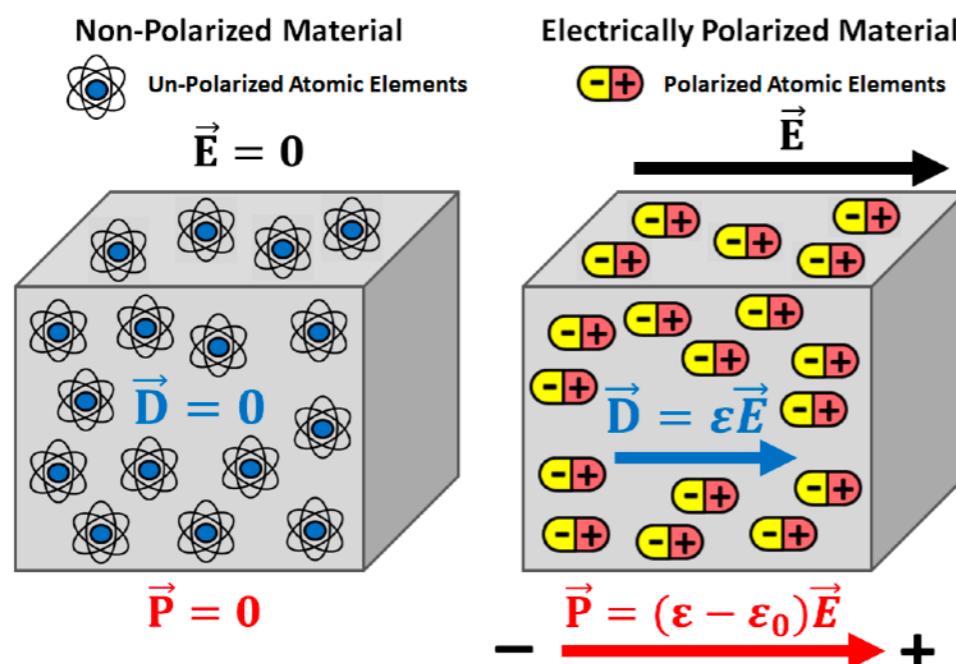


momentum conservation: $\mathbf{P}_i = \mathbf{P}_f + \mathbf{P}_{\text{dust}}$ $|\mathbf{P}_{\text{dust}}| = |\mathbf{P}_i - \mathbf{P}_f| = \frac{h\nu}{c} (1 - \cos \theta)$

- ▶ The momentum transferred to the grain is $\frac{F\sigma_{\text{rp}}}{c}$ for an incident beam of flux F (erg cm $^{-2}$ s $^{-1}$).

Dielectrics and Conductors

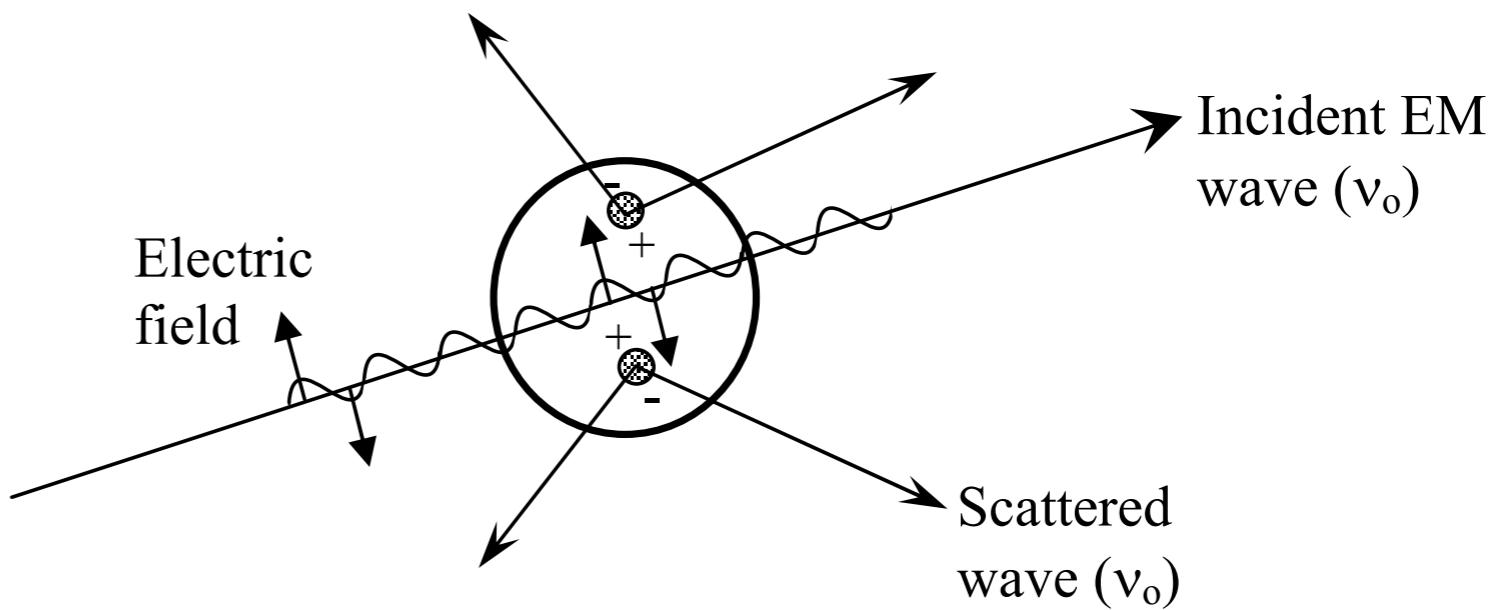
- Materials
 - ▶ **Dielectrics:** Dielectrics are substances which do not contain free charge carriers. They are isolators and no constant current can be sustained within them. Nevertheless, alternating currents produced by a time-variable electric field are possible. In these currents, the charges do not travel far from their equilibrium positions.
 - ▶ **Conductors:** The substances having free charge carriers are called the conductors. When a piece of metal is connected at its ends to the poles of a battery, a steady current flows under the influence of an electric field. When this piece of metal is placed in a static electric field, the charges accumulate at its surface and arrange themselves in such a way that the electric field inside vanishes and then there is no internal current. However, time-varying electric fields and currents are possible.
 - ▶ In the ISM, one finds both dielectric and metallic particles, but the latter are far from being perfect conductors.



Optical Properties of Grains

- Physical Basis for Scattering and Absorption
 - If an obstacle (which could be a single electron, an atom or molecule, a solid or liquid particle) is illuminated by an electromagnetic wave, electric charges in the obstacle are set into oscillatory motion with ***the same frequency*** as the electric field of the incident wave.
 - We consider the dielectric material to be made up of an infinite number of infinitely small electric and magnetic dipoles whose dipole strengths are proportional to the imposed field strengths. *The induced dipoles create their own field or wave in return. The dust particles emits its own field or waves in reaction to the imposed field of waves.*

scattering =
excitation + reradiating



- Accelerated electric charges radiate electromagnetic energy in all directions; it is this secondary radiation that is called ***the radiation scattered*** by the obstacle:

-
- In addition to reradiating electromagnetic energy, the excited elementary charges may transform part of the incident electromagnetic energy into other forms (thermal energy, for example), a process called ***absorption***.
 - ▶ ***Rayleigh scattering*** (Lord Rayleigh), applicable to small, dielectric (non-absorbing), spherical particles. ==> simple
 - ▶ $|m| \frac{2\pi a}{\lambda} \ll 1$ (m = the refractive index, a = radius of the spherical particle)
 - ▶ ***Mie scattering*** (Gustave Mie), the general solution for (absorbing or non-absorbing) spherical particles without a particular bound on particle size. ==> complex
 - ▶ Geometric optics regime: The particle is much larger than the wavelength, so that it can be regarded in the geometric optics regime. This does not mean that its scattering is simple. Reflection on the surface and refraction in the interior can still be quite complex (e.g., light passing through a rain drop), but it can be calculated using ray-tracing through the particle and off the particle's surface.

Electromagnetic Theory - Maxwell's equations

- Maxwell's eqs. (in macroscopic forms) relates fields to charge and current densities.

$$\nabla \cdot \mathbf{D} = 4\pi\rho_f$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \mathbf{H} = \frac{4\pi}{c} \mathbf{J}_f + \frac{1}{c} \frac{\partial \mathbf{D}}{\partial t}$$

Gauss's law

Gauss's law for magnetism
(no magnetic monopoles)

Maxwell-Faraday equation

Ampere-Maxwell equation

\mathbf{D}, \mathbf{H} : macroscopic fields

\mathbf{B}, \mathbf{E} : microscopic fields

$$\mathbf{D} = \epsilon \mathbf{E}$$

$$\mathbf{B} = \mu \mathbf{H}$$

ϵ : dielectric constant

μ : magnetic permeability

Here, f denotes the free charge or free current.

Dielectric material (절연체): an electrical insulator that can be polarized by an applied electric field. Electric charges do not flow through the material as they do in a conductor, but only slightly shift from their average equilibrium positions causing dielectric polarization.

Permeability (투자율): the degree of magnetization of a material in response to a magnetic field.

Note $\epsilon = \mu = 1$ in the absence of dielectric or permeability media.

D and E / H and B

- Griffiths, Introduction to Electrodynamics, 3rd
- **D** allows us to write Gauss's law in terms of the free charge alone.

The electric displacement provide a particularly useful way to express Gauss's law, in the context of dielectrics, because it makes reference only to free charges, and free charge is the stuff we control. Bound charge comes along for the ride: when we put the free charge in place, a certain polarization automatically ensues, and this polarization produces the bound charge.

- **H** plays a role in magnetostatics analogous to **D** in electrostatics:

H permits us to express Ampere's law in terms of the free current alone - and free current is what we control directly. Bound current, like bound charge, comes along for the ride - the material gets magnetized, and this results in bound currents; we cannot turn term on or off independently, as we can free currents.

Many authors call **H**, not **B**, the “magnetic field.” Then they have to invent a new word for **B**: the “flux density,” or magnetic “induction” (an absurd choice, since that term already has at least two other meanings in electrodynamics). Anyway, **B** is indisputably the fundamental quantity, so it would better to call it the “magnetic field,” as everyone does in the spoken language. **H** has no sensible name: just call it “**H**”.

Waves in a medium

In order to calculate scattering and absorption of electromagnetic waves by dust grains, we need to characterize the response of the target material to the local oscillating electric fields.

D electric displacement

Gauss

Macroscopic
Maxwell's equations

$$\nabla \cdot \mathbf{D} = 4\pi\rho$$

$$\nabla \cdot \mathbf{B} = 0$$

E electric field

B magnetic flux density
(magnetic induction)

H magnetic field strength
(magnetic field)

Faraday

$$\nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \mathbf{H} = \frac{4\pi}{c} \mathbf{J} + \frac{1}{c} \frac{\partial \mathbf{D}}{\partial t}$$

Ampere

Constitutive
Relations

$$\mathbf{D} = \epsilon \mathbf{E}$$

$$\mathbf{B} = \mu \mathbf{H}$$

$$\mathbf{J} = \sigma \mathbf{E}$$

Continuity Equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0$$

$$\nabla \cdot \left(\nabla \times \mathbf{H} = \frac{4\pi}{c} \mathbf{J} + \frac{1}{c} \frac{\partial \mathbf{D}}{\partial t} \right)$$

$$0 = 4\pi \nabla \cdot \mathbf{J} + \frac{\partial}{\partial t} \nabla \cdot \mathbf{D}$$

$$0 = \nabla \cdot \mathbf{J} + \frac{\partial \rho}{\partial t}$$

Assume a space and time variation of all quantities of the form $\exp [i(\mathbf{k} \cdot \mathbf{r} - \omega t)]$

ϵ = permittivity
 μ = permeability
 σ = conductivity

$$i\mathbf{k} \cdot \mathbf{D} = 4\pi\rho$$

$$i\mathbf{k} \cdot \mathbf{B} = 0$$

$$i\mathbf{k} \times \mathbf{E} = i\frac{\omega}{c} \mathbf{B}$$

$$i\mathbf{k} \times \mathbf{H} = \frac{4\pi}{c} \mathbf{J} - i\frac{\omega}{c} \mathbf{D}$$

$$-i\omega\rho + i\mathbf{k} \cdot \mathbf{J} = 0$$

$$\mathbf{k} \times (\mathbf{k} \times \mathbf{E}) = \frac{\omega}{c} \mathbf{k} \times \mathbf{B}$$

$$\mathbf{k}(\mathbf{k} \cdot \mathbf{E}) - \mathbf{E}(\mathbf{k} \cdot \mathbf{k}) = \frac{\omega\mu}{c} \mathbf{k} \times \mathbf{H}$$

$$k^2 \mathbf{E} = \frac{\omega^2 \epsilon \mu}{c^2} \left(1 + i \frac{4\pi\sigma}{\omega\epsilon} \right) \mathbf{E}$$

$$\mathbf{k} \times \mathbf{H} = -i\frac{4\pi}{c} \mathbf{J} - \frac{\omega}{c} \mathbf{D}$$

$$= -\frac{\omega\epsilon}{c} \left(1 + i \frac{4\pi\sigma}{\omega\epsilon} \right) \mathbf{E}$$

Dispersion Relation

$$k^2 = \frac{\omega^2}{c^2} m^2$$

$$m^2 = \mu \left(\epsilon + i \frac{4\pi\sigma}{\omega} \right)$$

m = complex index of refraction

m is sometimes referred to as the optical constants, or simply the "n and k".

- ▶ k is property of the wave, however, $\epsilon\mu$ is a property of the medium. Here, we will ignore the magnetic field, i.e., $\mu = 1$.
- ▶ These enter into the theory through the **complex index of refraction**, $m = n_r + in_i$, where the real and imaginary part are functions of the wavelength.
- ▶ Alternatively, the optical properties of a material can be expressed in terms of the **dielectric function** (or dielectric constant) $\epsilon = \epsilon_1 + i\epsilon_2$. The dielectric function and the complex index of refraction are related through.

$$m = n_r + in_i \quad (\text{or } m = n + ik)$$

$$\begin{aligned} \epsilon &= \epsilon_1 + i\epsilon_2 & \longrightarrow & \epsilon_1 = n_r^2 - n_i^2 \\ \epsilon &= m^2 & \epsilon_2 &= 2n_r n_i \end{aligned}$$

The electrical conductivity σ , if any, can be absorbed within the imaginary part of the dielectric function.

$$\mathbf{J} = \sigma \mathbf{E} \quad \epsilon \rightarrow \epsilon + \frac{4\pi i\sigma}{\omega}$$

- ▶ They are often referred to as **optical constants**.
- Consider a plane wave traveling in the z direction represented by

$$E = E_0 \exp [i(kz - \omega t)]$$

- ▶ In free space, the wave vector is given by

$$k = \omega/c = 2\pi/\lambda \quad (\lambda = \text{wavelength in vacuum})$$

-
- ▶ In a material with the index of refraction m , the wave vector is:

$$k = m\omega/c$$

The electric field becomes:

$$E = E_0 \exp\left(-\frac{n_i\omega}{c}z\right) \exp\left[-i\omega\left(t - \frac{n_r z}{c}\right)\right]$$

Thus, ***the real part of the index of refraction introduces a phase shift*** while the ***imaginary part results in damping***. The power of electromagnetic wave will decrease as it propagates through the material, with

$$|E|^2 \propto e^{-2n_i\omega z/c}$$

The attenuation coefficient will be

$$\kappa = 2n_i \frac{\omega}{c} = \frac{4\pi n_i}{\lambda}$$

- Examples:

- ▶ For transparent substances, the imaginary part of the index of refraction is much smaller than one.

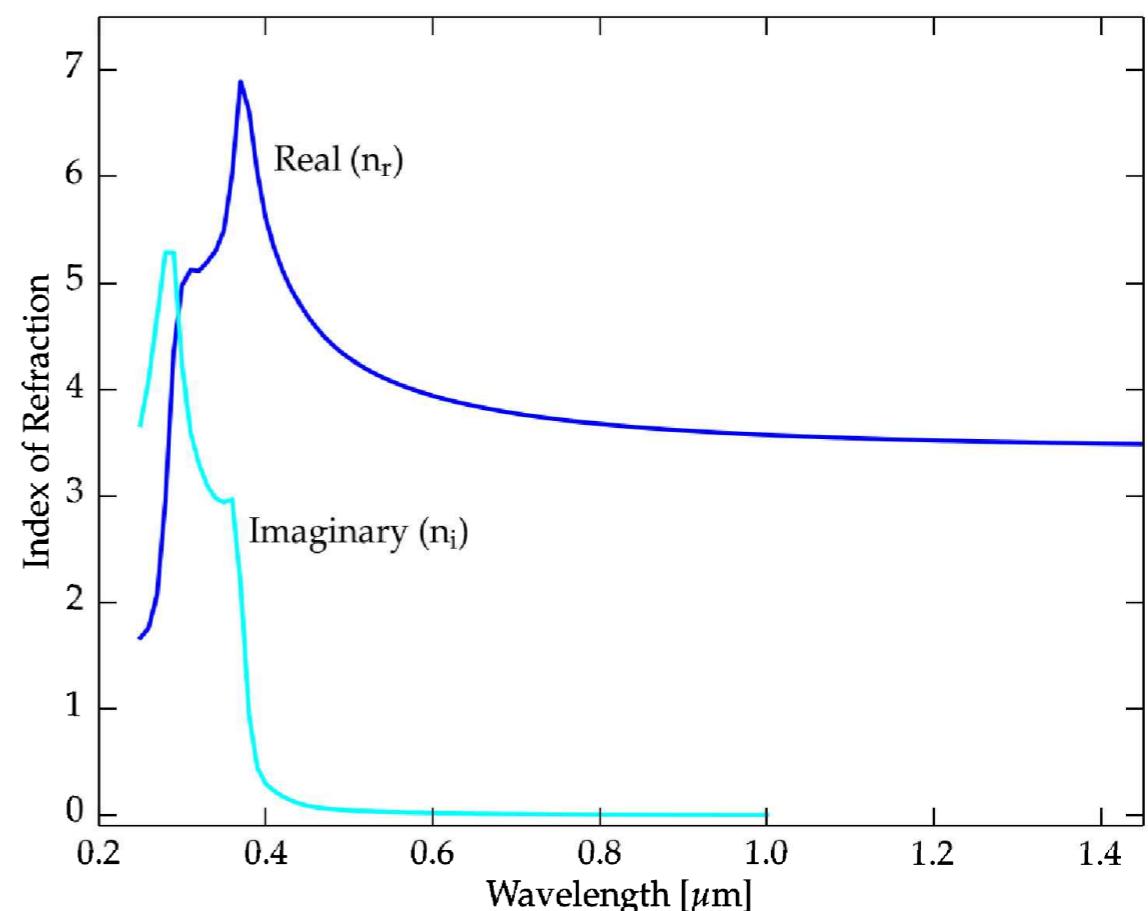
$$m = 1.31 + i(3.1 \times 10^{-9}) \quad \text{pure water ice, } \lambda = 5500\text{\AA}$$

- ▶ For highly reflective substances, the imaginary part of the index of refraction is comparable to or greater than one.

$$m = 0.36 + i2.69 \quad \text{gold, } \lambda = 5500\text{\AA}$$

- ▶ The index of refraction can be strongly dependent on wavelength.
- ▶ Silicon goes from being opaque in the UV to being transparent in the near IR.

The real (blue) and imaginary (cyan) components of the index of refraction for silicon at $T = 300$ K.



Mie Theory

- The derivation of the equations is somewhat elaborate.
 - See Chapter 4 of Bohren & Huffman [Absorption and Scattering of Light by Small Particles]
- Summary of the Results:
 - The interaction of an incident wave with a sphere of radius a causes the sphere to radiate electromagnetic waves. This outgoing wave can be written in terms of vector spherical harmonics. Like with spherical harmonics, this involves Legendre polynomials and Bessel functions.
 - The ***extinction and scattering cross sections*** can be written in terms of the scattering coefficients a_n and b_n :

$$Q_{\text{ext}} = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n+1) \operatorname{Re}\{a_n + b_n\}$$

$$Q_{\text{sca}} = \frac{2}{x^2} \sum_{n=1}^{\infty} (2n+1) (|a_n|^2 + |b_n|^2)$$

Here, x is the **size parameter**:

$$x = \frac{2\pi a}{\lambda} = \text{ratio of the size of the particle over the wavelength}$$

- The ***asymmetry factor*** is given by:

$$g = \frac{4}{x^2 Q_{\text{sca}}} \sum_{n=1}^{\infty} \left[\frac{n(n+2)}{n+1} \operatorname{Re}\{a_n^* a_{n+1} + b_n^* b_{n+1}\} + \frac{2n+1}{n(n+1)} \operatorname{Re}\{a_n^* b_n\} \right]$$

The scattering coefficients are expressed in terms of Riccati-Bessel functions ψ and ξ .

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

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

Recurrence relations:

$$\psi_n(x) = x j_n(x)$$

$$\psi'_n(x) = x j_{n-1}(x) - n j_n(x)$$

$$\xi_n(x) = x [j_n(x) + i y_n(x)]$$

$$\xi'_n(x) = x [j_{n-1}(x) + i y_{n-1}(x)] - n [j_n(x) + i y_n(x)]$$

The spherical Bessel functions satisfy the recurrence relation:

$$j_n(x) = -j_{n-2}(x) + \frac{2n-1}{x} j_{n-1}(x)$$

$$y_n(x) = -y_{n-2}(x) + \frac{2n-1}{x} y_{n-1}(x)$$

$$j_0(x) = \frac{\sin x}{x}$$

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}$$

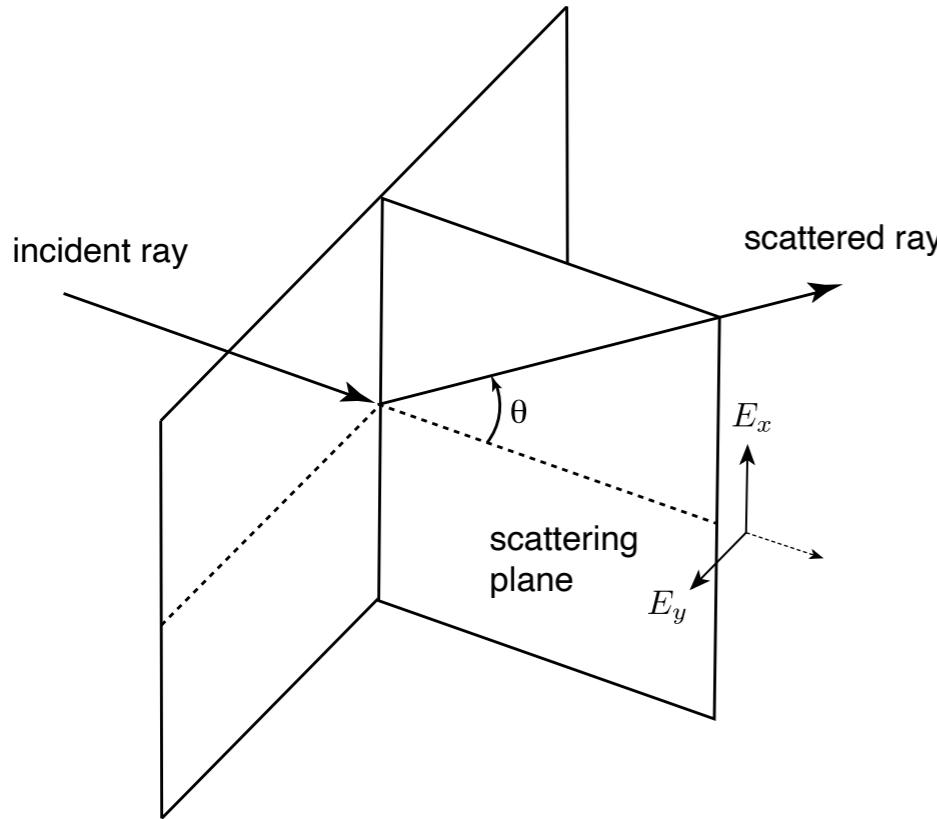
$$y_0(x) = -\frac{\cos x}{x}$$

$$y_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}$$

The larger the particle is compared to the wavelength, the more terms have to be included in the sum. A good Mie code is BHMIE of Bohren & Huffman, a version of which can be downloaded from the website of Bruce Draine (<http://www.astro.princeton.edu/~draine/scattering.html>). A python code: <https://miepython.readthedocs.io/en/latest/>

Scattering Phase Function

Let's define the scattering geometry as follows:



Scattering plane = the plane containing the incident and scattered beams

The scattering angle is defined in the scattering plane.

The functions π_n and τ_n are defined by

$$\pi_n(\cos \theta) = \frac{P_n^1(\cos \theta)}{\sin \theta}$$

$$\tau_n(\cos \theta) = \frac{dP_n^1}{d\theta}$$

Then, the scattered electric fields are given by:

$$\begin{pmatrix} E'_\parallel \\ E'_\perp \end{pmatrix} = \frac{e^{ik(r-z)}}{-kr} \begin{pmatrix} S_2 & 0 \\ 0 & S_1 \end{pmatrix} \begin{pmatrix} E_\parallel \\ E_\perp \end{pmatrix}$$

Here, the elements of the amplitude scattering matrix are

$$S_1 = \sum_n \frac{2n-1}{n(n+1)} (a_n \pi_n + b_n \tau_n)$$

$$S_2 = \sum_n \frac{2n-1}{n(n+1)} (a_n \tau_n + b_n \pi_n)$$

Definition of Bohren & Huffman

$E_x = E_\parallel^{\text{BH}}$ parallel to the scattering plane

$E_y = -E_\perp^{\text{BH}}$ perpendicular to the scattering plane

Recurrence relations:

$$\pi_n(\mu) = \frac{2n-1}{n-1} \mu \pi_{n-1} - \frac{n}{n-1} \pi_{n-2}$$

$$\tau_n(\mu) = n \mu \pi_n - (n+1) \pi_{n-1}$$

$$\pi_0 = 0 \quad \text{and} \quad \pi_1 = 1$$

$$\mu = \cos \theta$$

For an unpolarized incident light ($|E_{\parallel}| = |E_{\perp}|$) , the intensities of the incident and scattered radiation into the direction θ are related by

$$\begin{aligned} I &\equiv |E_{\parallel}|^2 + |E_{\perp}|^2 \\ I' &\equiv |E'_{\parallel}|^2 + |E'_{\perp}|^2 \end{aligned} \quad \longrightarrow \quad I'(\theta) = S_{11}I(\theta) \quad \text{where } S_{11} = \frac{1}{2}(|S_1|^2 + |S_2|^2)$$

$S_{11}(\cos \theta)$ is the scattering phase function, after a proper normalization.

When integrated over all directions, the S_{11} is related to the scattering efficiency:

$$\int_0^\pi \bar{S}_{11}(\cos \theta) \sin \theta d\theta = \frac{1}{2}x^2 Q_{\text{sca}}$$

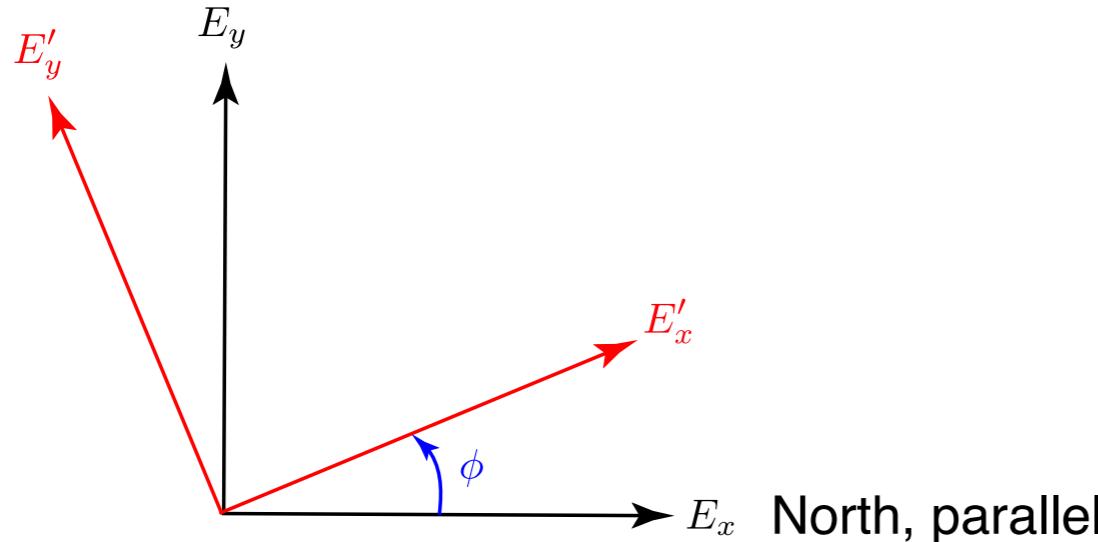
Then, the normalized phase function is given by

$$\mathcal{P}(\cos \theta) = \frac{2}{x^2 Q_{\text{sca}}} \bar{S}_{11}(\cos \theta) = S_{11}(\cos \theta) \quad \int_0^\pi \mathcal{P}(\cos \theta) \sin \theta d\theta = 1$$

Stokes Parameters

Definition of the Stokes parameters, according to the IAU recommendation:

East, perpendicular



$$\begin{aligned} I &= E_x E_x^* + E_y E_y^* \\ Q &= E_x E_x^* - E_y E_y^* \\ U &= E_x E_y^* + E_y E_x^* \\ V &= i(E_x E_y^* - E_y E_x^*) \end{aligned}$$

The Stokes parameters for scattered light for a spherical grain is then given by

$$\begin{pmatrix} I' \\ Q' \\ U' \\ V' \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} & 0 & 0 \\ S_{12} & S_{11} & 0 & 0 \\ 0 & 0 & S_{33} & S_{34} \\ 0 & 0 & -S_{34} & S_{33} \end{pmatrix} = \begin{pmatrix} I \\ Q \\ U \\ V \end{pmatrix}$$

$$S_{11} = \frac{1}{2}(|S_1|^2 + |S_2|^2)$$

$$S_{12} = \frac{1}{2}(|S_2|^2 - |S_1|^2)$$

$$S_{33} = \frac{1}{2}(S_1 S_2^* + S_2 S_1^*)$$

$$S_{34} = \frac{i}{2}(S_1 S_2^* - S_2 S_1^*)$$

$$\begin{pmatrix} I'_{\text{BH}} \\ Q'_{\text{BH}} \\ U'_{\text{BH}} \\ V'_{\text{BH}} \end{pmatrix} = \begin{pmatrix} S_{11}^{\text{BH}} & S_{12}^{\text{BH}} & 0 & 0 \\ S_{12}^{\text{BH}} & S_{11}^{\text{BH}} & 0 & 0 \\ 0 & 0 & S_{33}^{\text{BH}} & S_{34}^{\text{BH}} \\ 0 & 0 & -S_{34}^{\text{BH}} & S_{33}^{\text{BH}} \end{pmatrix} = \begin{pmatrix} I_{\text{BH}} \\ Q_{\text{BH}} \\ U_{\text{BH}} \\ V_{\text{BH}} \end{pmatrix}$$

Comparison with the definition of Bohren & Huffman

$$I = I_{\text{BH}} \qquad \qquad S_{11} = S_{11}^{\text{BH}}$$

$$Q = Q_{\text{BH}} \qquad \qquad S_{12} = S_{12}^{\text{BH}}$$

$$U = -U_{\text{BH}} \qquad \qquad S_{33} = S_{33}^{\text{BH}}$$

$$V = -V_{\text{BH}} \qquad \qquad S_{34} = S_{34}^{\text{BH}}$$

Extinction Efficiency

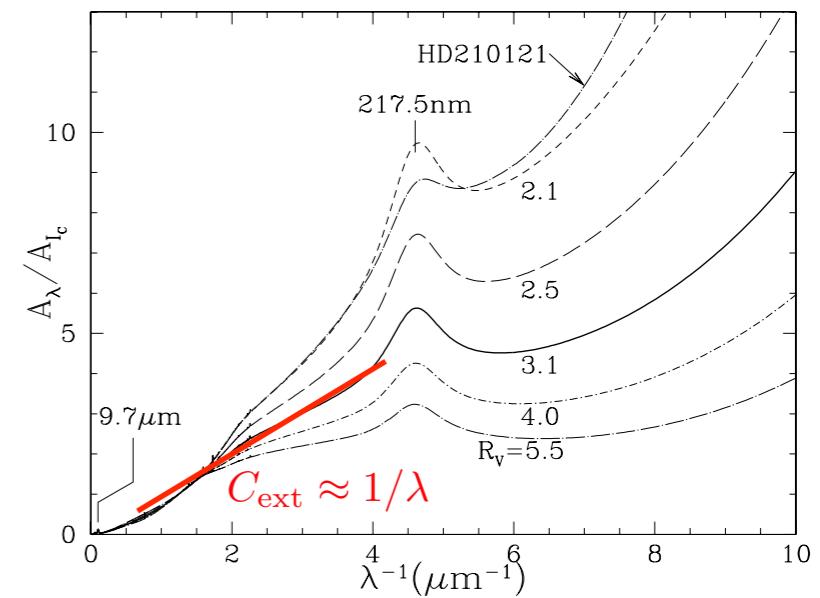
- **Rayleigh Limit:**

$$x = 2\pi a/\lambda \ll 1, \quad |m|x \ll 1$$

- Using only the lowest term of x , we obtain

$$\begin{aligned} a_1 &= -i \frac{2x^3}{3} \frac{m^2 - 1}{m^2 + 2} & Q_{\text{ext}} &\simeq \frac{6}{x^2} \operatorname{Re}(a_1) \\ b_1 &= -i \frac{x^5}{45} (m^2 - 1) & Q_{\text{sca}} &\simeq \frac{6}{x^2} |a_1|^2 \end{aligned}$$

$$\begin{aligned} Q_{\text{ext}} &\simeq 4 \left(\frac{2\pi a}{\lambda} \right) \operatorname{Im} \left(\frac{m^2 - 1}{m^2 + 2} \right) \simeq Q_{\text{abs}} \\ Q_{\text{sca}} &\simeq \frac{8}{3} \left(\frac{2\pi a}{\lambda} \right)^4 \left| \frac{m^2 - 1}{m^2 + 2} \right|^2 \end{aligned}$$



$$\begin{aligned} C_{\text{abs}} &= Q_{\text{abs}} \pi a^2 \propto \frac{a^3}{\lambda} \\ C_{\text{sca}} &\propto \frac{a^6}{\lambda^4} \quad C_{\text{sca}} \ll C_{\text{abs}} \end{aligned}$$

- ▶ The absorption coefficient is proportional to the fraction of the volume of space that is occupied by dust. ***Recall that $C_{\text{ext}} \approx 1/\lambda$ is approximately what is observed in the UV-to-NIR parts.***
- ▶ The scattering cross section is inversely proportional to $1/\lambda^4$, which is characteristic of Rayleigh scattering.
- ▶ ***As long as there is absorption ($n_i \neq 0$), absorption will dominate in the limit of small grain (in the infrared wavelengths).***

- Anomalous diffraction theory
 - When the refractive index of the particle is close to that of the environment, the particle is sometimes referred to as “soft” or “tenuous”.
 - For optically soft particles and large size parameter,

$$|m - 1| \ll 1, \quad x = 2\pi a/\lambda \gg 1$$

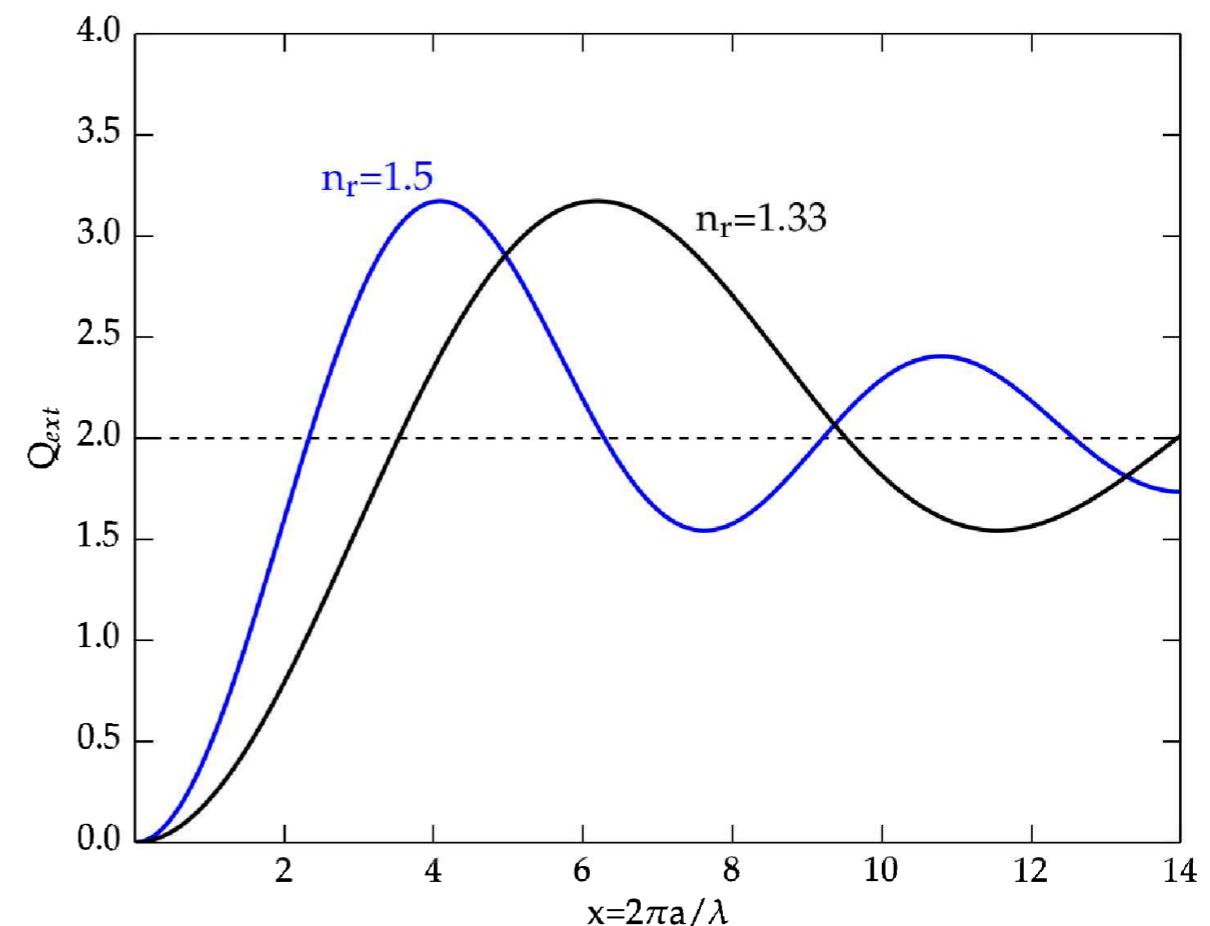
$$|m - 1| \ll 1 \rightarrow n_r \approx 1, \quad n_i \approx 0$$

This condition implies no significant attenuation.

- For the pure scattering case, the efficiency factor is

$$Q_{\text{ext}} = Q_{\text{sca}} = 2 - \frac{4}{\rho} \sin \rho + \frac{4}{\rho^4} (1 - \cos \rho)$$

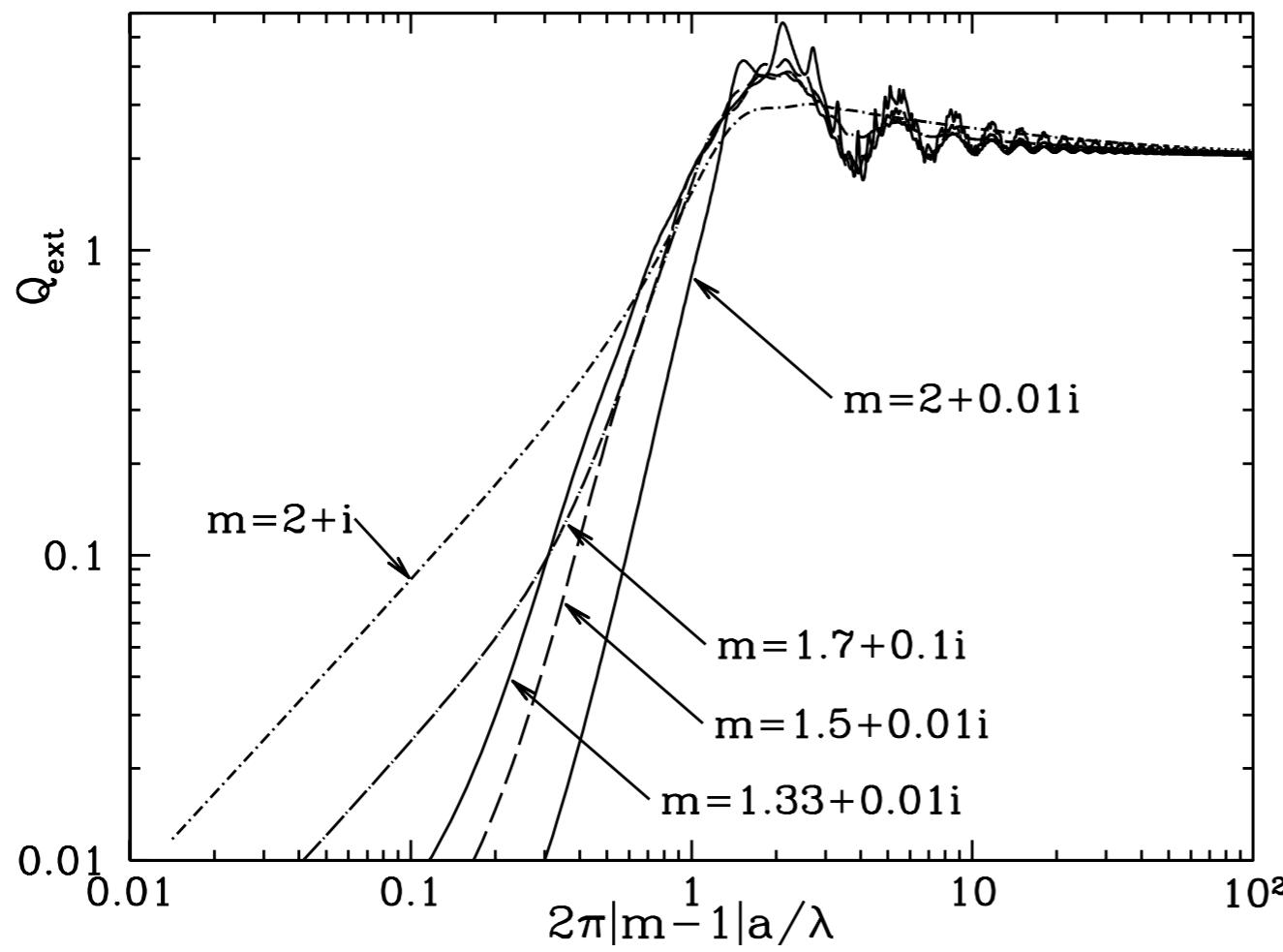
$$\text{where } \rho \equiv 2 \left(\frac{2\pi a}{\lambda} \right) |m - 1|$$



- ***In the short-wavelength limit,***

$$Q_{\text{ext}} \rightarrow 2 \quad (\text{as } |m - 1|x \rightarrow \infty) \quad \text{This is a general result.}$$

- ▶ The “**extinction paradox**” (or **Babinet’s theorem**): The extinction cross section approaches twice the geometric cross section. For more realistic spheres, that absorb as well as scatter, it is also found that $Q_{\text{ext}} \rightarrow 2$.



Extinction efficiency factors for spheres with various refractive indices.

Fig 22.3 [Draine]

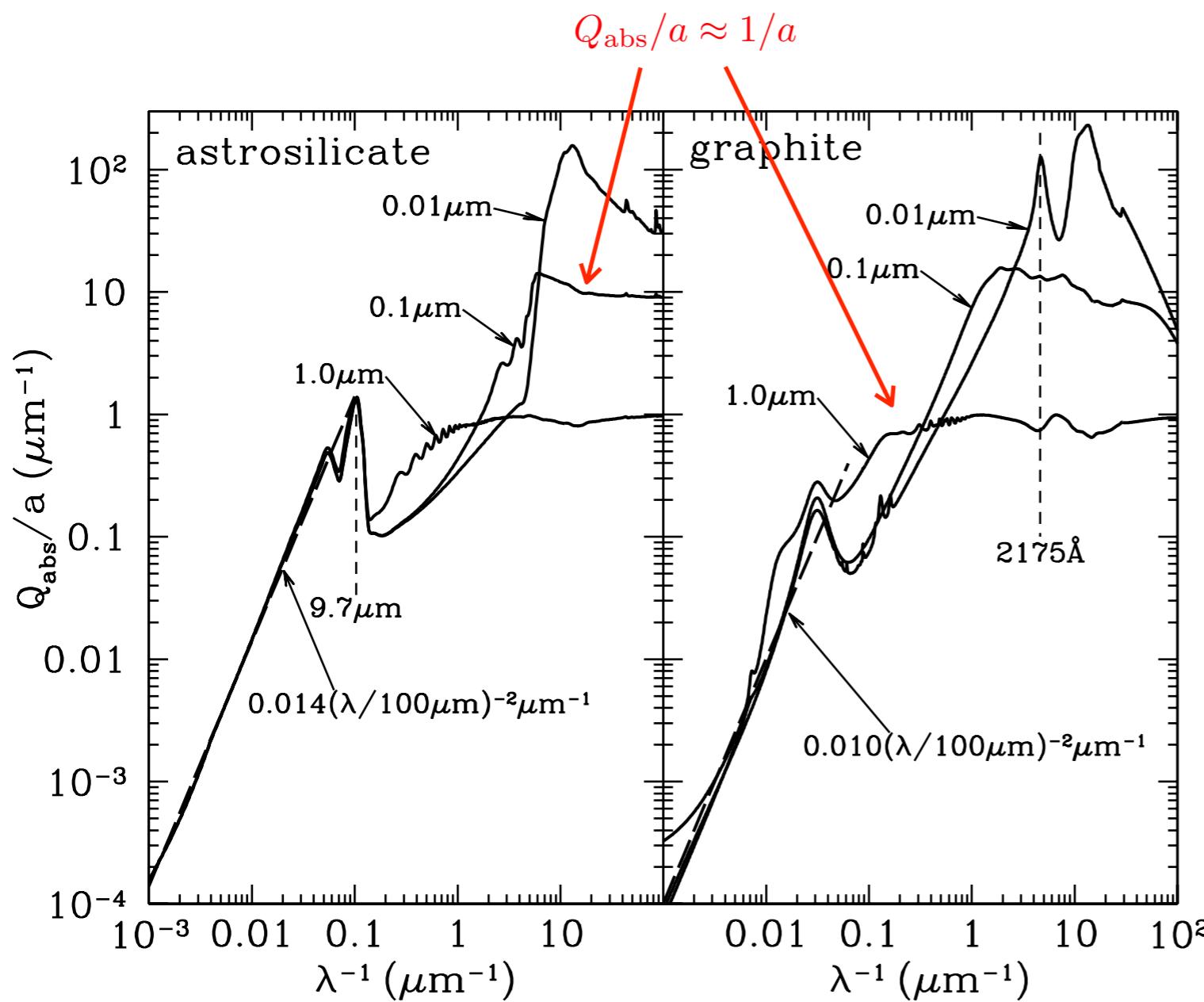
-
- Ray-tracing arguments would lead us to expect the extinction cross section to be equal to the geometric cross section in the limit $\lambda \ll a$.
 - ▶ However, *diffraction around the target leads to additional small-angle scattering*, with the total extinction cross section equal to twice the geometric cross section.
 - ▶ **Babinet's principle:** The diffraction pattern produced by an opaque object is identical to that from a hole of the same size and shape.
 - ▶ Scattering at the edge of a large obstacle is predominantly forward. At short distances, it will not be possible to recognize the diffraction effect from everyday experience so that a brick appears to remove only as much sunlight as falls onto its projected surface, and not twice as much. Therefore, $Q_{\text{ext}} = 2$ can only be verified at far distances; it is always valid for interstellar grains.
 - ▶ In the limit of opaque bowling balls, light is dimmed with efficiency factors:

$$Q_{\text{abs}} = 1$$

$$Q_{\text{sca}} = 1$$

Absorption Efficiencies for Silicate and Graphite

The figure shows the absorption efficiencies for the astrosilicate and graphite grains, with a size of $a \geq 0.01 \mu\text{m}$.



At short wavelengths ($\lambda \lesssim a$):

$$Q_{\text{abs}} \approx 1 \quad (x \gtrsim 2\pi)$$

At long wavelengths ($\lambda \gtrsim 20\mu\text{m}$):

$$Q_{\text{abs}} \approx 0.01(a/\mu\text{m})(\lambda/100\mu\text{m})^{-2}$$

[Fig 24.1, Draine]

Models for Interstellar Dust

- A model for interstellar dust must specify the **composition** of the dust as well as the **geometry (shape and size)** of the dust particles.
 - If the model is to reproduce the polarization of (extinguished) starlight, at least some of the grains should be nonspherical and aligned.
 - From the observational data available to us, **it is not yet possible to arrive at a unique grain model.**
- A class of models that has met with some success assumes the dust to consist of two materials: **(1) amorphous silicate, and (2) carbonaceous material.**
 - ***Mathis, Rumpl, and Nordsieck (1977; MRN)*** found that models using two components, silicate and graphite spheres with power-law size distributions, could reproduce the observed extinction from the near-IR to the UV ($\lambda = 0.11\mu\text{m} - 1\mu\text{m}$).

$$\frac{dn_{\text{gr}}}{da} da = A_i n_{\text{H}} a^{-3.5} da \quad \text{for } a_{\min} \leq a \leq a_{\max}$$

$a_{\min} \approx 0.025\mu\text{m}$

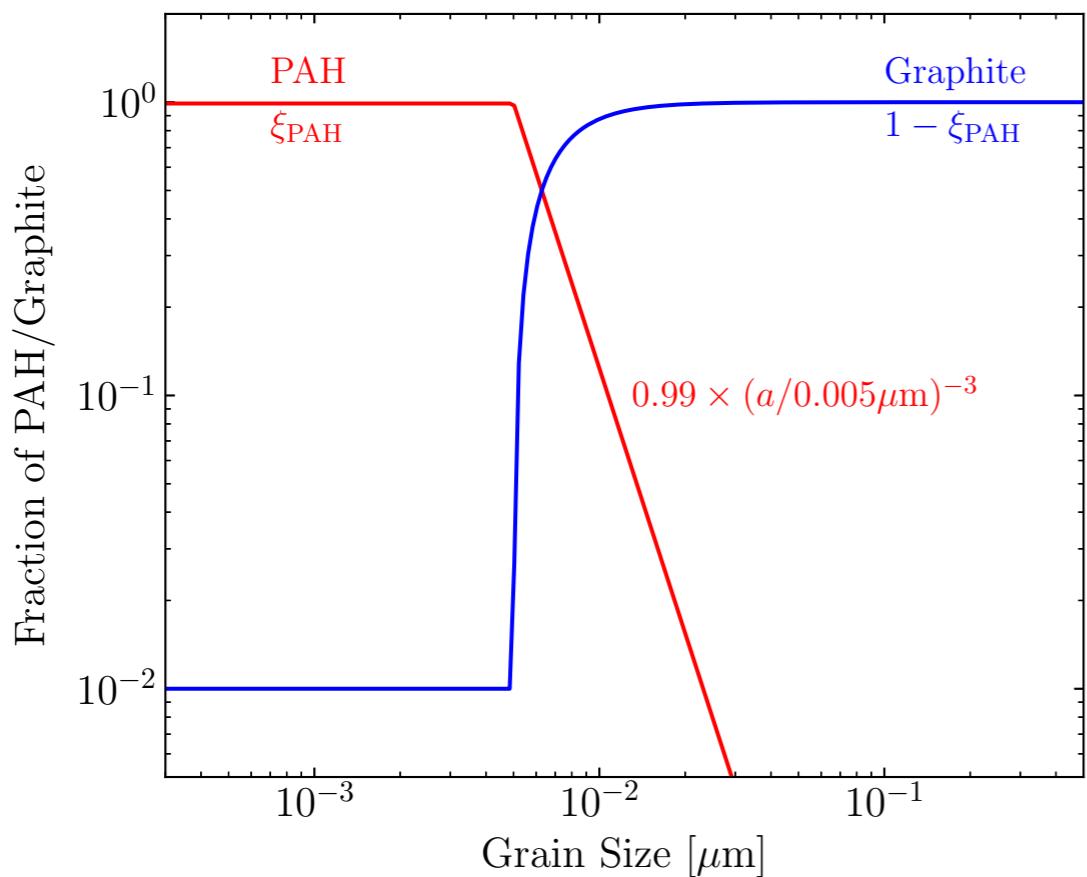
$$A_{\text{sil}} = 7.8 \times 10^{-26}, \quad A_{\text{gra}} = 6.9 \times 10^{-26} \text{ cm}^{2.5} (\text{H atom})^{-1}$$

$a_{\max} \approx 0.25\mu\text{m}$

- ▶ Graphite was a necessary component. The other could be silicon carbide (SiC), magnetite (Fe_3O_4), iron, olivine, or pyroxene.
- ***Draine and Collaborators***
 - ▶ Draine & Lee (1984) presented self-consistent dielectric functions for graphite and silicate, and showed that the graphite-silicate model appeared to be consistent with what was known about dust opacities in the Far-IR. (extended the MRN model to the Far-IR).

- They also included PAHs at small grain sized. PAHs should be added to the graphite-silicate model, either as a third component, or as the small-particle extension of the graphite model.
- The carbonaceous material is assumed to be PAH-like when the particles are small*, but when the particles are large, the carbonaceous material is approximated by graphite.

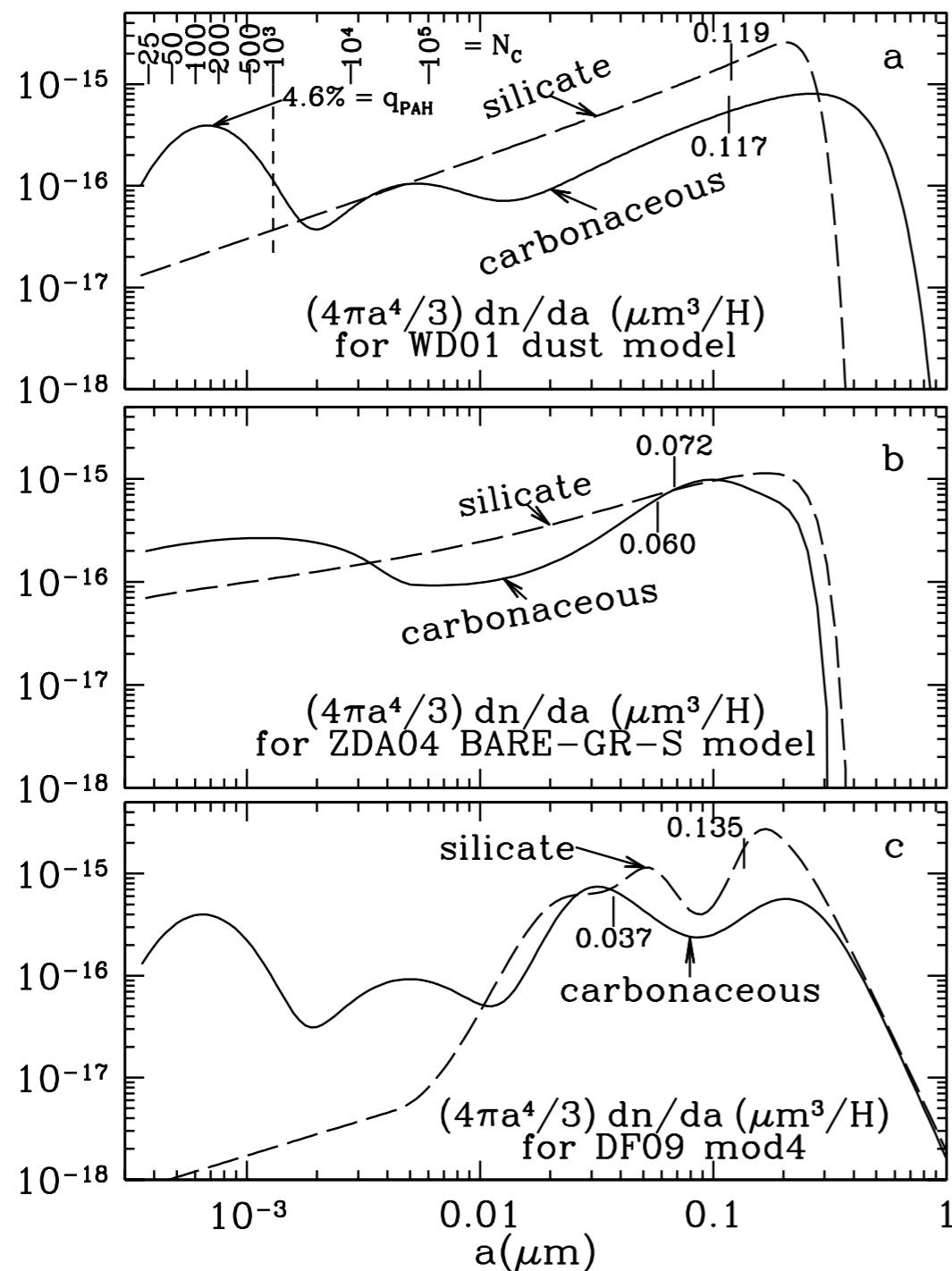
$$\sigma_{\text{abs}}^{\text{carb}}(a, \lambda) = \xi_{\text{PAH}} \sigma_{\text{abs}}^{\text{PAH}} + (1 - \xi_{\text{PAH}}) \sigma_{\text{abs}}^{\text{gra}}(a, \lambda)$$



- The size distributions should reproduce the observed extinction curve, using amounts of grain material that are consistent with the abundance limits.
- The model of **Weingartner & Draine (2001; WD01)** does a good job of reproducing the observed extinction, but the assumed mass in dust exceeds estimates based on elemental abundances and observed depletions.
- WD01 model contains 0.011g of dust per a gram of hydrogen. **In the WD01 model, 75% of the dust mass comes from silicate grains, while other 25% comes from carbon grains.**
- Draine & Fraisse (2009) used grain models with spheroidal graphite and silicate grains to reproduce both the observed extinction and polarization. The non spherical grains are sometimes able to account for the observed extinction using less mass.

- **Zubko et al. (2004)**

- The size distribution of the “BARE-GR-S” model of Zubko et al. (2004), composed of bare graphite grains, bare silicate grains, and PAHs, differs significantly from the WD01 size distribution.



A “typical” grain size may be taken as the half-mass grain size $a_{0.5}$, defined so that half the mass of dust is in grains of radius $a_{0.5}$ or greater.

In WD01 model, both carbonaceous and silicate grains have $a_{0.5} \approx 0.12 \mu\text{m}$.

In Zubko et al. model, $a_{0.5} \approx 0.60 - 0.72 \mu\text{m}$.

Size distributions for silicate and carbonaceous grains for dust models from (a) Weingartner & Draine (2001), (b) Zubko et al. (2004), and (c) Draine & Faisse (2009).

In each case, *tick-marks indicate the “half-mass” radii for the silicate grains and carbonaceous grains.*

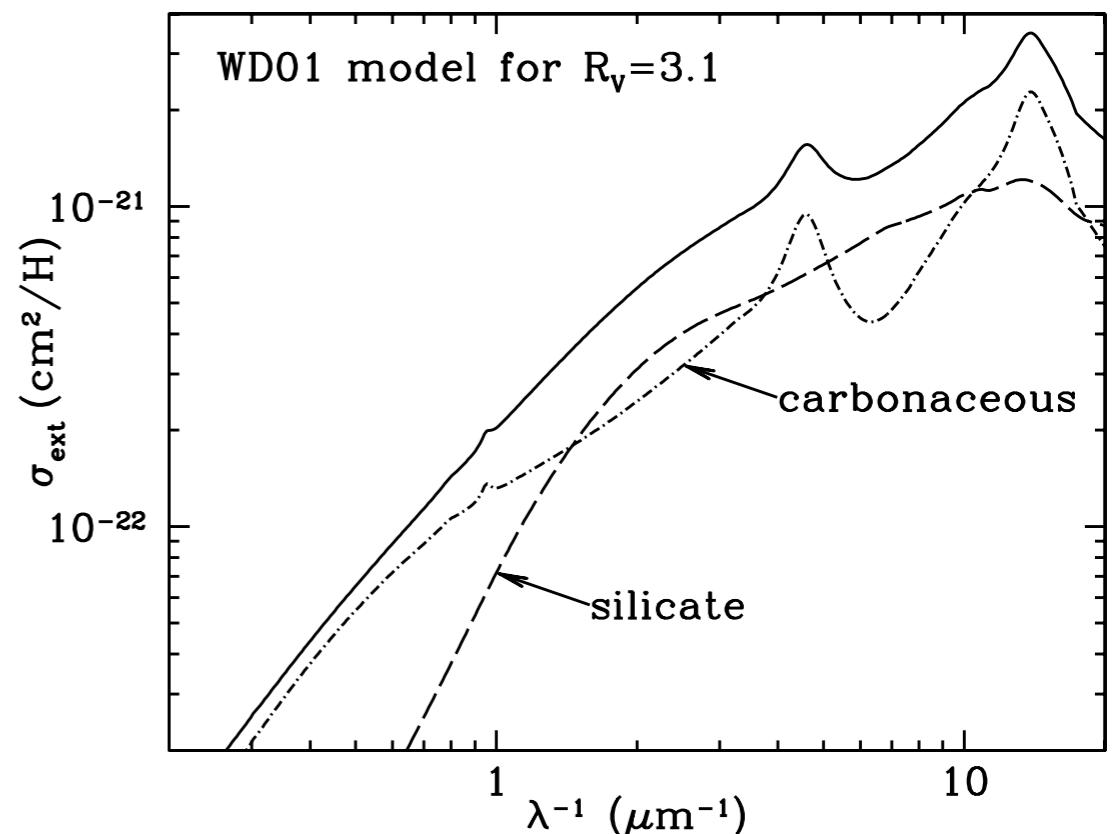
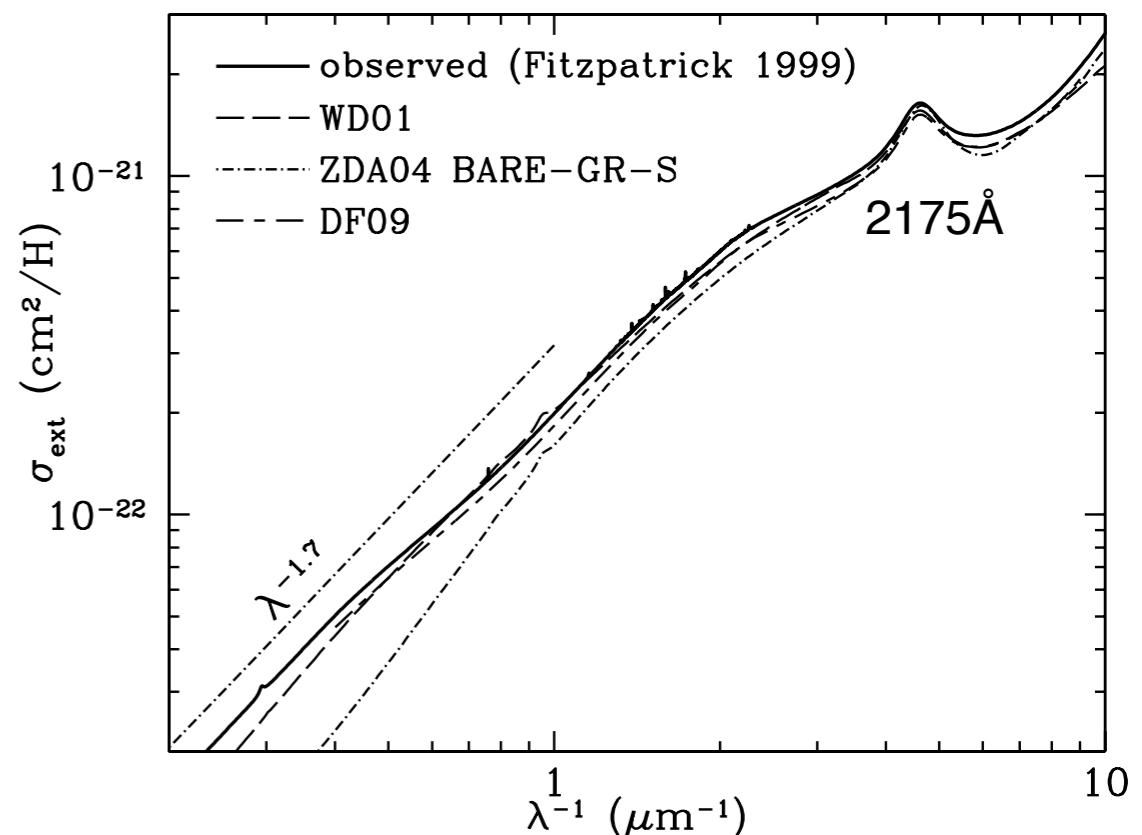
[Fig 23.10 Draine]

[Figure 23.11 Draine]

Averaged observed extinction for $R_V = 3.1$ (Fitzpatrick 1999) and extinction curves calculated for the Weingartner & Draine (2001) model and for the BARE-GR-S model of Zubko et al. (2004).

The Weingartner & Draine model provides considerably more extinction in the infrared (1 - 4 μm) than the Zubko et al. model.

Separate contributions of silicate and carbonaceous grains.



- Constraints on the small dust grains:
 - There is little constraint on the grain size distribution at the small end, because for small grains ($< 200 \text{ \AA}$) extinction is in the Rayleigh limit and independent of grain size. *The presence of very small grains and even large molecules is not derived from extinction measurements but rather inferred from studies of the mid-IR emission of the Galaxy.*
 - For very large grains ($\sim 1\mu\text{m}$), extinction in the visible is gray and dust abundances are mainly derived from abundance constraints on the elements making up these grains.
 - Despite these caveats, all dust models agree that ***the total dust volume is dominated by the large grains while the number density and surface area are dominated by the small grains.***

Dust models

- Li & Draine (2001a): pre-Spitzer model
amorphous silicate grains + graphite + PAHs
spherical grains: no polarization
- Draine & Li (2007) (DL07):
amorph. sil. and graphite from Li & Draine (2001a)
PAHs adjusted slightly to match early Spitzer results
spherical grains: no polarization
- Draine & Fraisse (2009):
DL07 materials
spheroidal grains grains with partial alignment
- Compiègne et al. (2011) (“DUSTEM” model)
amorph. silicate + amorph. C + PAHs
spherical grains: no polarization
- Jones et al. (2013):
amorph. silicate + Fe nanoparticles + amorph. C + PAHs
spherical grains: no polarization
- Hensley & Draine (2015):
amorph. silicate (new dielectric fn.) + Fe + graphite + PAHs
spheroidal grains with partial alignment

Temperatures of Interstellar Grains

- The “temperature” of a dust grain is a measure of ***the internal energy E_{int} present in vibrational modes and possibly also in low-lying electronic excitations.***
- Grain Heating
 - In diffuse regions, where ample starlight is present, grain heating is dominated by absorption of starlight photons.
 - In dense dark clouds, grain heating can be dominated by inelastic collisions with atoms or molecules from the gas (grain-grain collisions are too infrequent).
- When an optical or UV photon is absorbed by a grain, an electron is raised into an excited electronic state; three cases can occur.
 - If the electron is sufficiently energetic, it may be able to escape from the solid as a **“photoelectron.”**
 - In rare cases, the grain will “luminesce” (***luminescence = fluorescence*** when it occurs promptly + **phosphorescence** when it occurs slowly from a metastable level). The excited state will decay radiatively, emitting a photon of energy less than or equal to the energy of the absorbed photon.
 - ***In most solids or large molecules, however, the electronically excited state will deexcite nonradiatively, with the energy going into many vibrational modes - i.e., heat.***

- Large Grains
 - Grains with radii $a \gtrsim 0.03 \mu\text{m}$, can be considered “classical.” These grains are macroscopic - *absorption or emission of single quanta do not appreciably change the total energy in vibrational or electronic excitations.*
 - The temperature of a large dust grain can be obtained by equating the heating rate to the cooling rate.
- Very Small Grains
 - For ultra-small particles, ranging down to large molecules, quantum effects are important (this include the “spinning” dust grains responsible for microwave emission).
 - When a dust particle is very small, its temperature will fluctuate. This happens because whenever an energetic photon is absorbed, *the grain temperature jumps up by some not negligible amount* and subsequently declines as a result of cooling.
 - To compute their emission, *we need their optical and thermal properties.*
 - ▶ The optical behavior depends in a sophisticated way on the the complex index of refraction and on the particle shape.
 - ▶ The thermal behavior is determined more simply from the specific heat.
 - We need to calculate the distribution function of temperature.

Temperature - (1) Heating

- Radiative Heating rate (for a single particle):
 - Ignoring the small fraction of energy appearing as luminescence or photoelectrons, the rate of heating of the grain by absorption of radiation can be written.

$$\begin{aligned} \left(\frac{dE}{dt} \right)_{\text{abs}} &= \int \frac{u_\nu d\nu}{h\nu} \times c \times h\nu \times Q_{\text{abs}}(\nu) \pi a^2 \\ &= \int d\nu 4\pi J_\nu Q_{\text{abs}}(\nu) \pi a^2 \end{aligned}$$

Here, $u_\nu d\nu/h\nu$ is the number density of photons; the photons move at the speed of light c and carry energy $h\nu$.

- It is convenient to define a spectrum-averaged absorption cross section:

$$\langle Q_{\text{abs}} \rangle_* \equiv \frac{\int d\nu u_\nu Q_{\text{abs}}(\nu)}{u_*} = \frac{\int d\nu J_\nu Q_{\text{abs}}(\nu)}{J_*}, \quad u_* \equiv \int d\nu u_\nu, \quad J_* \equiv \int d\nu J_\nu$$

- The radiative heating rate is:

$$\left(\frac{dE}{dt} \right)_{\text{abs}} = \langle Q_{\text{abs}} \rangle_* \pi a^2 (u_* c) = \langle Q_{\text{abs}} \rangle_* \pi a^2 (4\pi J_*)$$

ISRF of Mathis et al.

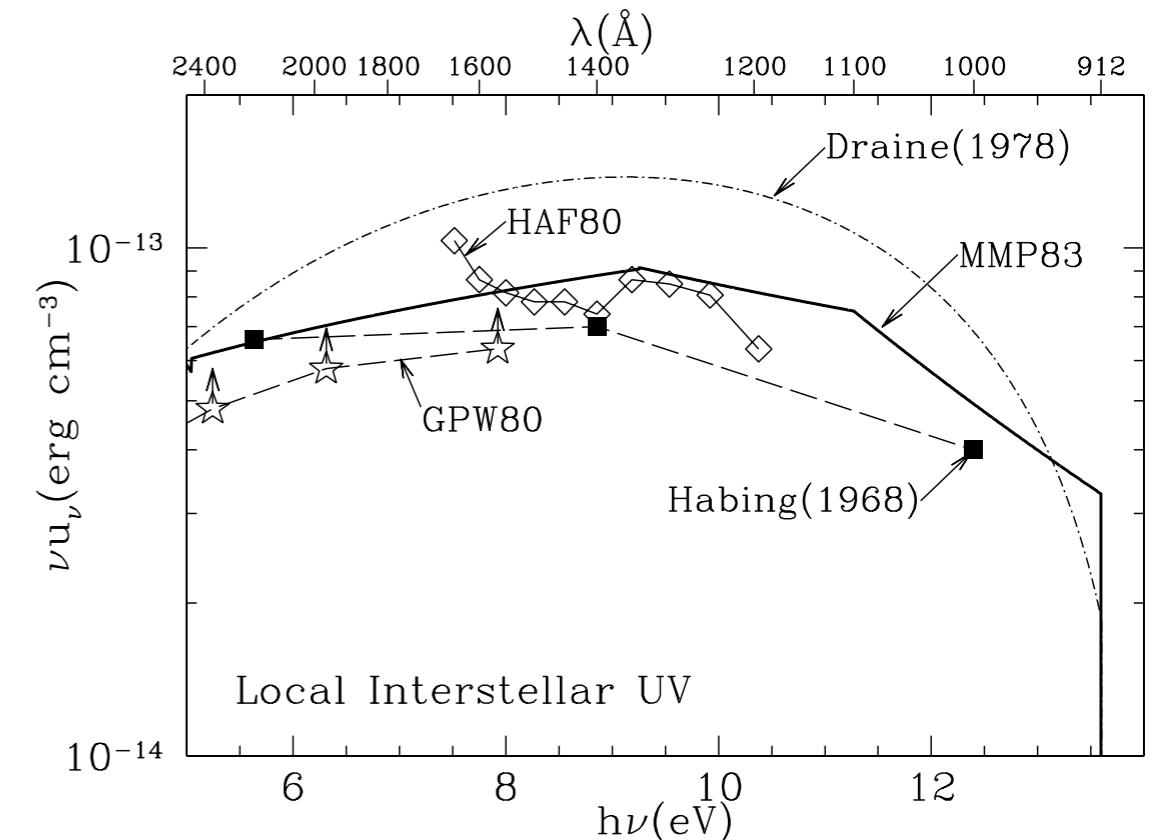
- Mathis et al. (1983, MMP83)
 - In the energy range 1 to 13.6 eV, most of the photons are starlight. Mathis et al. (1983) have approximated the local starlight background as a sum of three dilute blackbodies and a piecewise power-law approximation for UV.
 - To improve agreement with the COBE-DIRBE observation, Draine has increased the dilution factor W_1 by 40%.

$$\nu u_\nu = \sum_{j=1}^3 \frac{8\pi h\nu^4}{c^3} \frac{W_j}{e^{h\nu/kT_j} - 1} \quad \text{for } \lambda > 2450\text{\AA}$$

$$T_1 = 3000 \text{ K}, \quad W_1 = 7 \times 10^{-13}$$

$$T_2 = 4000 \text{ K}, \quad W_2 = 1.65 \times 10^{-13}$$

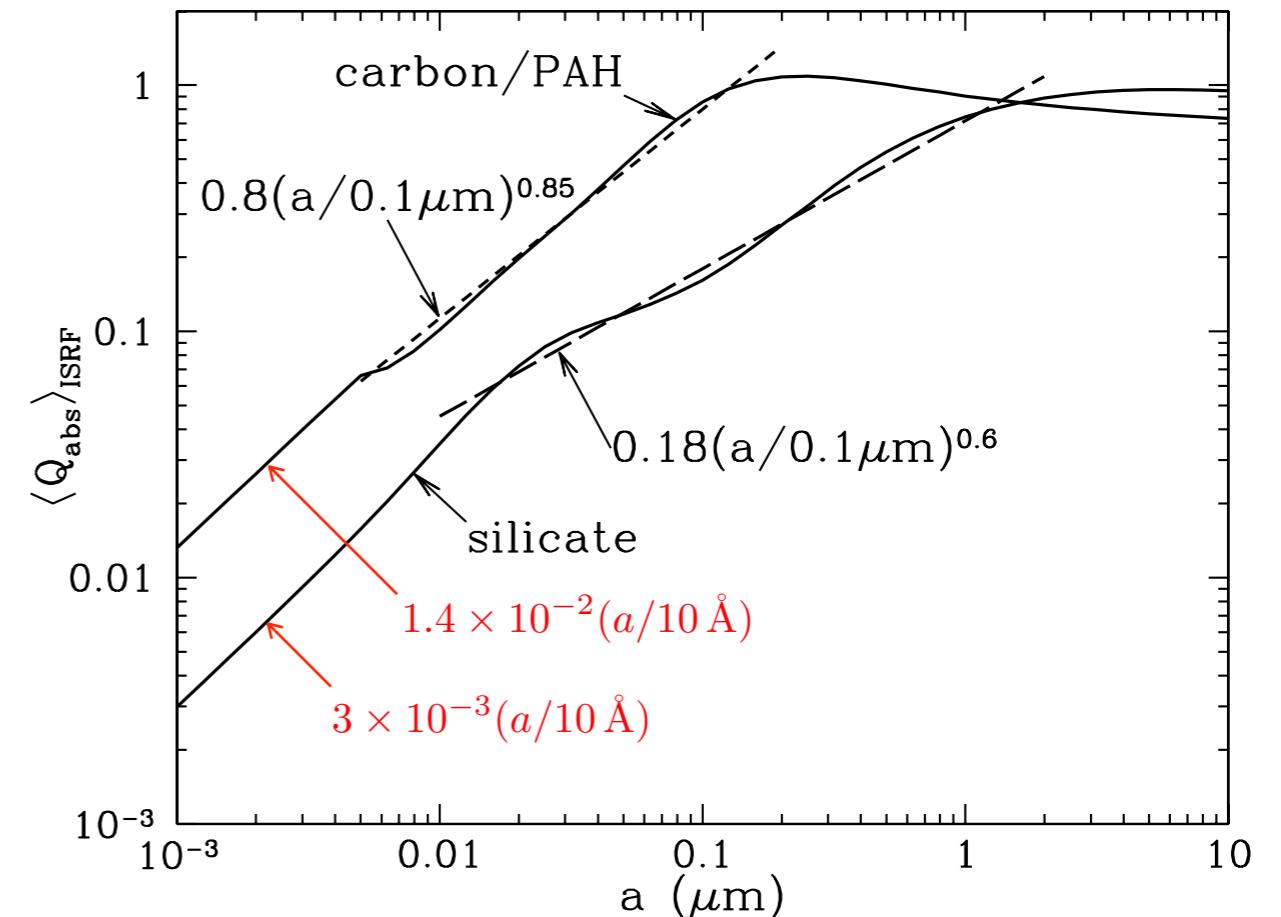
$$T_3 = 7500 \text{ K}, \quad W_3 = 1 \times 10^{-14}$$



[Fig 12.2, Draine]

$$\nu u_\nu = \begin{cases} 2.373 \times 10^{-14} (\lambda/\mu\text{m})^{-0.6678} \text{ erg cm}^{-3} & 1340 - 2460 \text{\AA} \\ 6.825 \times 10^{-13} (\lambda/\mu\text{m}) \text{ erg cm}^{-3} & 1100 - 1340 \text{\AA} \\ 1.287 \times 10^{-9} (\lambda/\mu\text{m})^{4.4172} \text{ erg cm}^{-3} & 912 - 1100 \text{\AA} \end{cases}$$

- The spectrum-averaged absorption cross section as a function of radius for graphite and silicate grains, and the spectrum of the interstellar radiation field (ISRF) from Mathis et al. (1983).



[Fig 24.2, Draine]

The numerical results can be approximated by

$$\begin{aligned}\langle Q_{\text{abs}} \rangle_{\text{ISRF}} &\approx 0.18(a/0.1\mu\text{m})^{0.6}, \quad \text{for silicate, } 0.01 \lesssim a \lesssim 1\mu\text{m} \\ &\approx 0.8(a/0.1\mu\text{m})^{0.85}, \quad \text{for graphite, } 0.005 \lesssim a \lesssim 0.15\mu\text{m}\end{aligned}$$

$$u_* = 1.05 \times 10^{-12} U \text{ [erg cm}^{-3}\text{]} \quad U = \text{strength of the ISRF in units of that of MMP83.}$$

Temperature - (2) Cooling

- Radiative Cooling rate (for a single particle)

- Kirchhoff's Law in LTE

j_ν = emissivity per unit volume

κ_ν = absorption coefficient per unit length

j_ν/n_d = emissivity per particle

$\kappa_\nu/n_d = C_{\text{abs}}(\nu)$ = absorption cross section

n_d = number density of dust particles

$$\frac{j_\nu}{\kappa_\nu} = B_\nu(T) \Rightarrow \frac{j_\nu}{n_d} = C_{\text{abs}}(\nu)B_\nu(T)$$

[$B_\nu(T)$ = Planck function, $\kappa_\nu = n_d C_{\text{abs}}(\nu)$]

- Grains lose energy by infrared emission at a rate:

$$\begin{aligned} \left(\frac{dE}{dt} \right)_{\text{emiss}} &= \int d\nu 4\pi j_\nu / n \\ &= \int d\nu 4\pi B_\nu(T_d) C_{\text{abs}}(\nu) \\ &= 4\pi a^2 \langle Q_{\text{abs}} \rangle_{T_d} \sigma_{\text{SB}} T_d^4 \end{aligned}$$

The Stephan-Boltzmann constant is:

$$\sigma_{\text{SB}} = \frac{2\pi^5 k_B^4}{15c^2 h^3} = 5.67 \times 10^{-5} \text{ erg cm}^2 \text{ s}^{-1} \text{ K}^{-4} \text{ sr}^{-1}$$

Here, the Planck-averaged emission efficiency is defined by

$$\langle Q_{\text{abs}} \rangle_T \equiv \frac{\int d\nu B_\nu(T) Q_{\text{abs}}(\nu)}{\int d\nu B_\nu(T)}$$

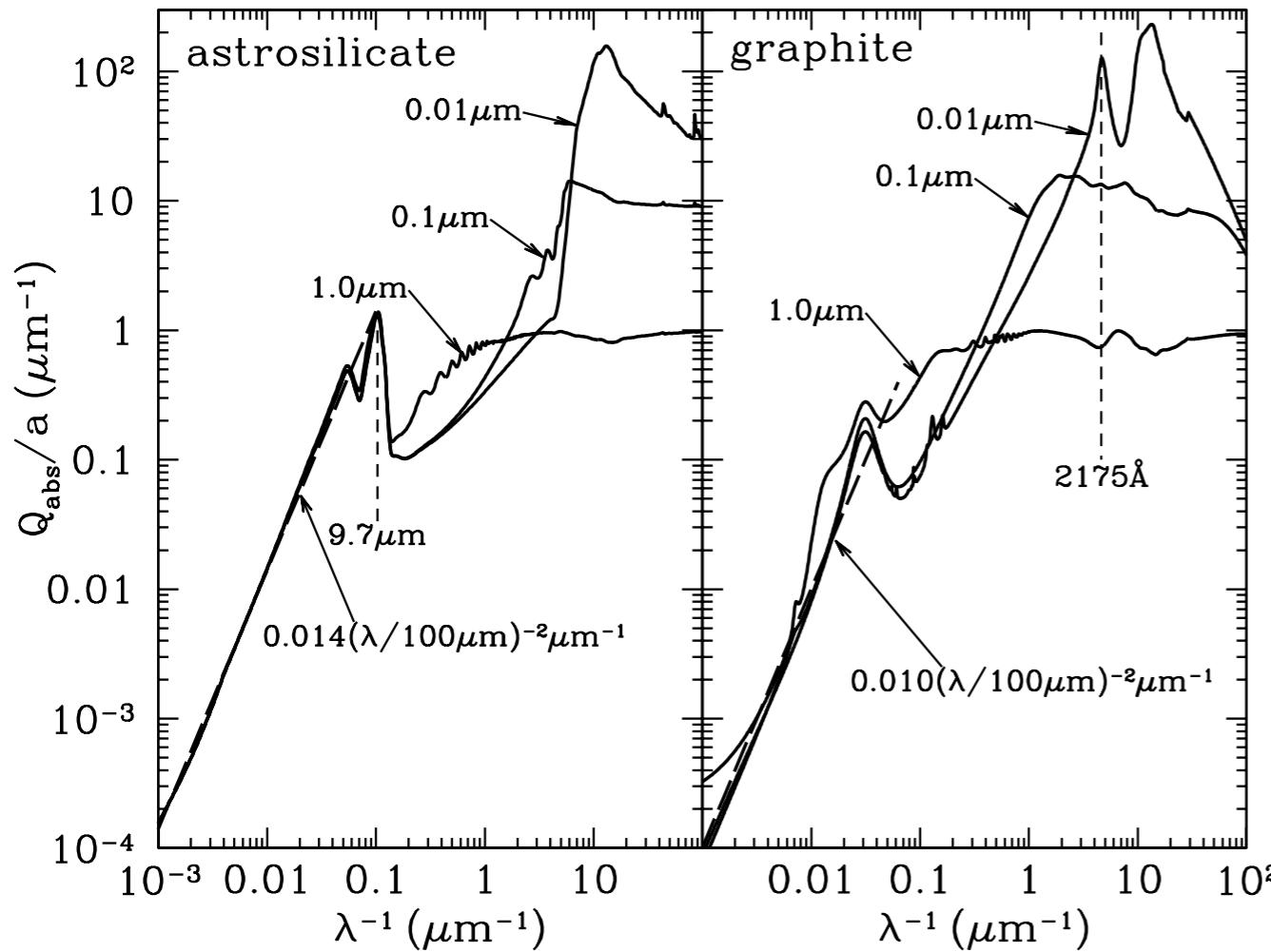
$$\int d\nu B_\nu(T) = \frac{\sigma_{\text{SB}}}{\pi} T_d^4$$

- In general, the absorption cross section in the far-IR can be approximated as a power-law in frequency,

$$Q_{\text{abs}}(\nu) = Q_0(\nu/\nu_0)^\beta = Q_0(\lambda/\lambda_0)^{-\beta} \quad (1 \lesssim \beta \lesssim 2)$$

in the far-IR

then the Planck average can be obtained analytically:



[Fig 24.1, Draine]

$$Q_{\text{abs}} \approx 1.4 \times 10^{-3} \left(\frac{a}{0.1\mu\text{m}} \right) \left(\frac{\lambda}{100\mu\text{m}} \right)^{-2}$$

silicate, $\lambda \gtrsim 20\mu\text{m}$

$$\approx 1.0 \times 10^{-3} \left(\frac{a}{0.1\mu\text{m}} \right) \left(\frac{\lambda}{100\mu\text{m}} \right)^{-2}$$

graphite, $\lambda \gtrsim 30\mu\text{m}$

Using the power-law approximation is valid because we are interested only in the Far-IR.

$$Q_{\text{abs}}(\nu) = Q_0 (\nu/\nu_0)^\beta$$

$$B_\nu(T) = \frac{2h\nu^3/c^2}{\exp(h\nu/k_B T) - 1}$$

$$\int_0^\infty d\nu B_\nu(T) Q_{\text{abs}}(\nu) = \left(\frac{2h}{c^2}\right) \left(\frac{kT}{h}\right)^4 \left(\frac{kT}{h\nu_0}\right)^\beta Q_0 \int_0^\infty dx \frac{x^{3+\beta}}{e^x - 1} \quad \leftarrow \quad x \equiv \frac{h\nu}{kT}$$

$$\begin{aligned} \int_0^\infty dx \frac{x^{3+\beta}}{e^x - 1} &= \int_0^\infty dx x^{3+\beta} e^{-x} (1 - e^{-x}) = \int_0^\infty dx x^{3+\beta} \sum_{n=1}^\infty e^{-nx} \\ &= \sum_{n=1}^\infty \frac{1}{n^{4+\beta}} \int_0^\infty dy y^{3+\beta} e^{-y} \quad \leftarrow \quad y \equiv nx \\ &= \zeta(4 + \beta) \Gamma(4 + \beta) \end{aligned}$$

$$\begin{aligned} \langle Q_{\text{abs}} \rangle_T &\equiv \frac{\int d\nu B_\nu(T) Q_{\text{abs}}(\nu)}{\int d\nu B_\nu(T)} \\ &= \frac{\left(\frac{kT}{h\nu_0}\right)^\beta Q_0 \zeta(4 + \beta) \Gamma(4 + \beta)}{\zeta(4) \Gamma(4)} \end{aligned}$$



$$\begin{aligned} \langle Q_{\text{abs}} \rangle_T &= \frac{15}{\pi^4} \Gamma(4 + \beta) \zeta(4 + \beta) Q_0 \left(\frac{kT}{h\nu_0}\right)^\beta \\ &= \left(\frac{40}{21}\pi^2\right) Q_0 \left(\frac{kT}{h\nu_0}\right)^2 \quad \text{for } \beta = 2 \end{aligned}$$

Riemann zeta-function

$$\zeta(4) = \sum_{n=1}^\infty \frac{1}{n^4} = \frac{\pi^4}{90}$$

$$\zeta(5) = \sum_{n=1}^\infty \frac{1}{n^5} = 1.03692$$

$$\zeta(6) = \sum_{n=1}^\infty \frac{1}{n^6} = \frac{\pi^6}{945}$$

gamma function

$$\Gamma(4) = 3! = 6$$

$$\Gamma(5) = 4! = 24$$

$$\Gamma(6) = 5! = 120$$

$$\begin{aligned} Q_0 &\approx 1.4 \times 10^{-3} (a/0.1 \mu\text{m}) \quad \text{silicate} \\ &\approx 1.0 \times 10^{-3} (a/0.1 \mu\text{m}) \quad \text{graphite} \end{aligned}$$

$$\lambda_0 = 100 \mu\text{m}$$

$$\begin{aligned} \langle Q_{\text{abs}} \rangle_T &\approx 1.3 \times 10^{-6} (a/0.1 \mu\text{m}) (T/\text{K})^2 \quad (\text{silicate}) \\ &\approx 9.1 \times 10^{-7} (a/0.1 \mu\text{m}) (T/\text{K})^2 \quad (\text{graphite}) \end{aligned}$$

Note typos in Equations (24.16) of Draine's book.

Equilibrium Temperature in the diffuse ISM

- Steady state temperature of large grains
 - The balance equation between the heating and cooling is:

$$\left(\frac{dE}{dt} \right)_{\text{abs}} = \left(\frac{dE}{dt} \right)_{\text{emiss}} \Rightarrow \pi a^2 \langle Q_{\text{abs}} \rangle_* (u_* c) = 4\pi a^2 \langle Q_{\text{abs}} \rangle_{T_d} \sigma_{\text{SB}} T_d^4$$

$$\Rightarrow \langle Q_{\text{abs}} \rangle_* (u_* c) = \frac{60}{\pi^4} \Gamma(4 + \beta) \zeta(4 + \beta) Q_0 \left(\frac{k}{h\nu_0} \right)^\beta \sigma_{\text{SB}} T_d^{4+\beta}$$

$$T_d = \left(\frac{h\nu_0}{k} \right)^{\beta/(4+\beta)} \left[\frac{\pi^4 \langle Q_{\text{abs}} \rangle_* c}{60\zeta(4+\beta)\Gamma(4+\beta)Q_0\sigma_{\text{SB}}} \right]^{1/(4+\beta)} u_*^{1/(4+\beta)}$$

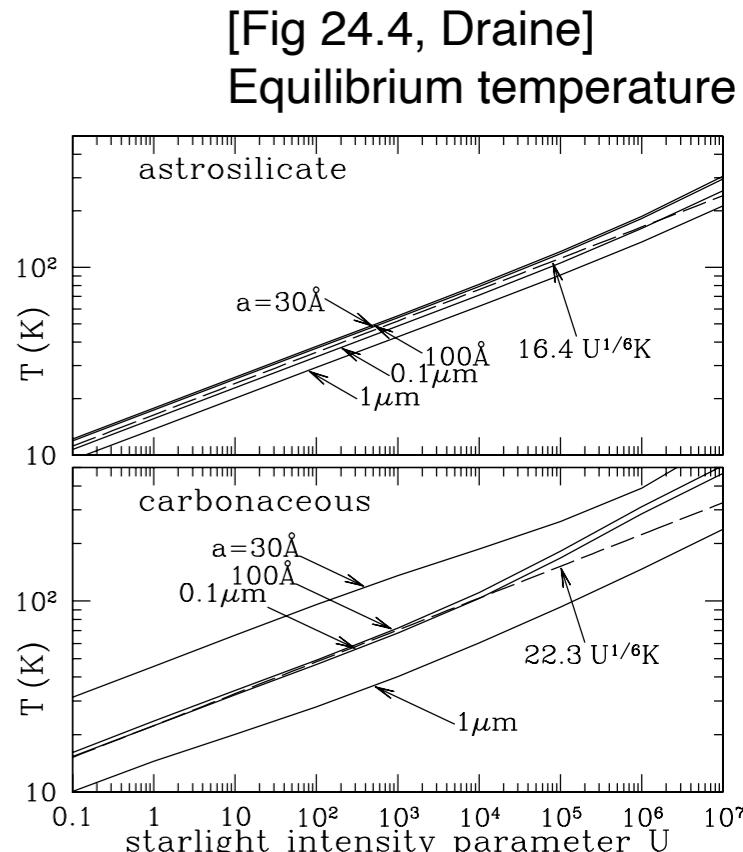
$$= \left(\frac{h\nu_0}{k} \right)^{1/3} \left[\frac{21 \langle Q_{\text{abs}} \rangle_* c}{160\pi^2 Q_0 \sigma_{\text{SB}}} \right]^{1/6} u_*^{1/6} \quad \text{for } \beta = 2$$

- Therefore, the temperature of a large grain is given by:

$$T_d \approx 16.4 (a/0.1 \mu\text{m})^{-1/15} U^{1/6} \text{ K, silicate} \quad (0.01 \lesssim a \lesssim 1 \mu\text{m})$$

$$\approx 22.3 (a/0.1 \mu\text{m})^{-1/40} U^{1/6} \text{ K, graphite} \quad (0.005 \lesssim a \lesssim 0.15 \mu\text{m})$$

for $Q_{\text{abs}} = Q_0(\lambda/\lambda_0)^{-2}$



-
- Implications
 - ▶ If the ISRF is doubled, the grain temperature increases by $\sim 12\%$. In order to increase the temperature by a factor of 2, 64 times stronger radiation is required.
 - ▶ ***There is also little dependence of the grain temperature on grain radius. Therefore, large grains can be regarded to be grains with a single size.***
 - ▶ If we assume $\beta = 1$ for the absorption cross section in the FIR, we obtain

$$T_d = \left(\frac{h\nu_0}{k} \right)^{1/5} \left[\frac{\pi^4 \langle Q_{\text{abs}} \rangle_* c}{60\zeta(5)\Gamma(5)Q_0\sigma_{\text{SB}}} \right]^{1/5} u_*^{1/5} \quad \text{for } Q_{\text{abs}} = Q_0(\lambda/\lambda_0)^{-1}$$

$$\begin{aligned} T_d &\approx 14.6 (a/0.1 \mu\text{m})^{-2/25} U^{1/5} \text{ K, silicate} \quad (0.01 \lesssim a \lesssim 1 \mu\text{m}) \\ &\approx 21.1 (a/0.1 \mu\text{m})^{-3/100} U^{1/5} \text{ K, graphite} \quad (0.005 \lesssim a \lesssim 0.15 \mu\text{m}) \end{aligned} \quad \text{for } \beta = 1$$

This indicates that *the steeper absorption cross section ($\beta = 2$) give a higher dust temperature.*

Example: Temperature of Grains exposed to a Star

- **Blackbody Particle (perfect absorber, $Q_{\text{abs}} = 1$)**

- If a blackbody particle is heated by a star with a temperature T_* and bolometric L_* at distance d , the balance between heating and cooling gives the dust temperature:

$$\int \pi a^2 Q_{\text{abs}}(\nu) \frac{L_\nu}{4\pi d^2} d\nu = 4\pi \int \pi a^2 Q_{\text{abs}}(\nu) B_\nu(T_d) d\nu \quad \longrightarrow \quad \frac{L_*}{4\pi d^2} = 4\sigma_{\text{SB}} T_d^4$$

Since the stellar luminosity can be expressed in terms of the stellar effective temperature.

$$L_* = 4\pi R_*^2 \int \pi B_\nu(T_*) d\nu = 4\pi R_*^2 (\sigma_{\text{SB}} T_*^4)$$

Here, R_* is the radius of the star.

We can find the equilibrium temperature of dust grains.

$$T_d = T_* \left(\frac{R_*}{2d} \right)^{1/2}$$

The dust temperature therefore decreases as the inverse square root of distance.

- Calculating the temperature at the distance of 1 AU from the Sun,

$$T_* = 5778 \text{ K}$$

$$R_* = 6.985 \times 10^{10} \text{ cm} = 4.669 \times 10^{-3} \text{ AU}$$

$$T_d = 279 \text{ K} \left(\frac{d}{\text{AU}} \right)^{-1/2}$$

This value is close to the average temperature of the surface of the Earth, although our planet does not emit like a perfect blackbody.

- ***Interstellar dust grains directly exposed to stars***
 - We assume that the absorption efficiency can be approximated as follows:

$$Q_{\text{abs}} \approx 1 \quad \text{at visible/UV wavelengths}$$

$$Q_{\text{abs}} \approx 0.01(a/\mu\text{m})(\lambda/100\mu\text{m})^{-2} \quad \text{in the FIR}$$

$$Q_0 = 0.01(a/\mu\text{m}), \lambda_0 = 100\mu\text{m}$$
 - The energy balance is

$$\int Q_{\text{abs}}(\nu) \frac{L_\nu}{4\pi d^2} d\nu = 4\pi \int Q_{\text{abs}}(\nu) B_\nu(T_d) d\nu$$

$$\frac{L_*}{4\pi d^2} = 4\pi \int Q_{\text{abs}}(\nu) B_\nu(T_d) d\nu \quad \longrightarrow \quad \left(\frac{R_*}{d}\right)^2 \sigma_{\text{SB}} T_*^4 = 4 \langle Q_{\text{abs}} \rangle_{T_d} \sigma_{\text{SB}} T_d^4$$

$$\langle Q_{\text{abs}} \rangle_{T_d} = \left(\frac{40}{21}\pi^2\right) Q_0 \left(\frac{kT_d}{h\nu_0}\right)^2$$

 - Using the Planck-averaged absorption efficiency, we can obtain the dust temperature:

$$T_d = \left(\frac{21}{160\pi^2} \frac{hc}{k_B \lambda_0} \frac{1}{Q_0}\right)^{1/6} \left(\frac{R_*}{d}\right)^{1/3} T_*^{2/3}$$

$$= 2.4 \left(\frac{a}{\mu\text{m}}\right)^{-1/6} \left(\frac{d}{R_*}\right)^{-1/3} T_*^{2/3}$$

$$= 129 \text{ K} \left(\frac{a}{\mu\text{m}}\right)^{-1/6} \left(\frac{d}{\text{AU}}\right)^{-1/3}$$

If there is extinction along the line of sight, one must replace the luminosity L_ν with $L_\nu e^{-\tau_\nu}$.

Stochastic Heating of Very Small Grains

- Temperature History:
 - ▶ Two effects become increasingly important with diminishing grain size: (1) the heat capacity of the dust becomes sufficiently small that single-particle hits can cause large spikes in the dust temperature and (2) the absorption rate with photons becomes sufficiently low that the cooling of the dust between successive collisions becomes important.
 - ▶ ***Therefore, it is clear that one cannot speak of a representative grain temperature under these conditions - one must instead use a temperature distribution function.***
 - ▶ ***As the grain size is increased, however, photon absorption events occur more frequently, the temperature rise at each event is reduced by the increased heat capacity, and temperature varies over only a small range.***

Heating and Cooling Time Scales

- Energy content:
 - When a grain is at a temperature T , the vibrational (internal) energy content of the grain (per unit volume) is
$$\frac{U(T)}{V} = \int_0^T C(T)dT$$
where $C(T)$ is the heat capacity of the grain (per unit volume) at temperature T .
 - Small grains are subject to temporal fluctuations in temperature, because their steady state internal energies are small compared with the energies of absorbed UV photons.
$$U(T) \ll h\nu$$
- Time Scales
 - There are three time scales to understand the temperature fluctuation of very small grains.
 - ▶ **Absorption time scale** : How often a grain will absorb a photon?
 - ▶ **Diffuse time scale** : How fast the absorbed energy is distributed over the whole grain?
 - ▶ **Cooling time scale** : How fast the excited vibration modes radiates back the energy to the interstellar space?

- **Absorption Time Scale:**

- The absorption rate of starlight photons by very small grains is

$$\left(\frac{dN_{\text{ph}}}{dt} \right)_{\text{abs}} = \int \frac{u_\nu d\nu}{h\nu} c Q_{\text{abs}}(\nu) \pi a^2 = \int d\nu \frac{4\pi J_\nu}{h\nu} Q_{\text{abs}}(\nu) \pi a^2$$

B. T. Draine does not provide an approximate formula for the absorption rate, but we can roughly estimate it from the heating rate.

$$\left(\frac{dN_{\text{ph}}}{dt} \right)_{\text{abs}} \approx \frac{1}{\langle h\nu \rangle} \left(\frac{dE}{dt} \right)_{\text{abs}} = (\pi a^2) \langle Q_{\text{abs}} \rangle_* \frac{u_* c}{\langle h\nu \rangle}$$

Here, $\langle h\nu \rangle$ is a typical photon energy of the ISRF.

We will take $\langle h\nu \rangle \approx 1 \times 10^{-11} \text{ erg}$ for $\lambda \approx 2000 \text{ \AA}$.

$$u_*/\langle h\nu \rangle \approx 1 \times 10^{-1} U [\text{cm}^{-3}]$$

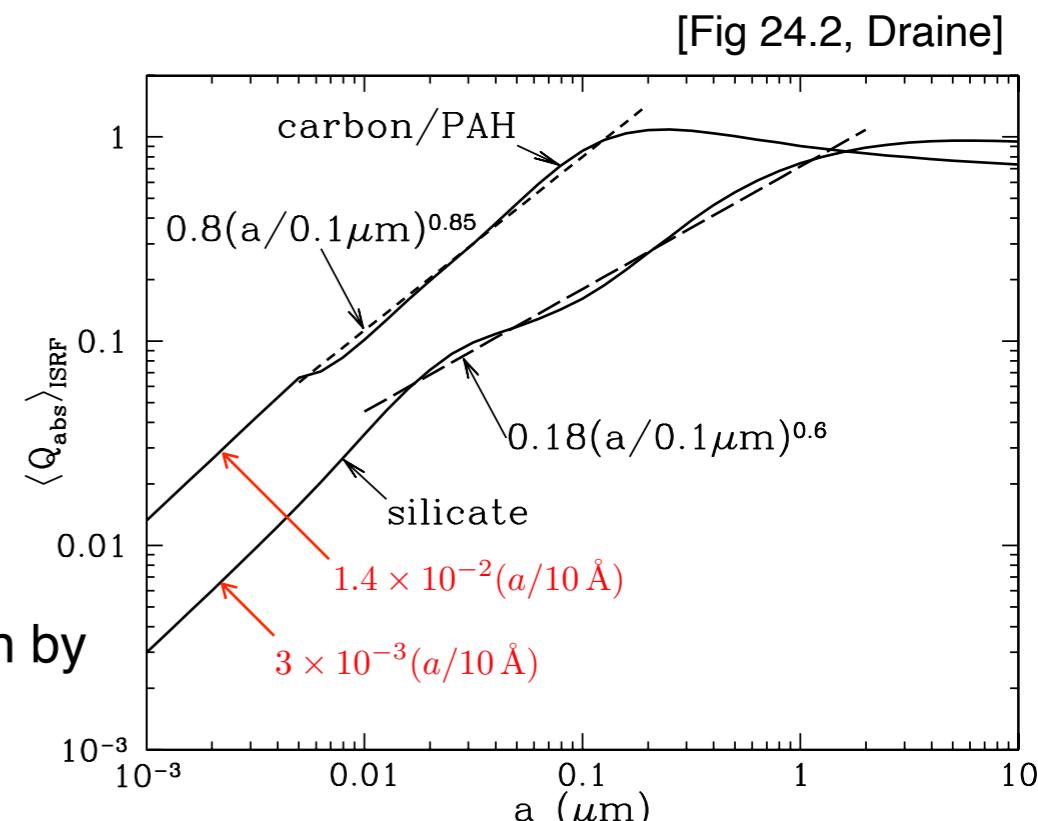
From the right figure, we take

$$\langle Q_{\text{abs}} \rangle_* \approx 1 \times 10^{-2} (a/10 \text{ \AA}) [\text{cm}^2]$$

Recall that the absorption efficiency is proportional to the grain size in the Rayleigh limit.

Hence, the photon absorption rate for small grains is given by

$$\left(\frac{dN_{\text{ph}}}{dt} \right)_{\text{abs}} \approx 1 \times 10^{-6} U (a/10 \text{ \AA})^3 [\text{s}^{-1}]$$



-
- Absorption Rate for Large grains (using the absorption cross-section in the figure)

$$\left(\frac{dN_{\text{ph}}}{dt} \right)_{\text{abs}} \approx (\pi a^2) \langle Q_{\text{abs}} \rangle_* \frac{u_* c}{\langle h\nu \rangle}$$

$$\approx 0.17 U(a/0.1\mu\text{m})^{2.6} [\text{s}^{-1}], \quad \text{for silicate}$$

$$\approx 0.75 U(a/0.1\mu\text{m})^{2.85} [\text{s}^{-1}], \quad \text{for graphite}$$

- ▶ Absorption time scale:

$$t_{\text{abs}} \equiv (dN_{\text{ph}}/dt)_{\text{abs}}^{-1}$$

$$\approx 1 \times 10^6 U^{-1} [\text{s}] \quad a \sim 10\text{\AA}$$

$$\approx 1.3 - 5.9 U^{-1} [\text{s}] \quad a \sim 0.1\mu\text{m}$$

- ▶ ***In diffuse interstellar space, the smaller component of interstellar dust will absorb star light photons once in two hours (for $a \sim 50\text{\AA}$) - 11 days (for $a \sim 10\text{\AA}$). Large dust grains ($a \sim 0.1\mu\text{m}$) will absorb photons once in a couple of seconds.***

- **Diffuse Time scale:** How long does it take to heat up the whole grain?

- ▶ The macroscopic diffuse equation:

$$\frac{\partial T}{\partial t} = D \nabla^2 T \quad \text{where } D = \text{diffusion coefficient}$$

$$t_{\text{diff}} \approx a^2/D$$

$$\approx 10^{-12} [\text{s}] (a/10 \text{\AA})^2 (10^{-2} \text{ cm}^2 \text{ s}^{-1}/D) \quad \text{a typical } D \text{ value from (Duley 1973, Ap\&SS, 23, 43)}$$

- ▶ Sound crossing time: Energy disturbance in a solid is transmitted to its lattice vibrational modes (photons) and phonons travel at the speed of sound, which is about a few 10^5 cm/s.

$$t_{\text{diff}} \approx 2a/c_s$$

$$\approx 2 \times 10^{-12} [\text{s}] (a/10 \text{\AA}) (10^5 \text{ cm s}^{-1}/c_s)$$

$c_s \sim 1 \text{ km s}^{-1}$ in a cold material.

- ▶ We may conclude that ***the grain is heated to a peak temperature instantaneously upon the absorption of a photon***, which is determined by:

$$h\nu = \frac{4\pi a^3}{3} \int_{T_0}^{T_p} C(T') dT' \quad C(T) = \text{heat capacity per unit volume}$$

where T_0 is the temperature just prior to the absorption event.

- Peak Temperature

- **Heat Capacity:** We need to know the **heat capacity** for dust grains to estimate the peak temperature.

In the low temperature limit: For a plausible grain material, the expected grain temperature would be in general lower than the Debye temperature; we may then use the *Debye approximation* for the heat capacity:

$$C(T) \approx \frac{N_a}{V} k_B \frac{12\pi^4}{5} \left(\frac{T}{\theta_D} \right)^3$$

$V = (4\pi/3)a^3$ = volume of a grain particle

N_a = number of atoms forming the grain particle

$n_a = N_a/V$ = number density of atoms in the grain.

$$\left(n_a = \frac{\rho}{\mu m_H}, \quad N_a = \frac{\rho}{\mu m_H} \frac{4\pi}{3} a^3 \right)$$

Here, **Debye temperature θ_D ~ temperature at which the highest-frequency mode is excited.**

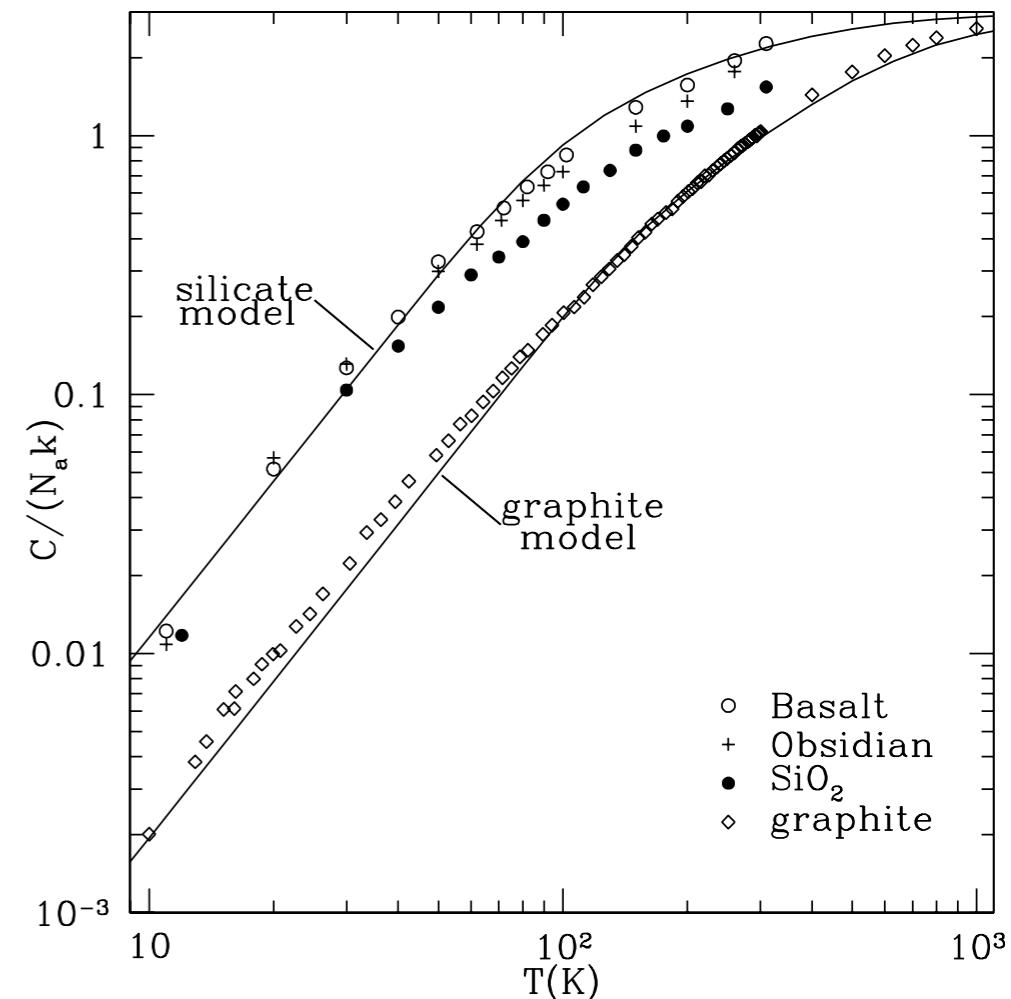
For graphite,

$$\mu = 12, \quad \rho = 2.24 \text{ g cm}^{-3}, \quad \theta_D = 420 \text{ K}$$

For silicate (olivine),

$$\mu = 170, \quad \rho = 3.8 \text{ g cm}^{-3}, \quad \theta_D = 665 \text{ K}$$

Heat capacity of graphite and silicate
Fig 2 of Draine & Li (2001, ApJ, 551, 807)



In the high temperature limit: the heat capacity is given by [the rule of Dulong-Petit](#):

$$C(T) \simeq 3 \frac{N_a}{V} k_B$$

- **Internal Energy:** The internal energy at T is then given by

$$U(T) \equiv V \int_0^T C(T') dT'$$

$$\begin{aligned} U(T) &\approx \frac{3\pi^4}{5} N_a k_B T \left(\frac{T}{\theta_D} \right)^3 && \text{at low temperature} \\ &\approx 3N_a k_B T && \text{at high temperature} \end{aligned}$$

The internal energy in the low temperature limit,

$$\begin{aligned} U(T) &\approx \frac{4\pi^5}{5} k_B \frac{a^3 \rho}{\mu m_H} \frac{T^4}{\theta_D^3} \\ &\approx 5.1 \times 10^{-16} [\text{erg}] \left(\frac{a}{10 \text{\AA}} \right)^3 \left(\frac{12}{\mu} \right) \left(\frac{\rho}{2.24 \text{ g cm}^{-3}} \right) \left(\frac{420 \text{ K}}{\theta_D} \right)^3 \left(\frac{T}{10 \text{ K}} \right)^4 \\ &\approx 1.5 \times 10^{-17} [\text{erg}] \left(\frac{a}{10 \text{\AA}} \right)^3 \left(\frac{170}{\mu} \right) \left(\frac{\rho}{3.8 \text{ g cm}^{-3}} \right) \left(\frac{665 \text{ K}}{\theta_D} \right)^3 \left(\frac{T}{10 \text{ K}} \right)^4 \end{aligned}$$

Therefore, ***the internal energy of a very small grain is much smaller than the absorbed photon energy.***

$$h\nu = 1.0 \times 10^{-11} \text{ [erg]} \left(\frac{2000 \text{ \AA}}{\lambda} \right) \longrightarrow \begin{cases} U(T_0) \ll h\nu & \text{for } a \ll 270 \text{ \AA} \\ U(T_0) \gg h\nu & \text{for } a \gg 270 \text{ \AA} \end{cases}$$

Now, the peak temperature can be estimated from:

$$h\nu = U(T_p) - U(T_0)$$

The peak temperature can be estimated as follows:

$$h\nu = U(T_p) - U(T_0) \longrightarrow U(T_p) \simeq h\nu$$

$$T_p \simeq 118 \text{ K} \left(\frac{2000 \text{ \AA}}{\lambda} \right)^{1/4} \left(\frac{a}{10 \text{ \AA}} \right)^{-3/4} \left(\frac{\mu}{12} \right)^{1/4} \left(\frac{\rho}{2.24 \text{ g cm}^{-3}} \right)^{-1/4} \left(\frac{\theta_D}{420 \text{ K}} \right)^{3/4}$$

The peak temperature for a small grain is in general much higher than the equilibrium temperature.

However, the internal energy of a large grain is much larger than the absorbed photon energy.
Therefore, **large grains will stay in a steady state with an equilibrium temperature.**

- ***The cooling time scale***

- The time evolution of grain temperature can be calculated by solving

$$\frac{dU}{dt} = -(4\pi)(\pi a^2) \int Q_{\text{abs}} B_\nu d\nu = -4\pi a^2 \langle Q_{\text{abs}} \rangle_T \sigma_{\text{SB}} T^4$$

$$\frac{dT}{dt} = -\frac{3}{aC(T)} \langle Q_{\text{abs}} \rangle_T \sigma_{\text{SB}} T^4$$

$$\begin{aligned} dU &= \frac{4\pi a^3}{3} C(T) dT \\ \leftarrow \quad \int Q_{\text{abs}} B_\nu d\nu &= \frac{\sigma_{\text{SB}}}{\pi} T^4 \end{aligned}$$

- The initial cooling time scale can be estimated by

$$\begin{aligned} t_{\text{cool}} &\approx \frac{U(T_p)}{|dU/dt|} \\ &\approx \frac{h\nu}{\Lambda} \end{aligned}$$

$$\begin{aligned} h\nu &= 1.0 \times 10^{-11} [\text{erg}] \left(\frac{2000 \text{ \AA}}{\lambda} \right) \\ \Lambda &= \left| \frac{dU}{dt} \right|_{T_p} = 4\pi a^2 \langle Q_{\text{abs}} \rangle_T \sigma_{\text{SB}} T_p^4 \end{aligned}$$

- We will assume an approximate, absorption efficiency, following S. S. Hong (1979, JKAS):

$$Q_{\text{abs}}(\nu) = \frac{4\pi a}{\lambda} = Q_0 (\lambda_0 / \lambda) \quad \leftarrow \quad Q_{\text{abs}}(\nu) = 4 \frac{2\pi a}{\lambda} \text{Im} \left(\frac{m^2 - 1}{m^2 + 2} \right) \quad \text{Rayleigh limit}$$

Here, $Q_0 \approx 6.283 \times 10^{-2} \chi(a/10 \text{ \AA})$

$$\lambda_0 = 2000 \mu\text{m}$$

$$\beta = 1$$

$$\chi \simeq 1$$

From the previous formula for

$$Q_{\text{abs}}(\nu) = Q_0(\lambda_0/\lambda)^{-\beta}$$

the planck-averaged absorption efficiency is given by

$$\begin{aligned}\langle Q_{\text{abs}} \rangle_T &= \frac{15}{\pi^4} \Gamma(4 + \beta) \zeta(4 + \beta) Q_0 \left(\frac{kT}{h\nu_0} \right)^\beta \\ &= 3.83220 Q_0 \left(\frac{kT}{h\nu_0} \right) \quad \text{for } \beta = 1 \\ &\approx 3.950 \times 10^{-2} \chi(a/10 \text{\AA})(\lambda/2000 \text{\AA})(T/118 \text{K})\end{aligned}$$

The cooling rate is:

$$\begin{aligned}\Lambda &= 4\pi a^2 \langle Q_{\text{abs}} \rangle_T \sigma_{\text{SB}} T^4 \\ &= 5.46 \times 10^{-11} [\text{erg s}^{-1}] \chi(a/10 \text{\AA})^3 (\lambda/2000 \text{\AA}) (T/118 \text{K})^5\end{aligned}$$

The cooling time scale at the peak temperature is:

$$\begin{aligned}t_{\text{cool}} &\approx \frac{U(T_p)}{|dU/dt|} = \frac{h\nu}{\Lambda} \\ &\approx 0.18 [\text{s}] \chi^{-1} (10 \text{\AA}/a)^3 (118 \text{K}/T)^5\end{aligned}$$

Because of the strong temperature dependence of the cooling rate, **the grain actually needs much longer time (up to 10^4 sec) to radiate its excess (absorbed) energy back** to the interstellar space.

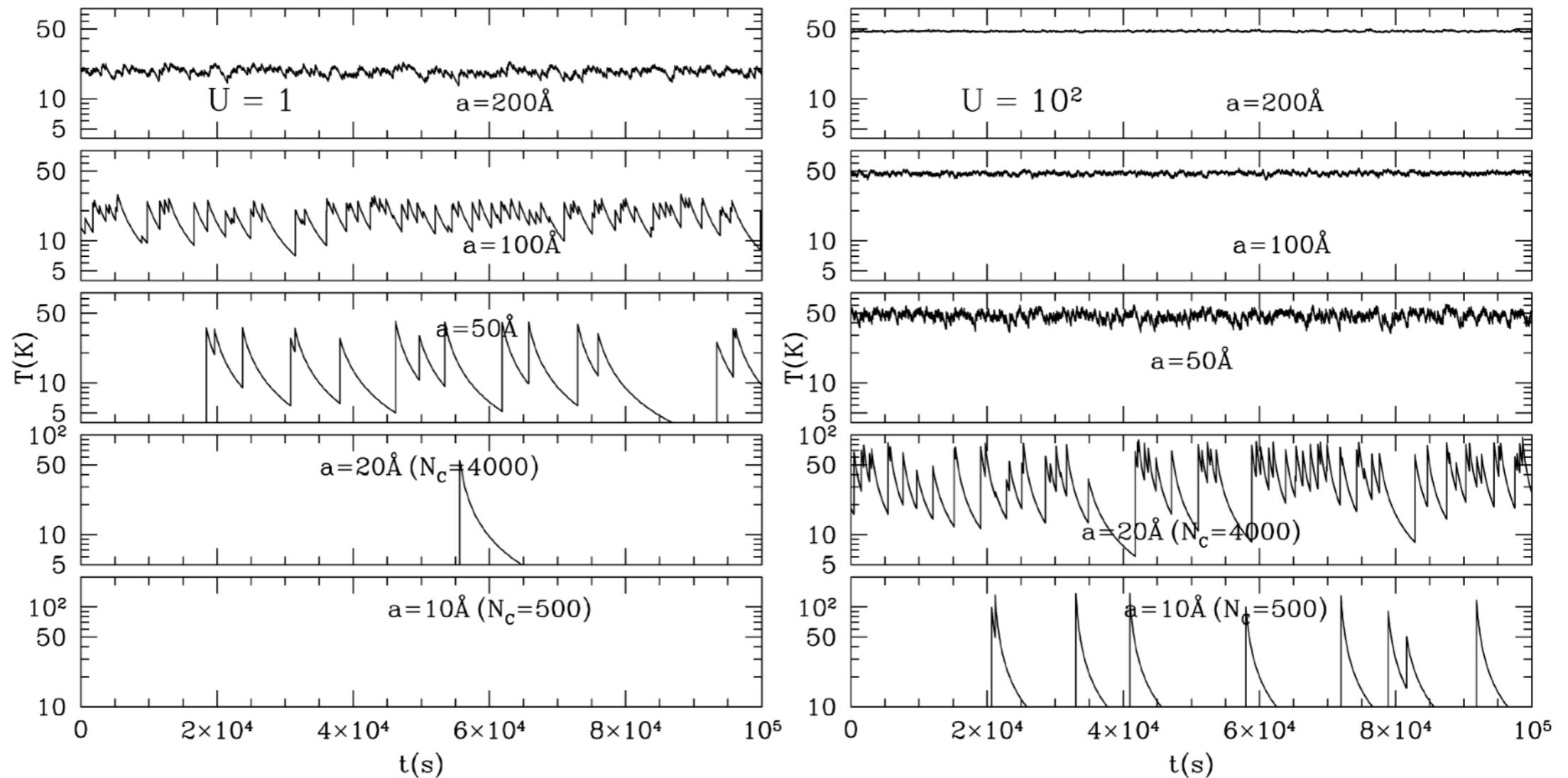
In summary,

$$t_{\text{abs}} \gg t_{\text{diff}}, \quad t_{\text{abs}} \gg t_{\text{cool}}, \quad t_{\text{cool}} \gg t_{\text{diff}}$$

The Stochastic Time Evolution of Grain Temperature

Monte-Carlo simulations of the temperature fluctuation:

See Draine & Anderson (1985, ApJ, 292, 494) and Krugel (The Physics of Interstellar Dust, IoP).



Temperature versus time during 10^5 s (~1 day) for five carbonaceous grains in two radiation fields: the local starlight intensity ($U = 1$; left panel) and 10^2 times the local starlight intensity ($U = 10^2$; right panel). The importance of quantized stochastic heating is evident for the smallest sizes.

[Fig 24.5, Draine]

-
- Temperature History:
 - ▶ Two effects become increasingly important with diminishing grain size: (1) **the heat capacity of the dust becomes sufficiently small that single-particle hits can cause large spikes in the dust temperature** and (2) **the absorption rate with photons becomes sufficiently low that the cooling of the dust between successive collisions becomes important.**
 - ▶ ***For very small dust grains, one cannot speak of a representative grain temperature under these conditions - one must instead use a temperature distribution function.***
 - Temperature Distribution Function:
 - ▶ Consider a large ensemble of identical grains in some interstellar environment. Let us define:
$$P(T)dT = \text{the probability that its temperature lies in the interval from } T \text{ and } T + dT.$$
The probability density is of course normalized:
$$\int_0^\infty P(T)dT = 1$$
 - ▶ The temperature distribution will depend on grain size, composition, and the intensity (and spectrum) of the radiation illuminating the grains.

- ▶ **For normal interstellar grains of average size**, the temperature oscillates only a little around an equilibrium value T_{eq} and in the limit of large grains, the distribution density function approaches the delta-function:

$$P(T) \rightarrow \delta(T - T_{\text{eq}})$$

where the equilibrium temperature follows from the steady-state balance between emission and absorption:

First, calculate the equilibrium temperature.

$$\int Q_{\nu}^{\text{abs}} J_{\nu} d\nu = \int Q_{\nu}^{\text{abs}} B_{\nu}(T_{\text{eq}}) d\nu \quad \rightarrow$$

Second, the emissivity per solid angle:

$$\epsilon_{\nu} = \pi a^2 Q_{\nu}^{\text{abs}} B_{\nu}(T_{\text{eq}})$$

- ▶ **Even for a very small particle** we will assume that its radiation obeys at any time Kirchhoff's law, so in the case of a sphere of radius a , we can express the average monochromatic emission per solid angle by

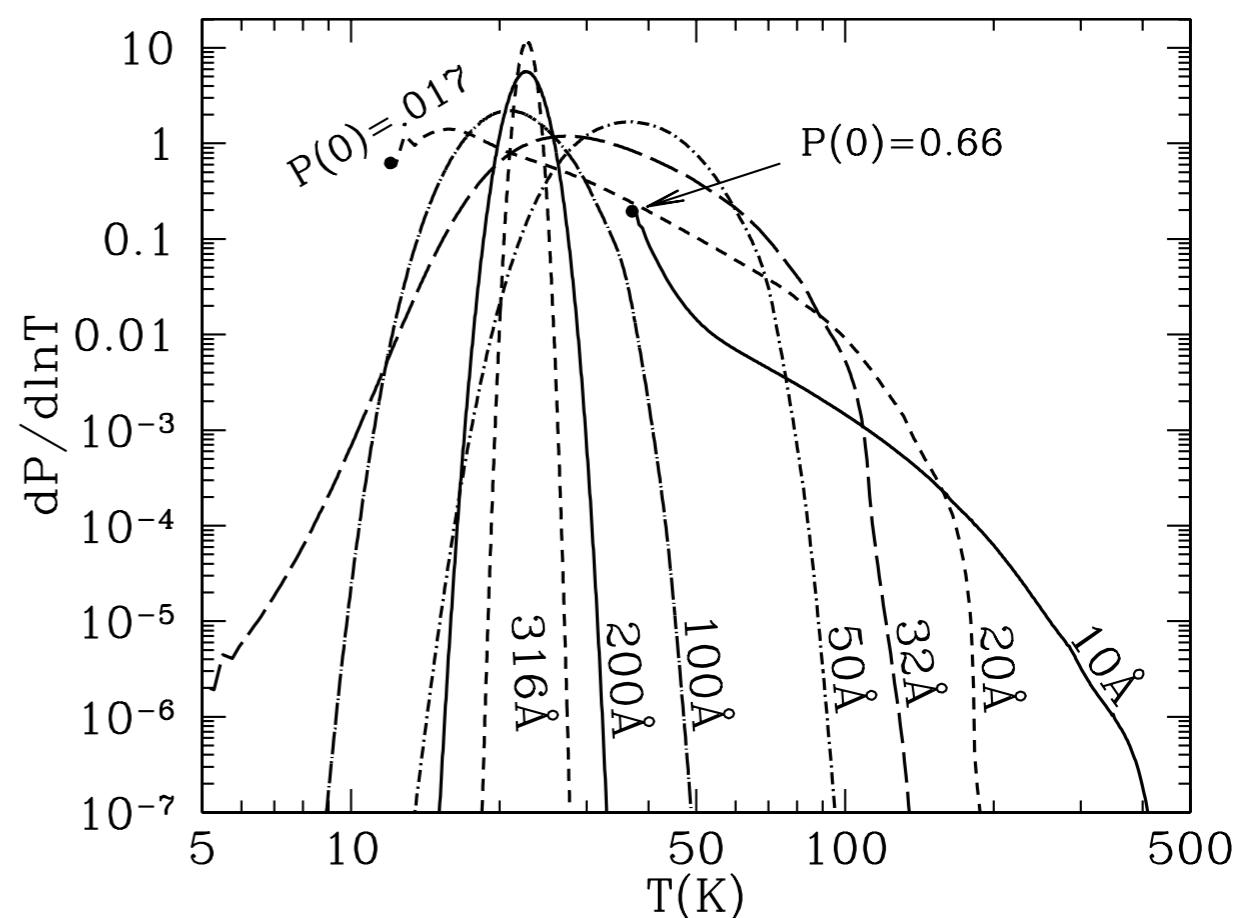
$$\epsilon_{\nu} = \pi a^2 Q_{\nu}^{\text{abs}} \int B_{\nu}(T) P(T) dT$$

Although the emission of a single such grain is not time-constant, the whole ensemble radiates at any frequency at a steady state.

- The following figure shows temperature distribution functions calculated for graphite/PAH dust grains of selected radii, exposed to the ISRF of Mathis et al. (1983).
 - ▶ We see that the distribution function for a grain with $a = 10\text{\AA}$ extends to $T = 400\text{ K}$ - this is the temperature that this grain will be heated to when it absorbs a single photon with energy just below the Lyman limit cutoff at 13.6 eV.
 - ▶ Most of the energy radiated by the grain is radiated while it is at temperature above 100 K - the typical absorbed photon raises the grain temperature to $T > 200\text{ K}$. Such grains radiate strongly in the PAH features at 7.7, 8.6, and 11.3 μm .

Temperature distribution function for seven carbonaceous grains in ISRF with $U = 1$. Curves are labeled by grain radius. For $a = 10$ and 20\AA curves, the dot indicates the first excited state and $P(0)$ is the fraction in the ground state.

[Fig 24.6, Draine]



Method of Calculation

- **Monte-Carlo simulation** (Draine & Anderson 1985)

- The cooling flux of low energy infrared photons and heating by photons with $\lambda > \lambda_c$ ($= 1000\mu\text{m}$) are assumed to be continuous. However, ***heating by photons with $\lambda < \lambda_c$ must be treated as a sequence of stochastic absorptions of single energetic photons.***
- The probability a photon is absorbed by a grain in a time interval $(t, t + dt)$ is given by

$$P(t)dt = \dot{p}e^{-\dot{p}t}dt$$

$$\dot{p} = \int_0^{\lambda_c} \pi a^2 Q_\lambda^{\text{abs}} \frac{u_\lambda c}{h\nu} d\lambda \quad [\text{s}^{-1}] \quad \rightarrow$$

$$t = -\frac{1}{\dot{p}} \ln \xi \quad (0 \leq \xi < 1)$$

ξ = uniform random number

- The energy (wavelength) of the absorbed photon is randomly determined according to

$$\frac{1}{\dot{p}} \frac{d\dot{p}}{d\lambda} d\lambda = \frac{Q_\lambda^{\text{abs}} (u_\lambda c / h\nu)}{\int Q_\lambda^{\text{abs}} (u_\lambda c / h\nu) d\lambda} d\lambda$$

- The temperature of the grain is then assumed to be immediately increased to that estimated from:

$$\frac{hc}{\lambda} = \frac{4\pi a^3}{3} \int_{T_0}^T C(T')dT'$$



$$dU = \frac{4\pi a^3}{3} C(T) dT$$

Here, T_0 is the temperature just prior to the absorption event.

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- For each grain type and size, the temperature evolution can be followed by solving the differential equation:

$$\frac{dU}{dt} = 4\pi^2 a^2 \left[\int_{\lambda_c}^{\infty} Q_{\lambda}^{\text{abs}} J_{\nu}(t) d\lambda - \int_0^{\infty} Q_{\lambda}^{\text{abs}} B_{\lambda}(T(t)) d\lambda \right]$$

continuous heating continuous cooling

$$\frac{dU}{dt} = \frac{4\pi a^3}{3} C(T) \frac{dT}{dt}$$

$$\longrightarrow \frac{dT}{dt} = \frac{3\pi}{aC(T)} \left[\int_{\lambda_c}^{\infty} Q_{\nu}^{\text{abs}} J_{\nu}(t) d\nu - \int_0^{\infty} Q_{\nu}^{\text{abs}} B_{\nu}(T(t)) d\nu \right]$$

The right side describes the difference between the power absorbed from the radiation field J_{ν} and the cooling rate.

- Having followed $U(t)$ or $T(t)$ over a long period, one can obtain the probability density $P(T)$ from the fraction of time that the grain has spent in the temperature interval T and $T + dT$.

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- Discretized steady state distribution function
 - It is far more efficient to solve directly for the discretized steady state distribution function.
 - ▶ **Guhathakurta & Draine (1989, ApJ, 345, 230)** developed a fast method to calculate the temperature distribution function. Draine & Li (2001, ApJ 551, 807) presented a statistically exact, and quantum-mechanical treatment.
 - ▶ **Desert et al. (1986, A&A, 160, 295)** also developed a different method to compute the temperature distribution function, which is publicly available (**DustEM**; <https://www.ias.u-psud.fr/DUSTEM/>; Campiegne et al. 2010, A&A, 724, 44).
 - ▶ **Dwek (1986, ApJ, 302, 363)** presented a method to calculate the temperature fluctuations in dust particles when they collide with low-density, X-ray emitting electrons.
 - Guhathakurta & Draine (1989)
 - ▶ When a grain absorbs or emits a photon, its internal energy $U(T)$, which is a function of temperature, changes. We bin $U(T)$ into N states (bins) U_j of width ΔU_j .

Let P_j the probability for a grain to be within the j th state.

Let A_{fi} the transition probability that a single grain changes from state i to f .

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- ▶ In statistical equilibrium, for each level j the number of populating and depopulating events must be equal.

$$\sum_{k \neq j} A_{jk} P_k = P_j \sum_{k \neq j} A_{kj}$$

population de-population

Note that P_j is proportional to the energy width ΔU_j

With the purely mathematical definition:

$$A_{jj} = - \sum_{k \neq j} A_{kj}$$

We can write the equilibrium equation as the following matrix equation:

$$\sum_{k=1}^N A_{jk} P_k = 0$$

- ▶ Only $N - 1$ of these N equations are linearly independent.

One may first put $P_1 = 1$ (or $P_N = 1$) and then solve for P_2, \dots, P_N (or P_1, \dots, P_{N-1}), and then rescale them:

$$\sum_{j=1}^N P_j = 1$$

- Matrix Elements

 - ▶ Heating:

$$A_{kj} = \frac{4\pi C_\nu^{\text{abs}} J_\nu}{h\nu} \Delta U_k \quad \text{where } h\nu = |U_k - U_j| \quad (j < k)$$

 - ▶ Cooling:

$$A_{kj} = \frac{4\pi C_\nu^{\text{abs}} B_\nu(T_j)}{h\nu} \Delta U_k \quad \text{where } h\nu = |U_j - U_k| \quad (j > k)$$

 - ▶ Above the main diagonal stand the cooling elements, below those for heating. The energy balance requires for the cooling and heating rate for each level j :

heating: $\sum_{k>j} A_{kj} |U_k - U_j| = \int_0^\infty 4\pi C_\nu^{\text{abs}} J_\nu d\nu$

cooling: $\sum_{k<j} A_{kj} |U_k - U_j| = \int_0^\infty 4\pi C_\nu^{\text{abs}} B_\nu(T_j) d\nu$

 - ▶ ***“Thermal Continuous” Cooling Approximation:*** As cooling proceeds via infrared photons which have low energy, their emission changes the grain temperature very little. ***This suggests that in cooling one needs to consider only the transitions to the levels immediately below*** ($k = j - 1, j \rightarrow j - 1$).

One can, therefore, put all matrix elements A_{fi} above the main diagonal to zero, except $A_{j-1,j}$. Then, in order to fulfill the energy equation, the cooling elements have to be written as:

$$\sum_{k>j} A_{kj} |U_k - U_j| = \int_0^\infty 4\pi C_\nu^{\text{abs}} J_\nu d\nu$$

$$A_{j-1,j} |U_{j-1} - U_j| = \int_0^\infty 4\pi C_\nu^{\text{abs}} J_\nu d\nu$$

$$\rightarrow A_{j-1,j} = \frac{1}{|U_j - U_{j-1}|} \int_0^\infty 4\pi C_\nu^{\text{abs}} B_\nu(T_j) d\nu$$

$$A_{kj} = 0 \text{ if } k < j - 1$$

- ▶ However, heating should not be reduced to single transitions $j \rightarrow j + 1$.
- ▶ GD1989 describes a simple trick to avoid numerical rounding errors in calculating the temperature distribution.

Setting $X_j = P_j/P_1$ ($X_1 = 1$), we can obtain the steady state solution for the distribution function:

$$\frac{d}{dt} \left(\sum_{j=1}^{f-1} P_j \right) = A_{f-1,f} P_f - \sum_{j=1}^{f-1} P_j \sum_{k=f}^N A_{k,j} \quad \xrightarrow{\quad}$$

$$X_f = \frac{1}{A_{f-1,f}} \sum_{j=1}^{f-1} B_{f,j} X_j \quad \text{where} \quad B_{f,j} \equiv \sum_{k=f}^N A_{k,j} \quad (f > j)$$

However, in practice, even adopting the trick, calculating the temperature distribution function is a bit tricky; it is hard to define a proper interval for U or T .

- Infrared Emission from Grains
 - In a typical spiral galaxy, perhaps 1/3 of the energy radiated by stars is absorbed by dust grains, and reemitted in the IR. The spectrum of this emission is determined by the temperatures and composition of the dust grains.
 - IR emission is a quantum process - a radiative transition between an upper and lower vibrational level of the grain. However, it has been shown (Draine & Li 2001) that a “thermal” approach provides an excellent approximation.
 - In the approximation, the emissivity of a population of grains can be written:

$$4\pi j_\nu = 4\pi \sum_i \int da \frac{dn_i}{da} \int dT \left(\frac{dP}{dT} \right)_{i,a} C_\nu^{\text{abs}}(i, a) B_\nu(T)$$

where $(dn_i/da)da$ is the number density of grains of type i with radii in $[a, a + da]$.

- ▶ We, therefore, need a grain model to provide the size distribution for each composition, the absorption cross sections and temperature distribution functions.
- ▶ For large grains, the temperature distribution is sufficiently narrow that it may be approximated by a delta function $dP/dT \rightarrow \delta(T - T_{\text{eq}})$, where T_{eq} is the steady-state temperature for which the time-averaged cooling equals the time-averaged heating.
- ▶ But for $a \lesssim 0.01 \mu\text{m} = 100 \text{ \AA}$, one should use a realistic temperature distribution dP/dT rather than a delta-function.