

Astrophysics

Lecture 16

December 14 (Wed.), 2022

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UST / KASI

Dust / Solid Particles

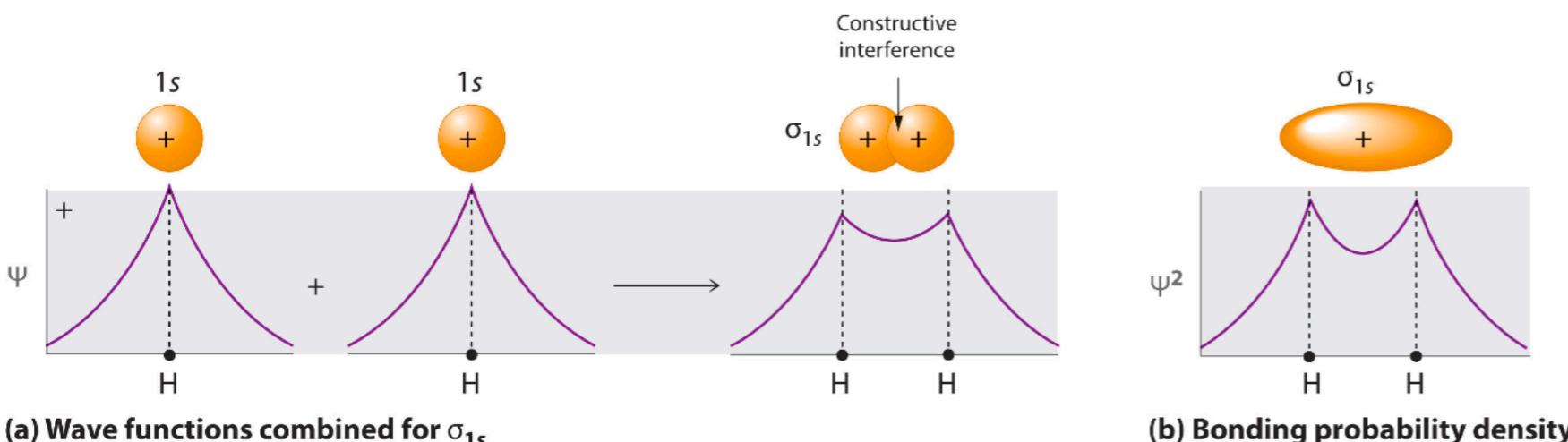
[Bonding and Antibonding Orbitals]

- **Molecular Orbital Method:** The molecular orbitals are created via the linear combinations of atomic orbitals. For instance, for a diatomic molecule,

$$|\psi\rangle = C_A|1s_A\rangle + C_B|1s_B\rangle$$

Since the two protons are identical, the probability that the electron is near A must equal the probability that the electron is near B.

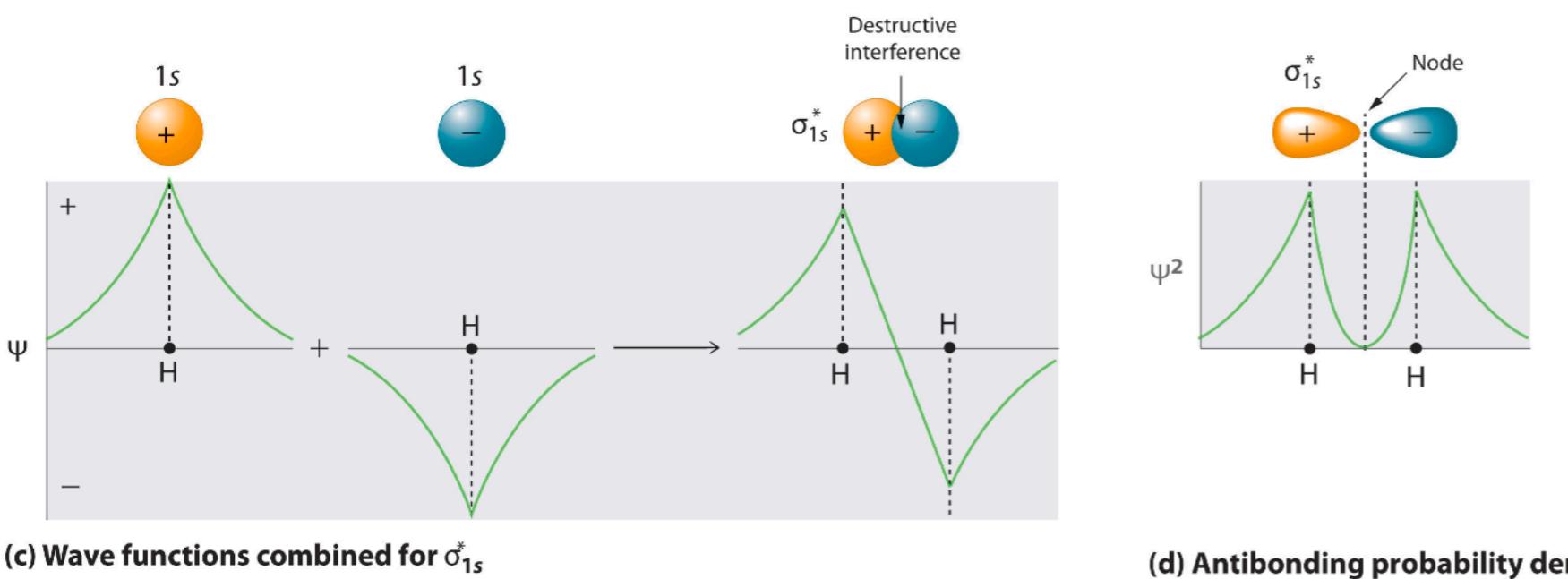
$$|C_A|^2 = |C_B|^2 \Rightarrow C_A = \pm C_B$$



We have two possibilities that satisfy the above condition.

$$|\sigma_{1s}\rangle = \frac{1}{\sqrt{2}} (|1s_A\rangle + |1s_B\rangle)$$

This is called a bonding orbital.



$$|\sigma_{1s}^*\rangle = \frac{1}{\sqrt{2}} (|1s_A\rangle - |1s_B\rangle)$$

This is called a antibonding orbital.

- **Bonding orbitals** are formed when atomic orbitals combine in ways that lead to predominantly constructive interference.

In the bonding orbitals, the electron density is found between the atoms. This leads to the idea that covalent bonding is “shared” electrons. The electrons have a high probability of being between the nuclei in the molecule.

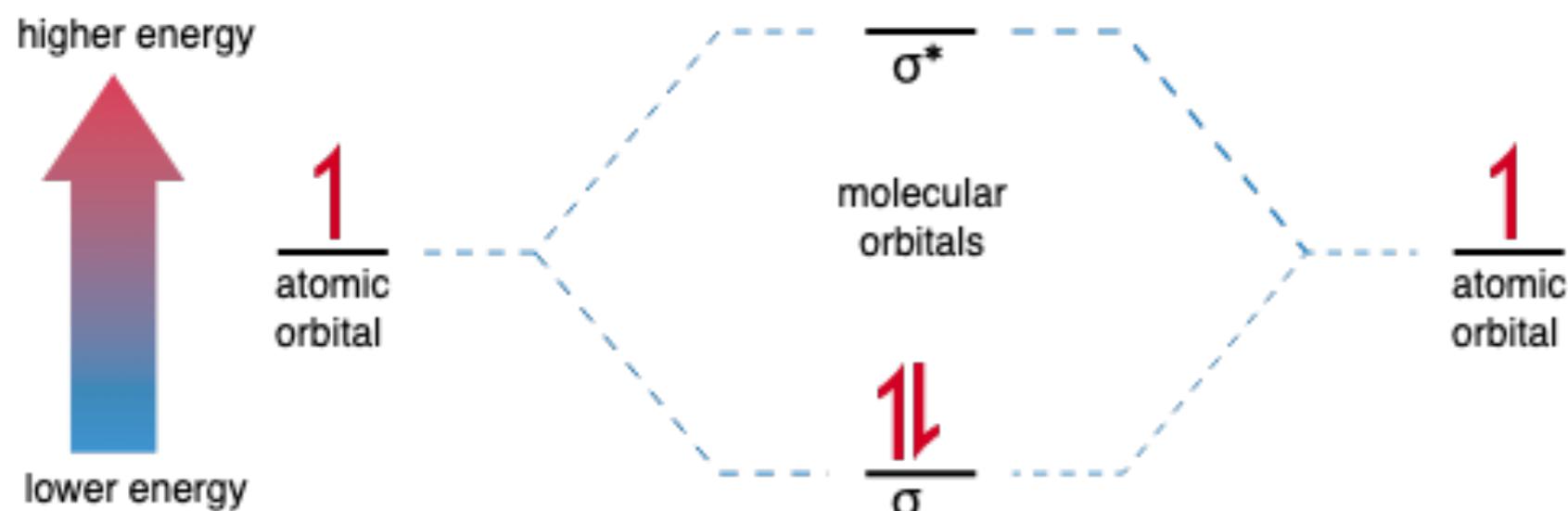
The molecular orbital has a lower energy than the separated atoms.

- **Anti-bonding orbitals** are formed when atomic orbitals combine in ways that lead to predominantly destructive interference.

In this bonding, a “node” or place of zero electron density exists between the atoms.

The molecular orbital has a higher energy than the separated atomic orbitals.

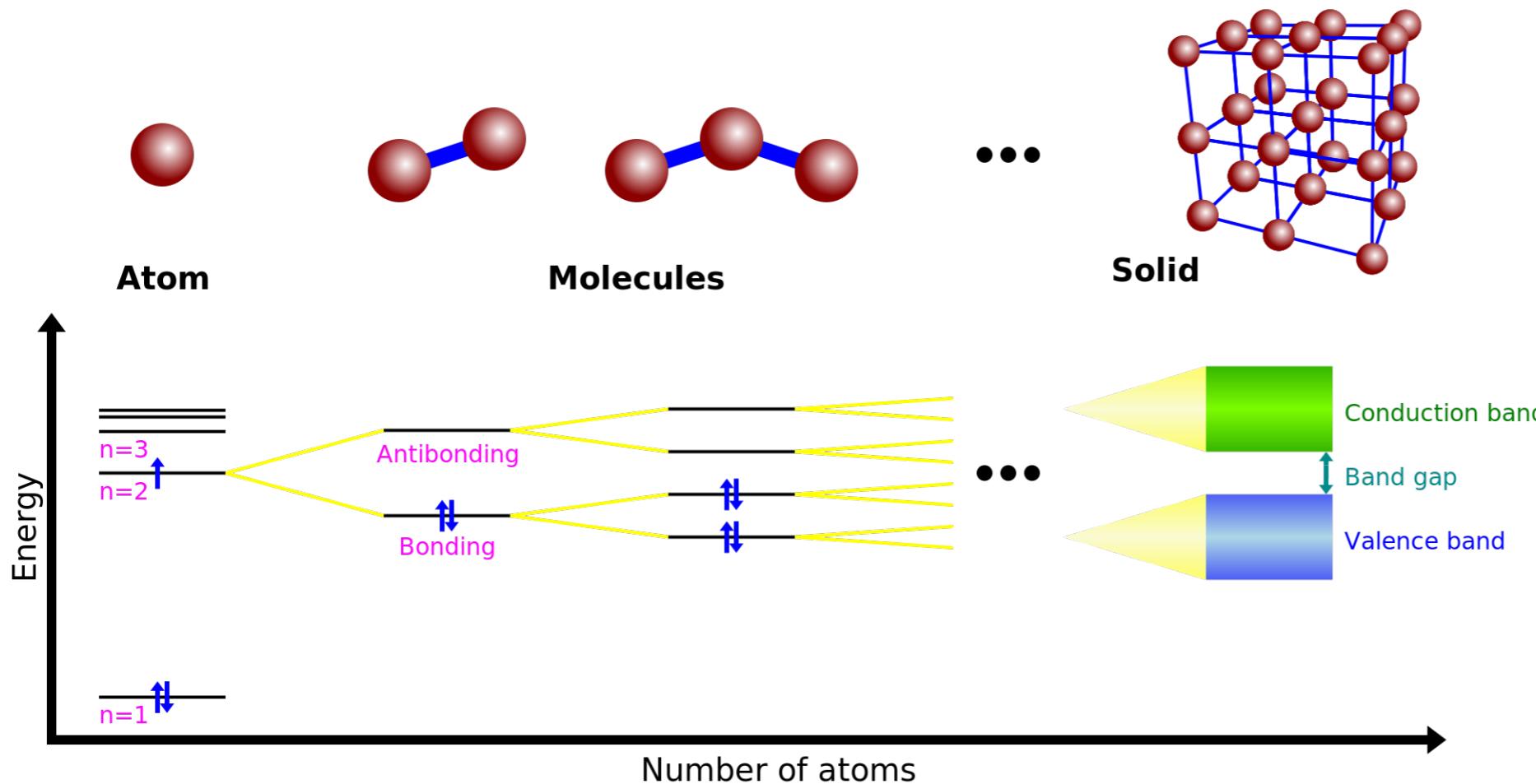
We denote anti-bonding orbitals with a * symbol.



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σ -bonding is due to the end-to-end overlap of orbitals having constructive interference (in phase). All σ -bonding is “on axis” meaning the electron density is centered directly between the two bonding nuclei.

[Band Structure of Solids]



From the left to the right, we represents: (i) typical discrete atomic levels, (ii) the successive splitting of molecular orbitals, (iii) resulting in the quasi-continuous distribution of levels in bands. Electrons are represented with a vertical blue arrow (up or down), corresponding to their spin.

Origin of the band structure of a solid

A solid can be idealized as a periodic lattice of atoms bonded to each other. The permitted energy levels of a single valence electron, in the periodic electrostatic potential created by this lattice, are a series of continuous functions, also called bands. This can be viewed as a generalization of the molecular level splitting. The spacing between a large number of levels is so small that it appears continuous.

The valence band is the highest energy band populated by valence electrons (at $T = 0 \text{ K}$).

The conduction band is the lowest energy band where electrons can move freely through the solid. It is the band immediately superior to the valence band.

The energy difference between them is called **the band gap** (often denoted to be E_g).

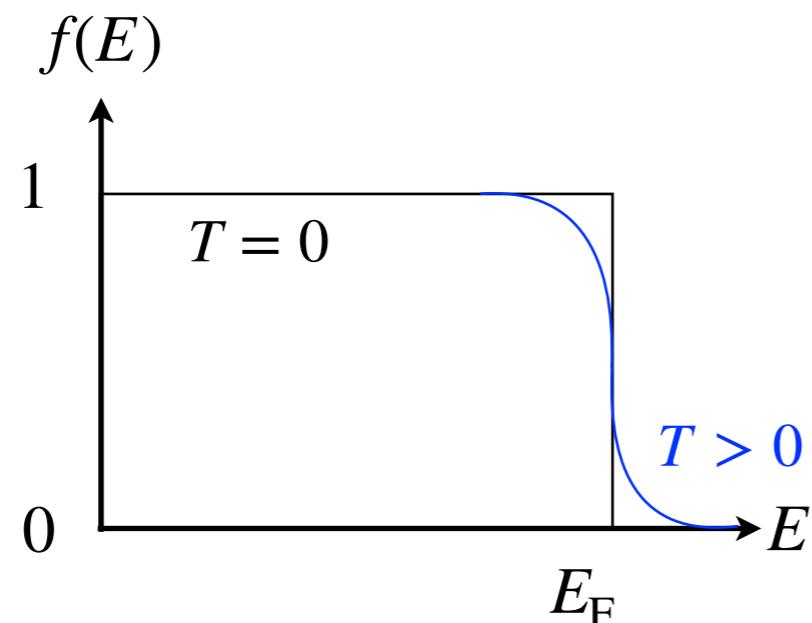
[The Fermi Level]

- The probability distribution of identical fermions, such as electrons in a solid, over the energy states of a system at temperature T , is given by the **Fermi-Dirac distribution**:

$$f(E) = \frac{1}{\exp\left(\frac{E-E_F}{k_B T}\right) + 1}$$

Here E_F is the Fermi level, which is the energy required to add an electron to the system and an intrinsic quantity characterizing a solid.

At $T = 0$ K, it gives a probability to electrons to occupy energy levels $E \leq E_F$, whereas zero probability to energy levels $E > E_F$

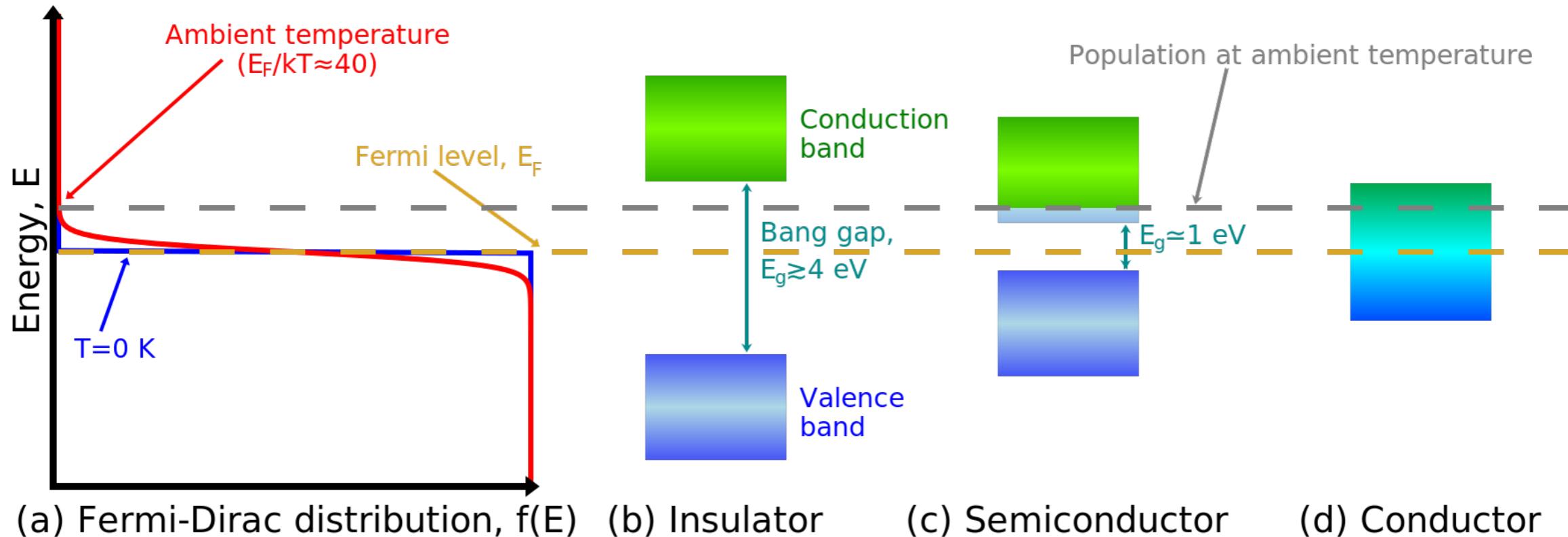


at $T = 0$ K

$$f(E > E_F) = \frac{1}{\exp(+\infty) + 1} = 0$$

$$f(E < E_F) = \frac{1}{\exp(-\infty) + 1} = 1$$

[Types of Solid]



- **Insulators** have their valence and conduction bands widely spread apart. At ambient temperature, no electron will populate the conduction band.
- **Semiconductors** have their valence and conduction bands close to each other. They are insulators at $T = 0$ K, but their conduction band can be populated at ambient temperature (kT gets close to E_F).
- **Conductors** are solids for which valence and conduction bands are the same. The Fermi level is within the band. In other words, the valence electrons are free to move through the lattice at any temperature.

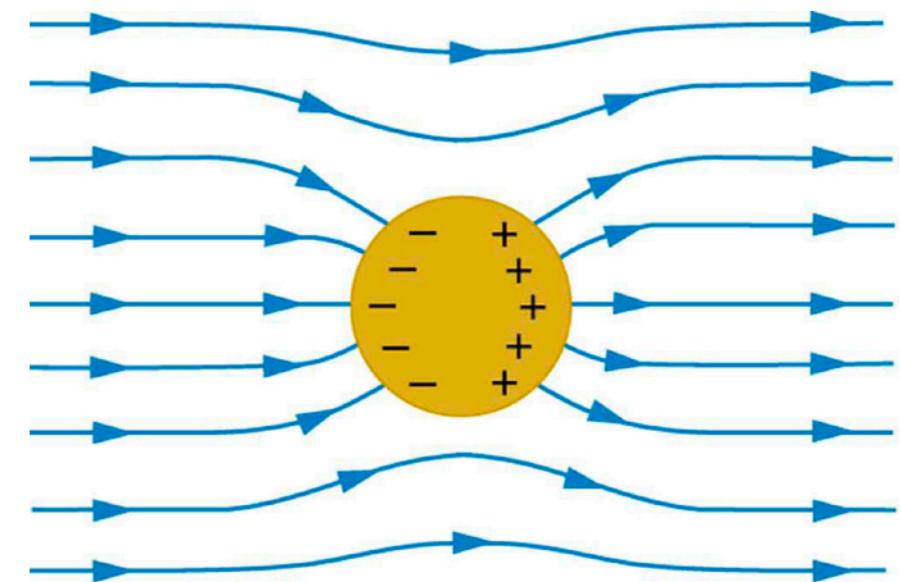
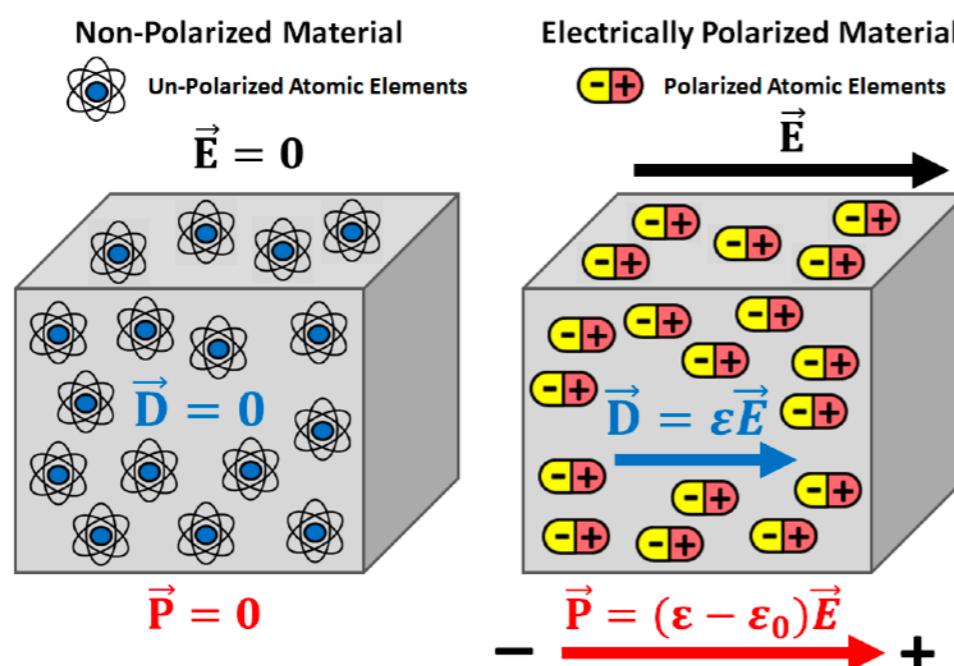
The Fermi level and the different types of solid.

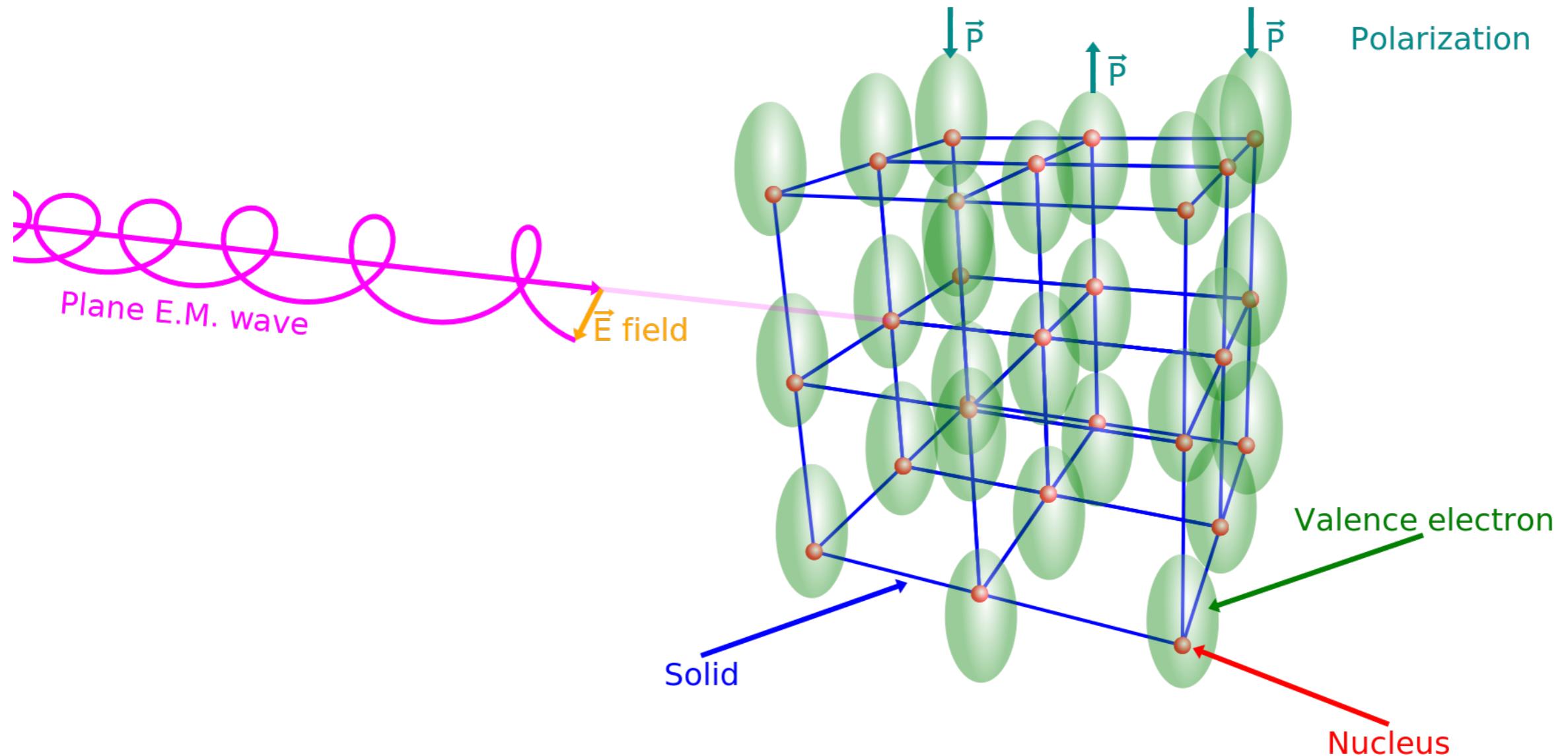
In the figure, the left plot shows the rotated Fermi-Dirac distribution, for two values of the temperature, $T = 0$ K and $T \approx 300$ K.

The three diagrams on the right show the valence and conduction bands relative to the Fermi level, E_F , for insulators, semiconductors and conductors. For conductors, the valence band is also the conduction band.

Dielectrics and Conductors

- Materials
 - **Dielectrics (Insulators)**: 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 (Metals)**: 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.





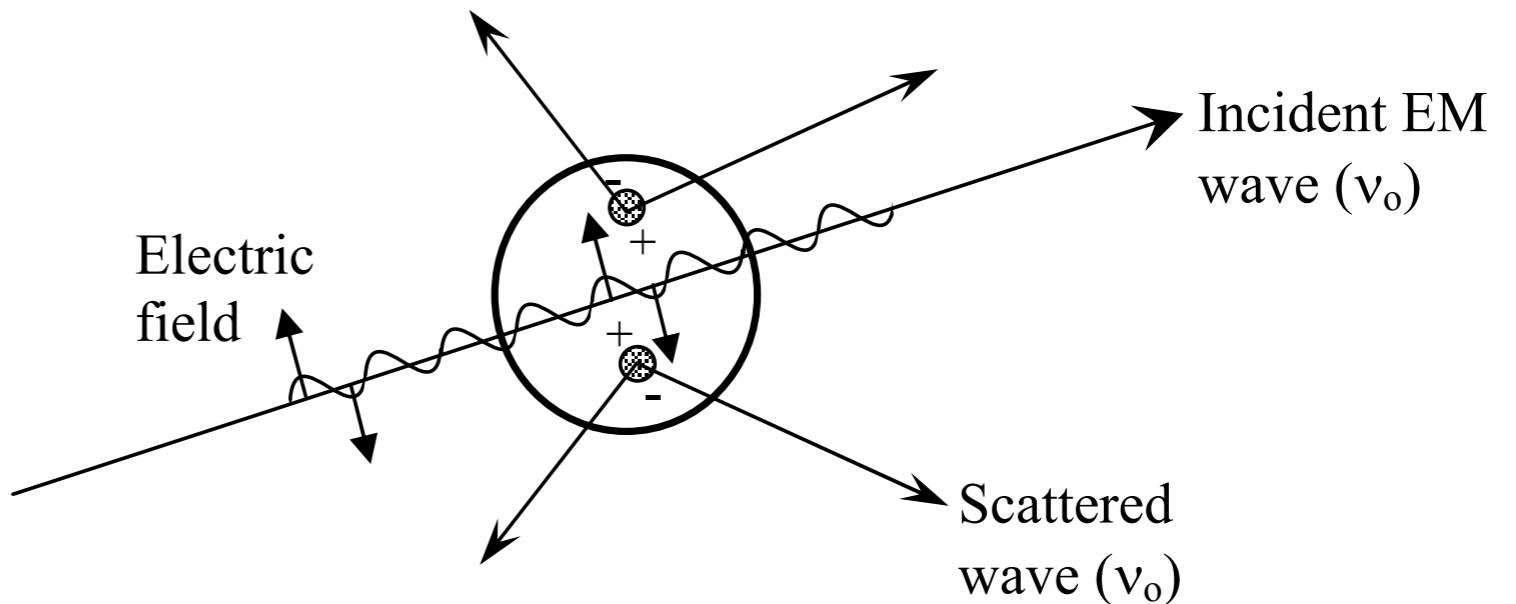
Effect of an electromagnetic wave on a dielectric. An incoming, circularly polarized, electromagnetic wave is figured in magenta. The cube on the right represents a solid. The nuclei, assumed to be fixed, are the red spheres. The valence electrons are the green ellipsoids. They are displaced out of their equilibrium positions by the electromagnetic wave, inducing a time-dependent polarization.

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

$$|m| \frac{2\pi a}{\lambda} \ll 1 \quad (m = \text{the refractive index}, \quad a = \text{radius of the spherical particle})$$

- ▶ ***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.

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

E electric field

B magnetic flux density
(magnetic induction)

H magnetic field strength
(magnetic field)

Gauss

Faraday

Ampere

Macroscopic
Maxwell's equations

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

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

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

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

Constitutive
Relations

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

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

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

Continuity Equation

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

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

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

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

ϵ = permittivity (유전율)

μ = permeability (투자율)

σ = conductivity (전도율)

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

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

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

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

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

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

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

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

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

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

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

Dispersion Relation

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

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

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., $\mu = 1$ and consider a dielectric material ($\sigma = 0$).**
 - ▶ 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.

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

$\epsilon = \epsilon_1 + i\epsilon_2$	\longrightarrow	$\epsilon_1 = n_r^2 - n_i^2$
$\epsilon = m^2$		$\epsilon_2 = 2n_r n_i$

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

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

- ▶ The refractive index is often referred to as optical constants, or simply the “ n and k ”.
- 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.

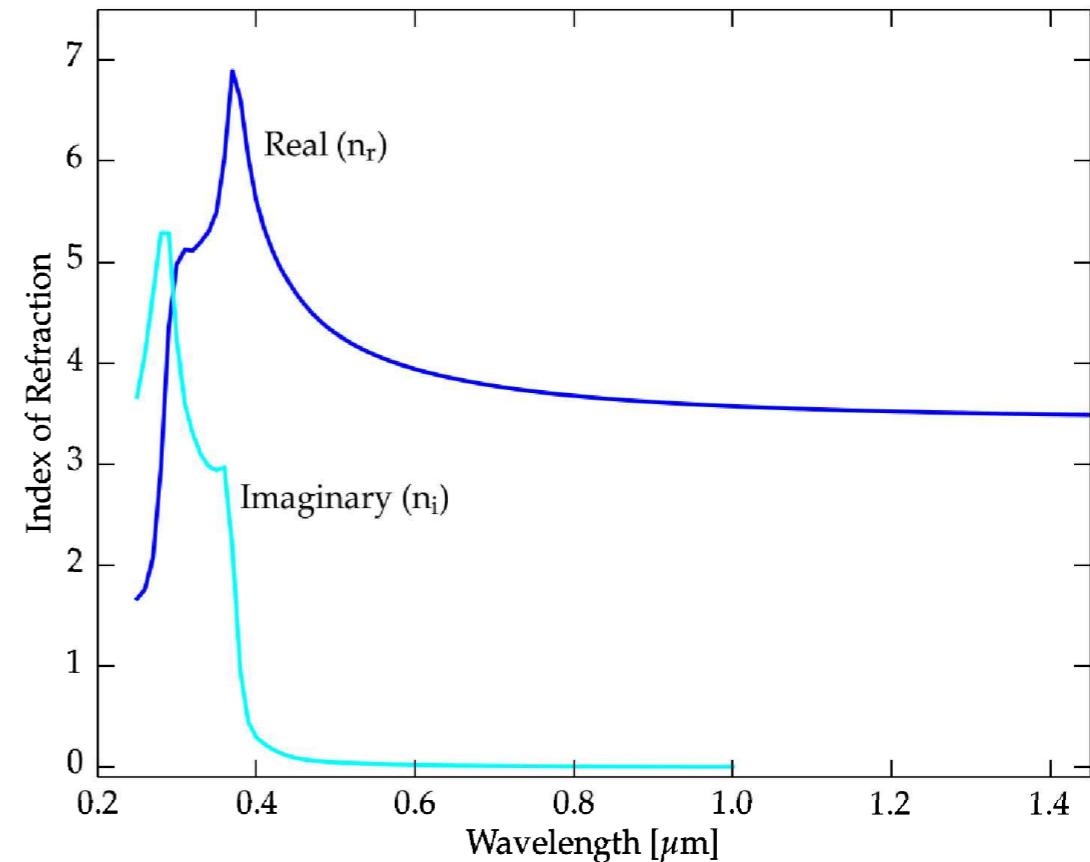
$$m = 1.31 + i(3.1 \times 10^{-9}) \quad \text{pure water ice, } \lambda = 5500\text{\AA}$$

- ▶ 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:

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

- 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:

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

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

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

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

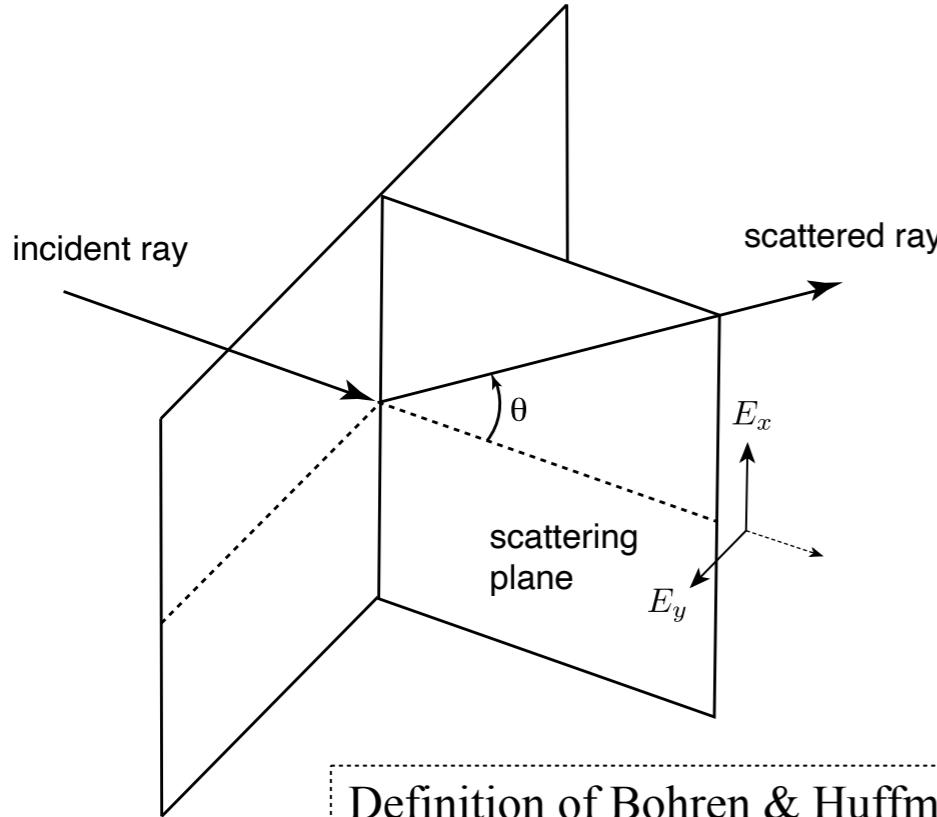
$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}$$

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

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>).

Scattering Phase Function

Let's define the scattering geometry as follows:



Definition of Bohren & Huffman

$$\begin{aligned} E_x &= E_{\parallel}^{\text{BH}} && \text{parallel to the scattering plane} \\ E_y &= -E_{\perp}^{\text{BH}} && \text{perpendicular to the scattering plane} \end{aligned}$$

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

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

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

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:

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

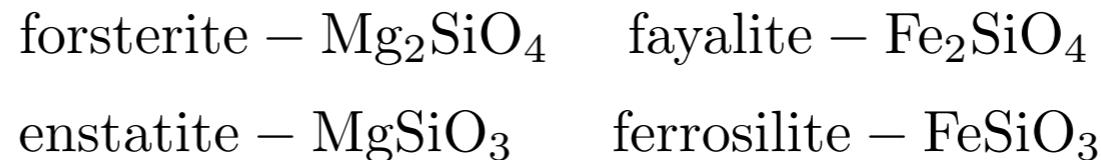
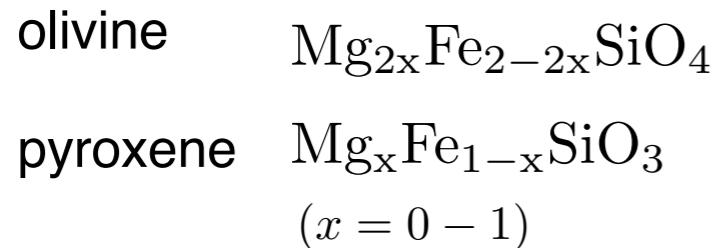
Then, the normalized phase function is given by

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

[Interstellar Dust]

- 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.

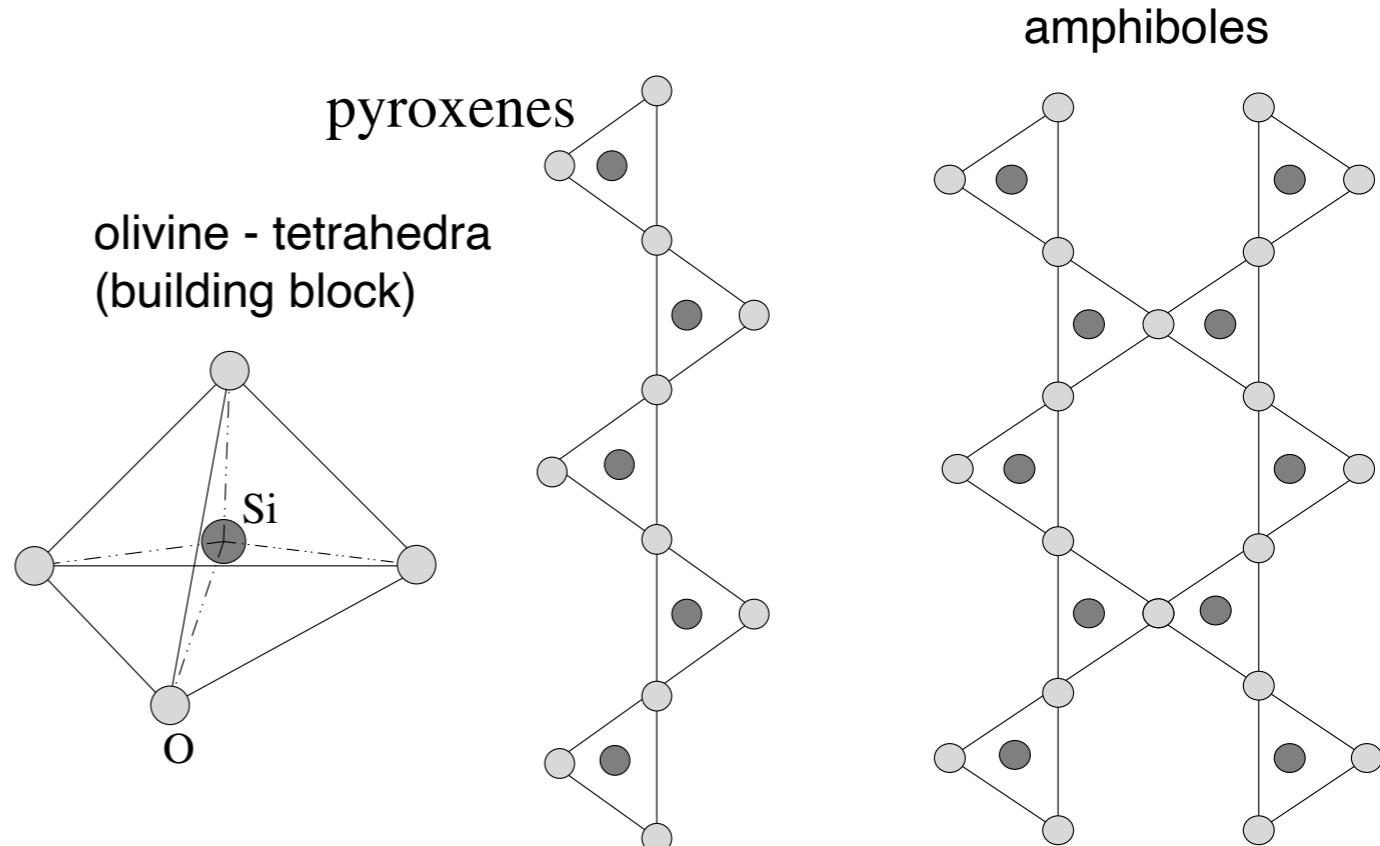
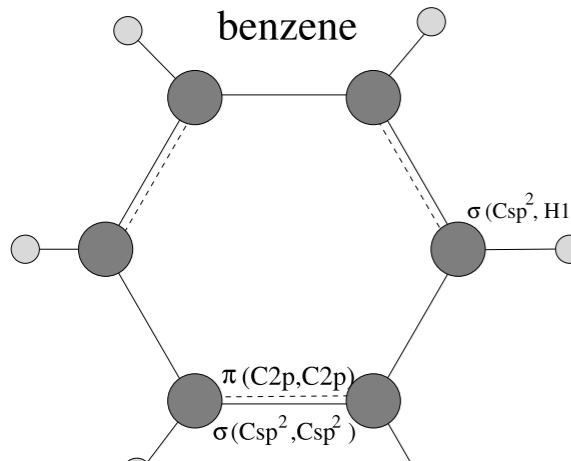


Fig 5.9 Krugel
[An Introduction to the Physics of Interstellar Dust]

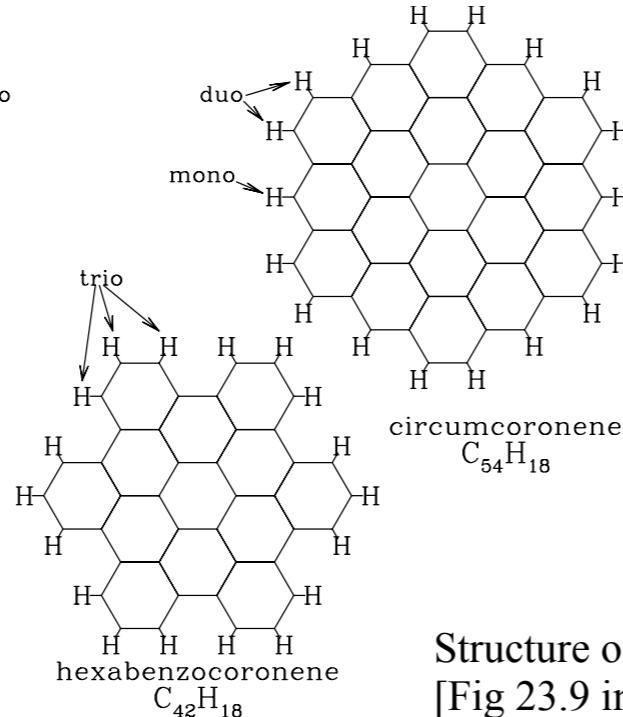
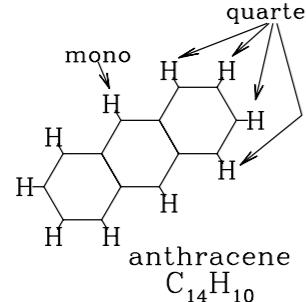
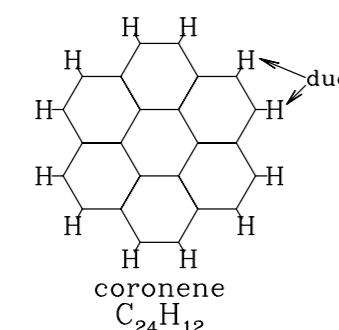
• Polycyclic Aromatic Hydrocarbons

- 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.

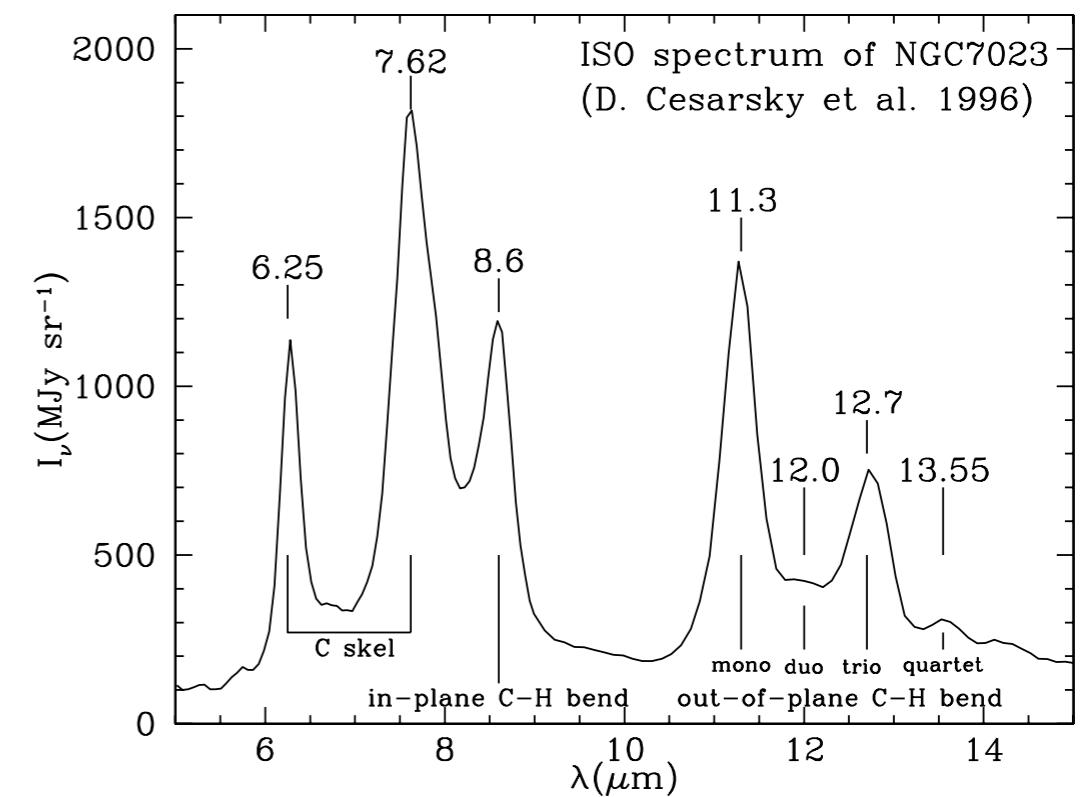


Bezene ring (C_6H_6)
The simplest type of PAHs.

[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)

- Graphite (흑연)

- Graphite is the most stable form of carbon (at low pressure), consisting of infinite parallel sheets of sp^2 -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 1.421\AA .
 - ▶ Crystalline graphite consists of regularly stacked graphene sheets.
 - ▶ The sheets are weakly bound to one another by van der Waals forces.

- Nanodiamond

- Diamond consists of sp^3 -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 premolar origin.
- But, its abundance in the ISM is not known.

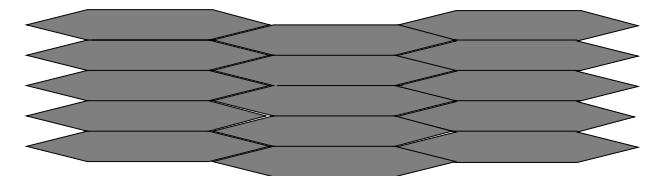
- Amorphous carbon

- Hydrogenated amorphous carbon (HAC)

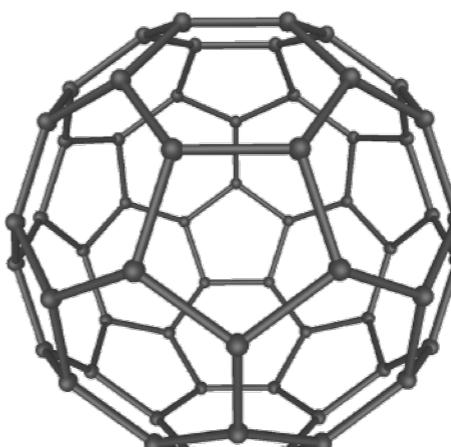
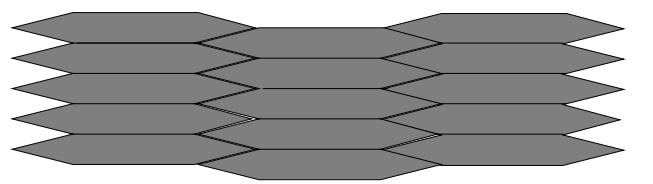
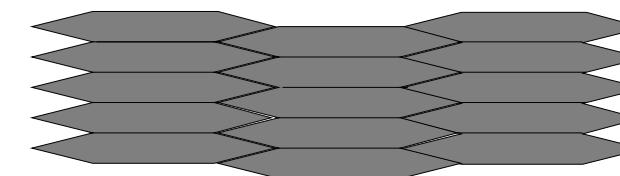
- Fullerenes



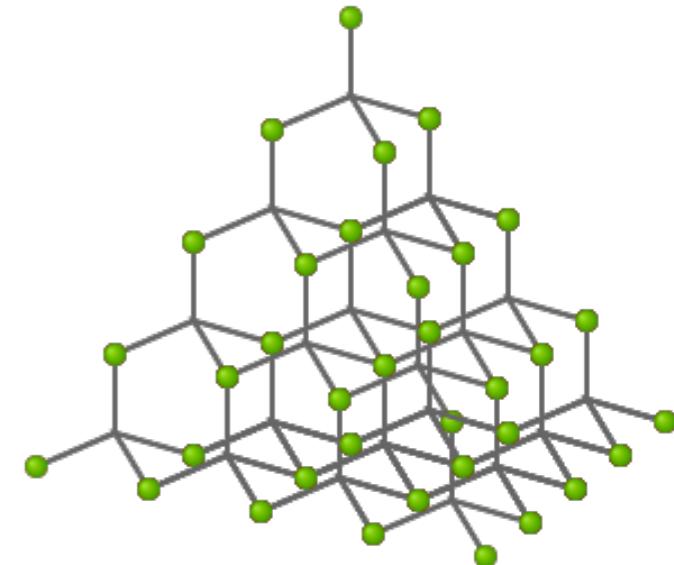
graphite sheets



3.35\AA



Buckminsterfullerene (C_{60})

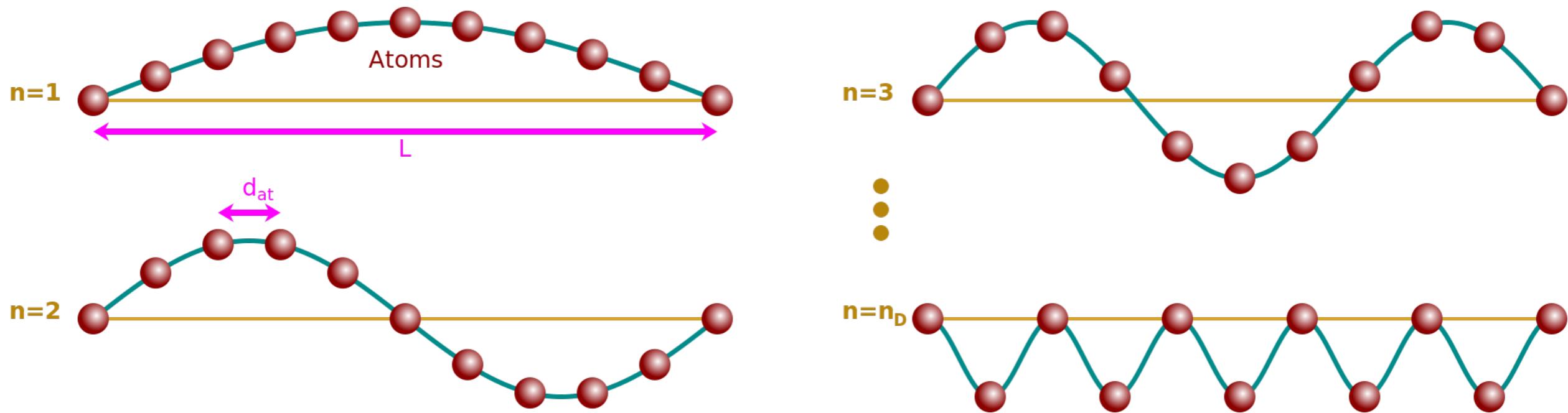


Structure of diamond.

[Temperatures of Interstellar Grains]

- The “temperature” of a dust grain is a measure of the internal energy 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 most solids or large molecules, however, the electronically excited state will deexcite nonradiatively, with the energy going into ***many vibrational modes - i.e., heat.***

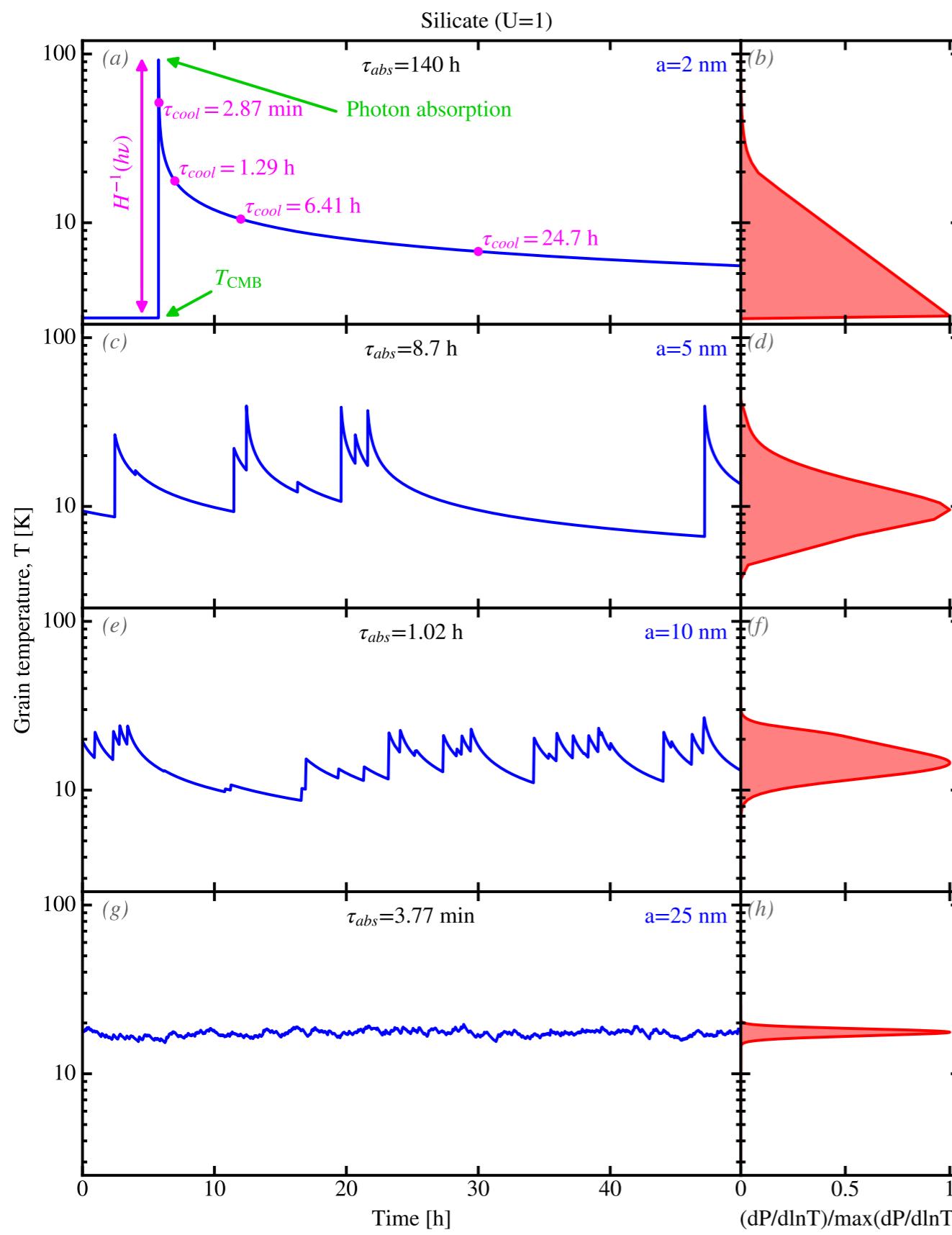
- The atoms in a solid may oscillate along the chain (longitudinal wave) or perpendicular to it (transverse wave). These collective vibrational modes are sound waves.



Phonon modes. We represent the simplest case of a string of atoms (red spheres). The total length of the solid is materialized by the yellow horizontal line. The two atoms at each end of this line are fixed. The modes are thus quantified. The shortest possible wavelength is $2d_{at}$, corresponding to the $n = n_D$ mode.

[Temperature of Large Grains and Small Grains]

- 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 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 fluctuations of grains with different radii.

The left panels show the time variation of the temperature of silicate grains (Draine 2003b,c), exposed to the Mathis et al. (1983) interstellar radiation field with $U = 1$. The radius of the grain a increases downward.

The right panels show the corresponding probability distribution of the temperature.

The simulation were performed using the Draine & Anderson (1985) Monte-Carlo method.

See Draine (2003a) for a similar simulation with graphite.

[credit: Federic Galliano]