

Astrophysics

Lecture 16

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Dust / Solid Particles

[Bonding and Antibonding Orbitals]

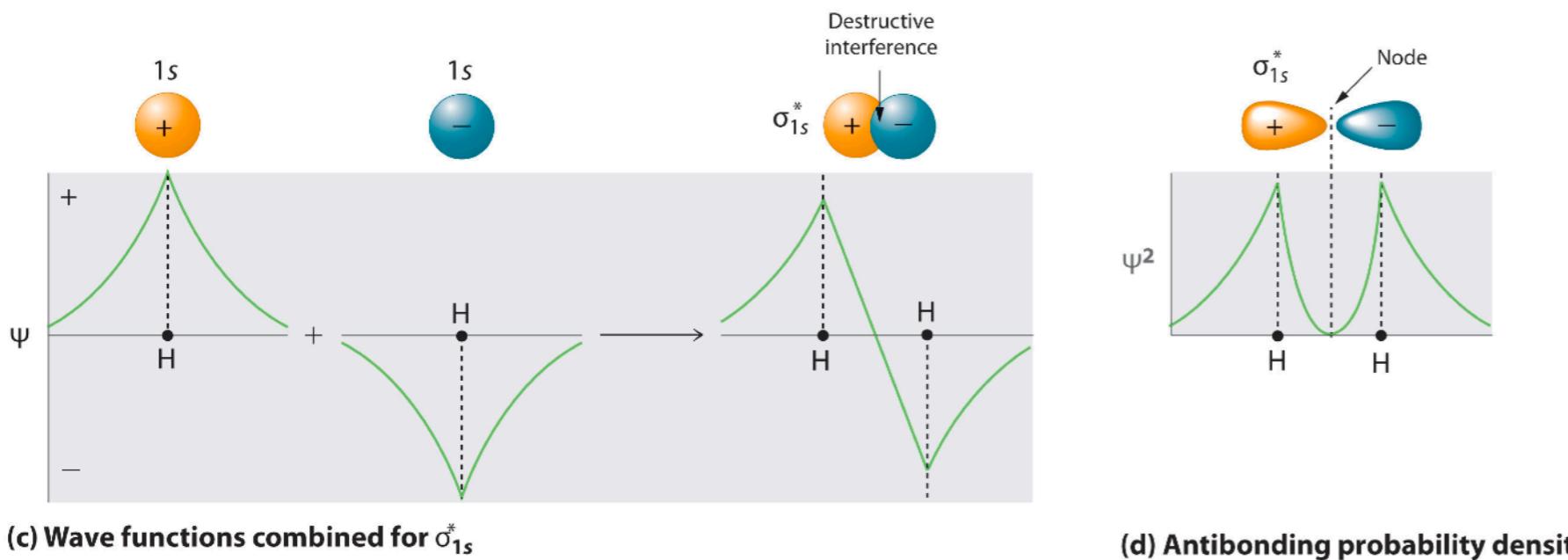
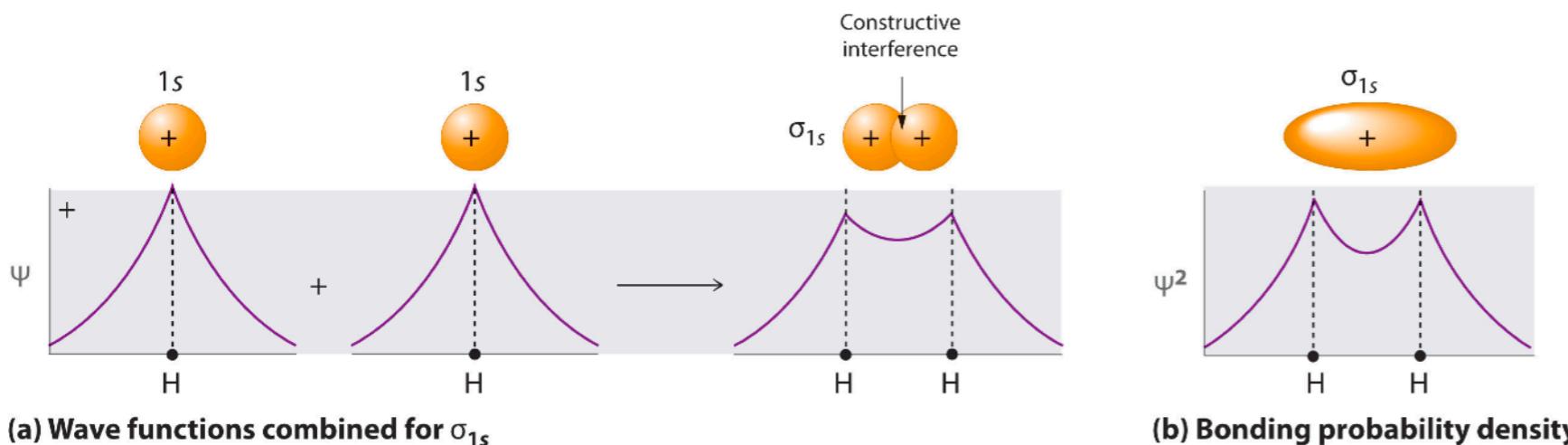
- **Molecular Orbital Method:** The molecular orbitals are created via the linear combinations of atomic orbitals. For instance, for a diatomic molecule,

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

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

$$|C_A|^2 = |C_B|^2$$

We have two possibilities that satisfy the above condition.



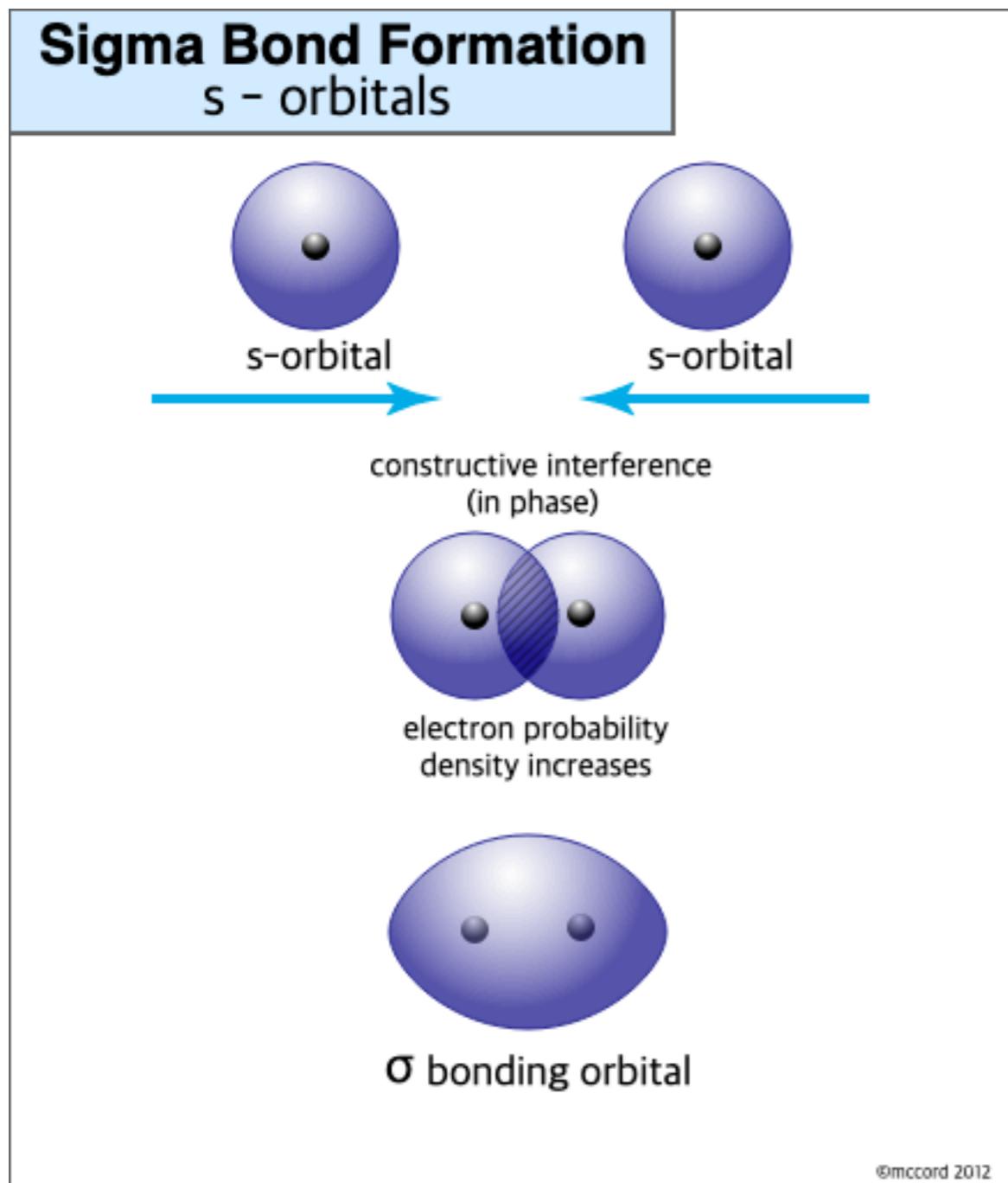
$$|\sigma_{1s}\rangle = \frac{1}{\sqrt{2}} (|1s_A\rangle + |1s_B\rangle)$$

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

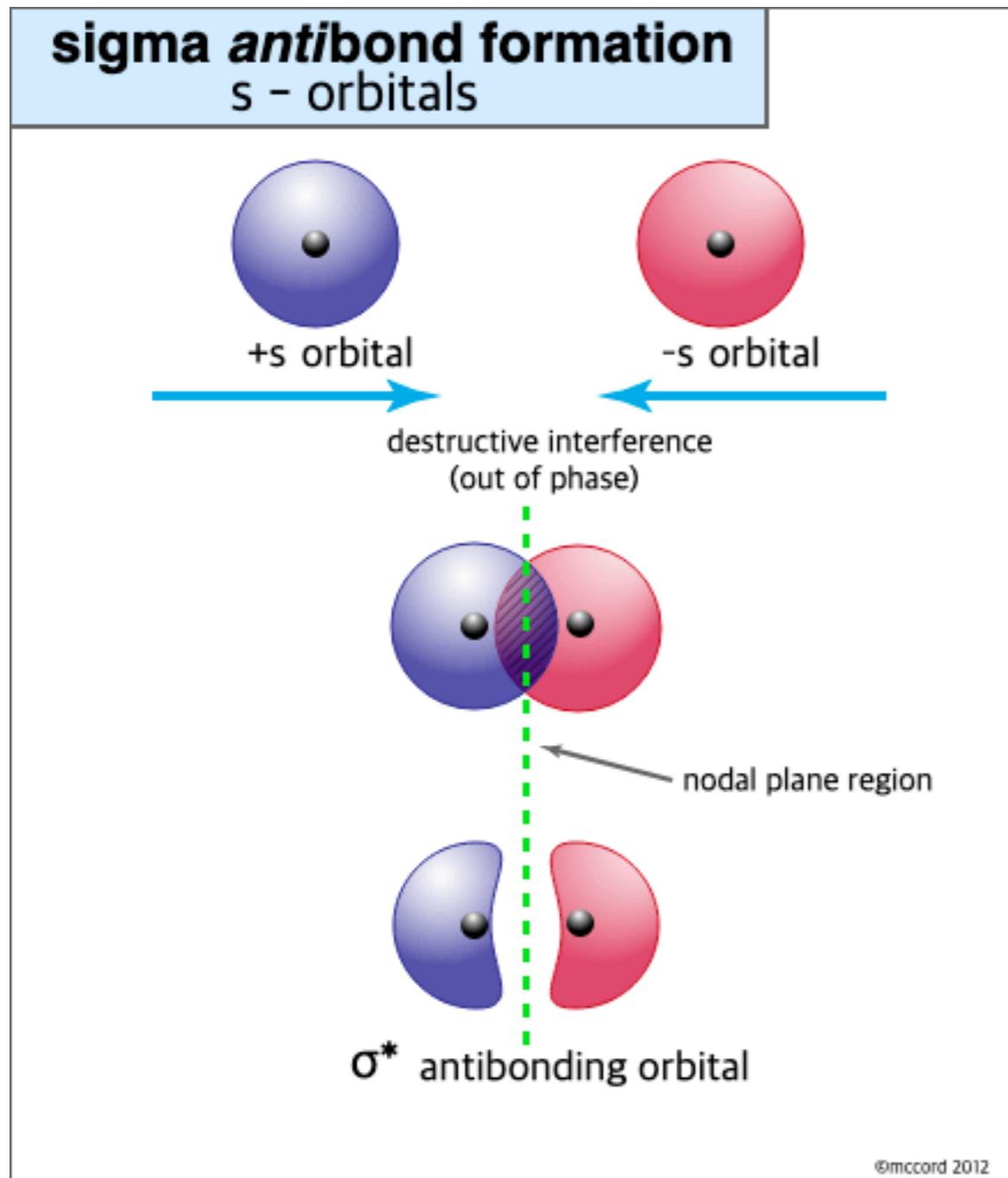


- Bonding orbitals are formed when atomic orbitals combine in ways that lead to predominantly constructive interference.

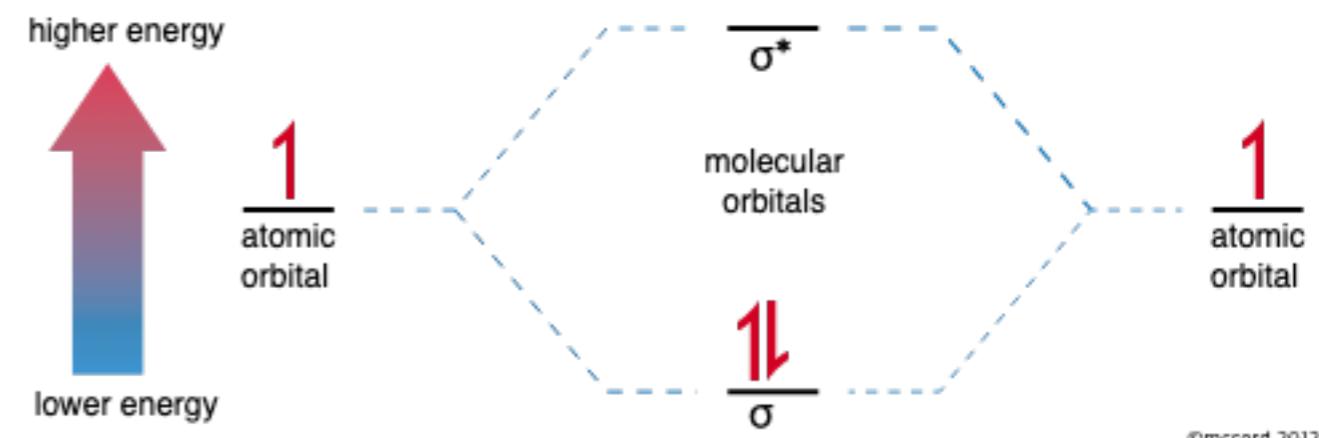
In the bonding orbitals, the electron density is found between the atoms. This leads to the idea that covalent bonding is “shared” electrons. The electrons have a high probability of being between the nuclei in the molecule.

The molecule has a lower energy than the separated atoms.
- 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.

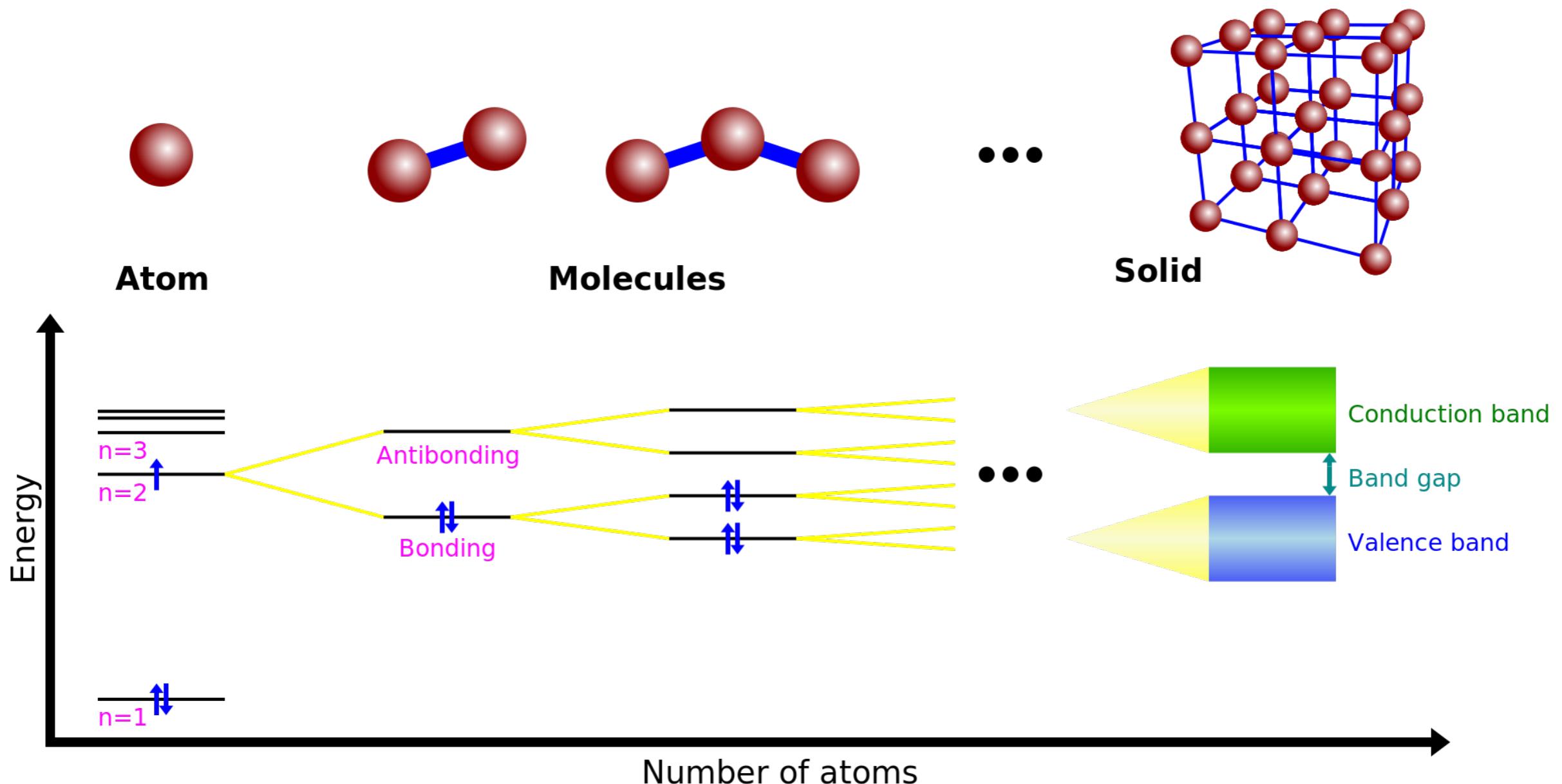
Antibonding Orbitals



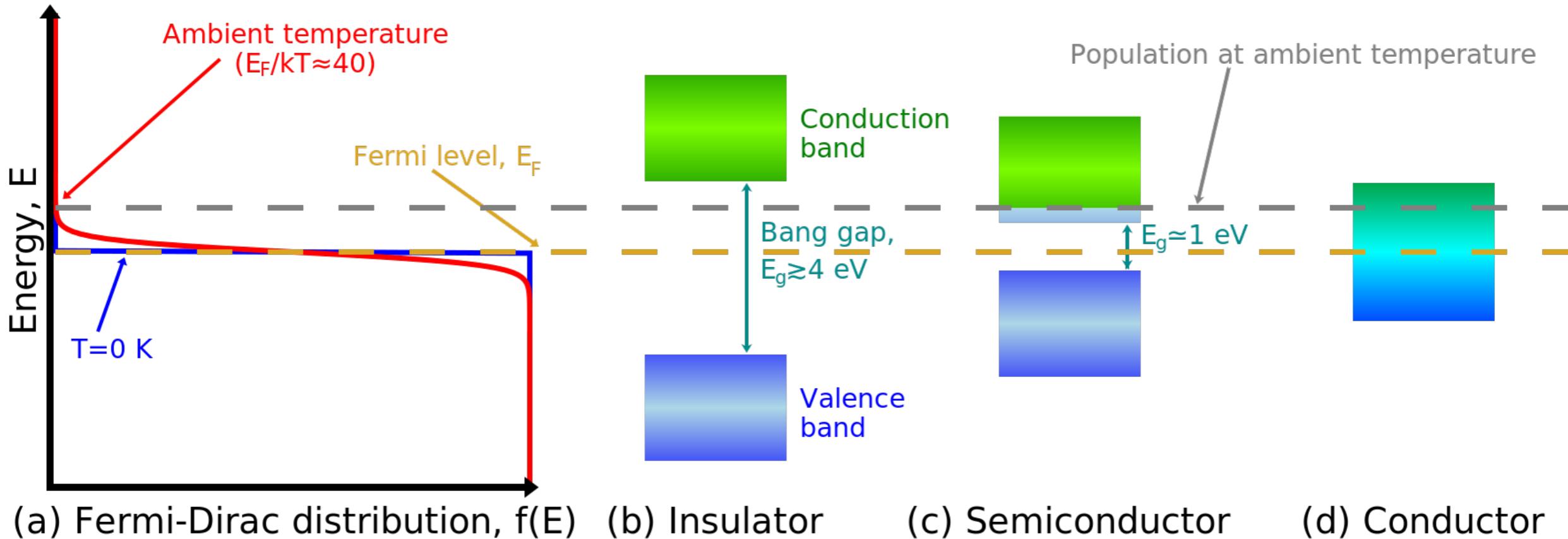
- Anti-bonding orbitals are formed when atomic orbitals combine in ways that lead to predominantly destructive interference. In this bonding, a “node” or place of zero electron density exists between the atoms.
- The molecular orbitals have a higher energy than the corresponding atomic orbitals.
- We denote anti-bonding orbitals with a * symbol.



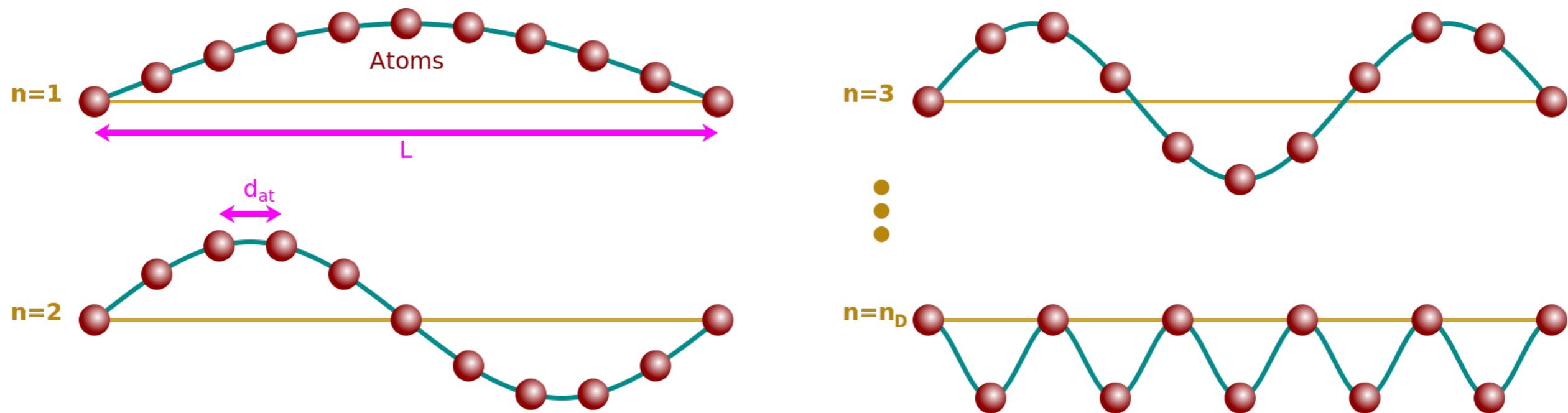
[Band Structure of a Solid]



Origin of the band structure of a solid. From the left to the right, we represent: (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.



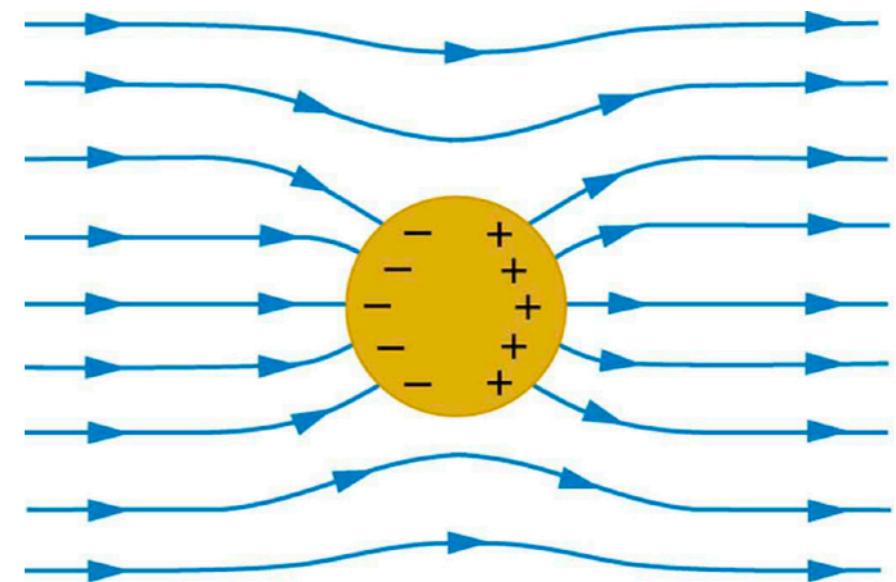
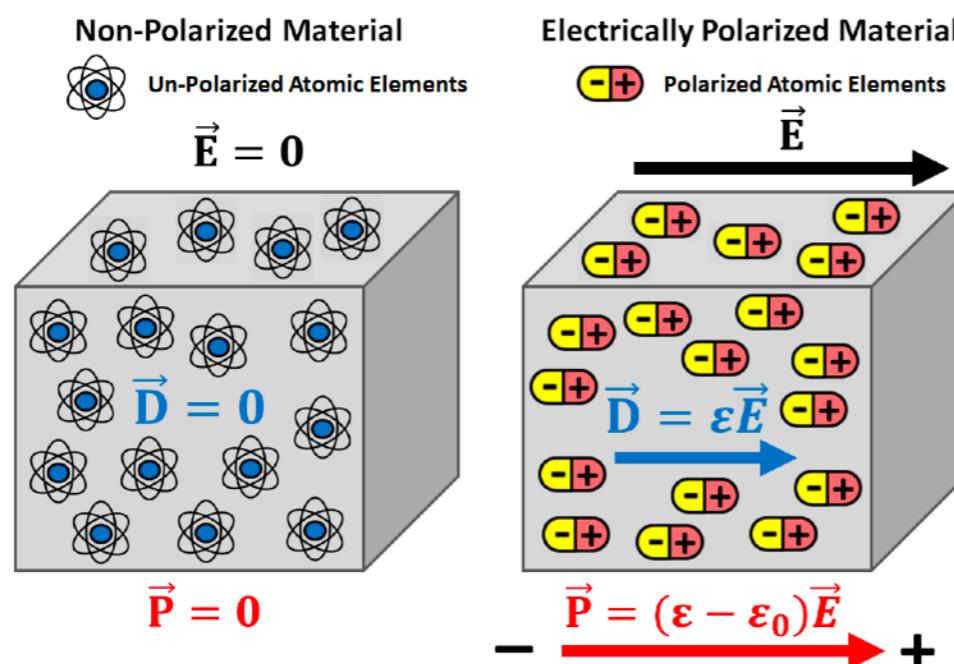
The Fermi level and the different types of solid. The left plot shows the rotated Fermi-Dirac distribution, for two values of the temperature, $T = 0 \text{ K}$ and $T \approx 300 \text{ K}$. The three diagrams on the right show the valence and conduction bands relative to the Fermi level, E_F , for insulators, semiconductors and conductors. For conductors, the valence band is also the conduction band.

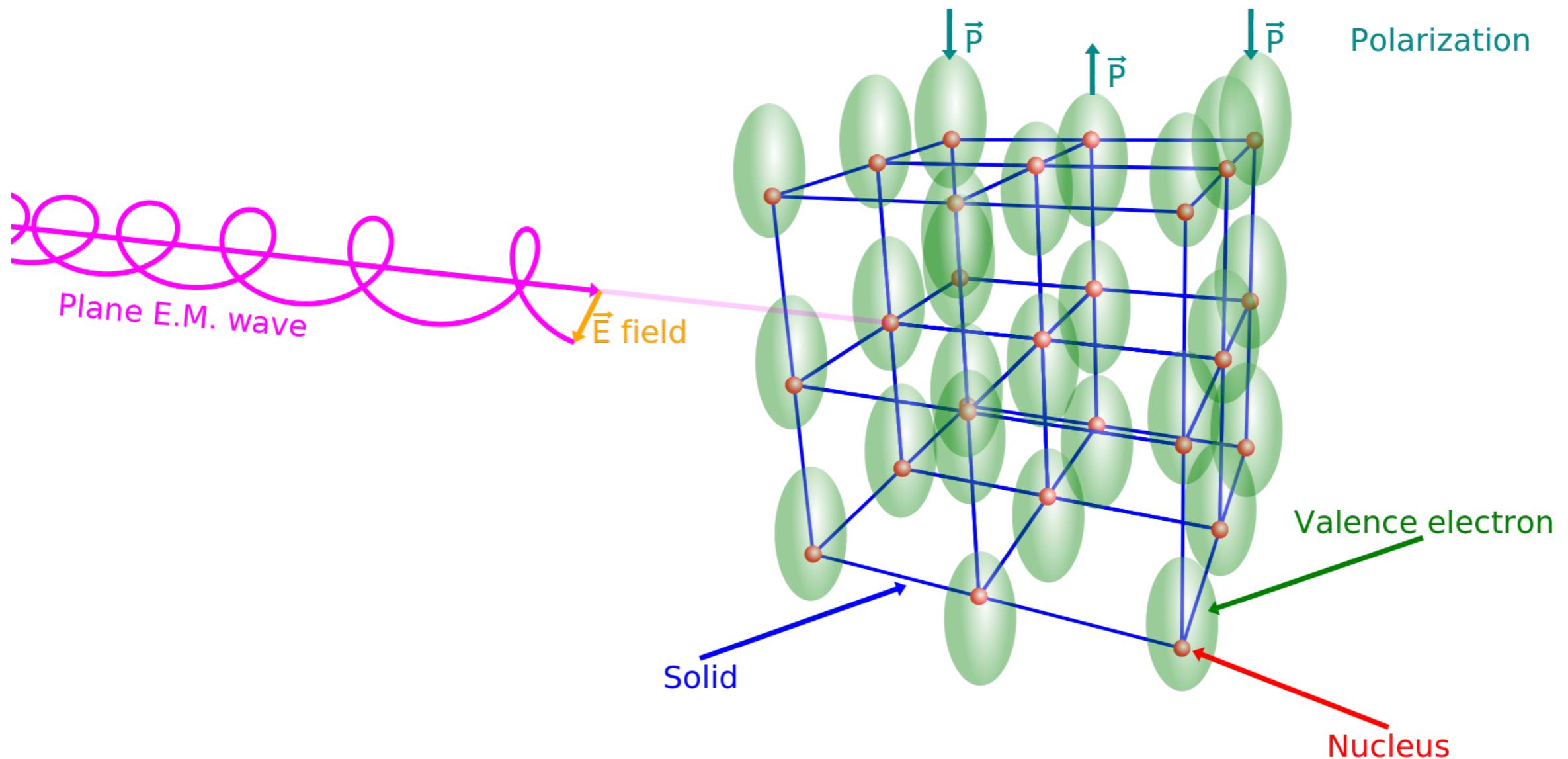


Phonon modes. We represent the simplest case of a string of atoms (red spheres). The total length of the solid is materialized by the yellow horizontal line. The two atoms at each end of this line are fixed. The modes are thus quantified. The shortest possible wavelength is $2d_{at}$, corresponding to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

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**: 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.



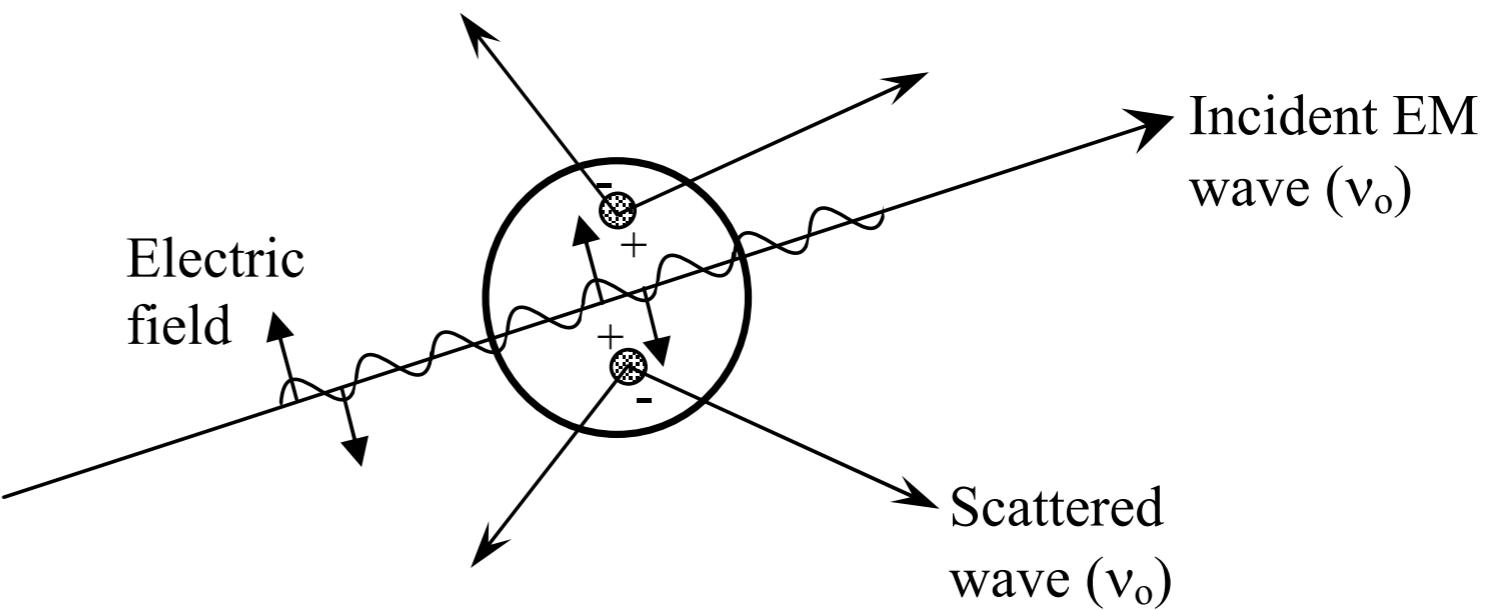


Effect of an electromagnetic wave on a dielectric. An incoming, circularly polarized, electromagnetic wave is figured in magenta. The cube on the right represents a solid. The nuclei, assumed to be fixed, are the red spheres. The valence electrons are the green ellipsoids. They are displaced out of their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

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- 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.

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

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

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

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

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

E electric field

B magnetic flux density
(magnetic induction)

H magnetic field strength
(magnetic field)

Faraday

Ampere

Constitutive
Relations

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

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

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

Continuity Equation

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

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

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

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

ϵ = permittivity

μ = permeability

σ = conductivity

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

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

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

- ▶ 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.

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

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

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

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- ▶ 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.

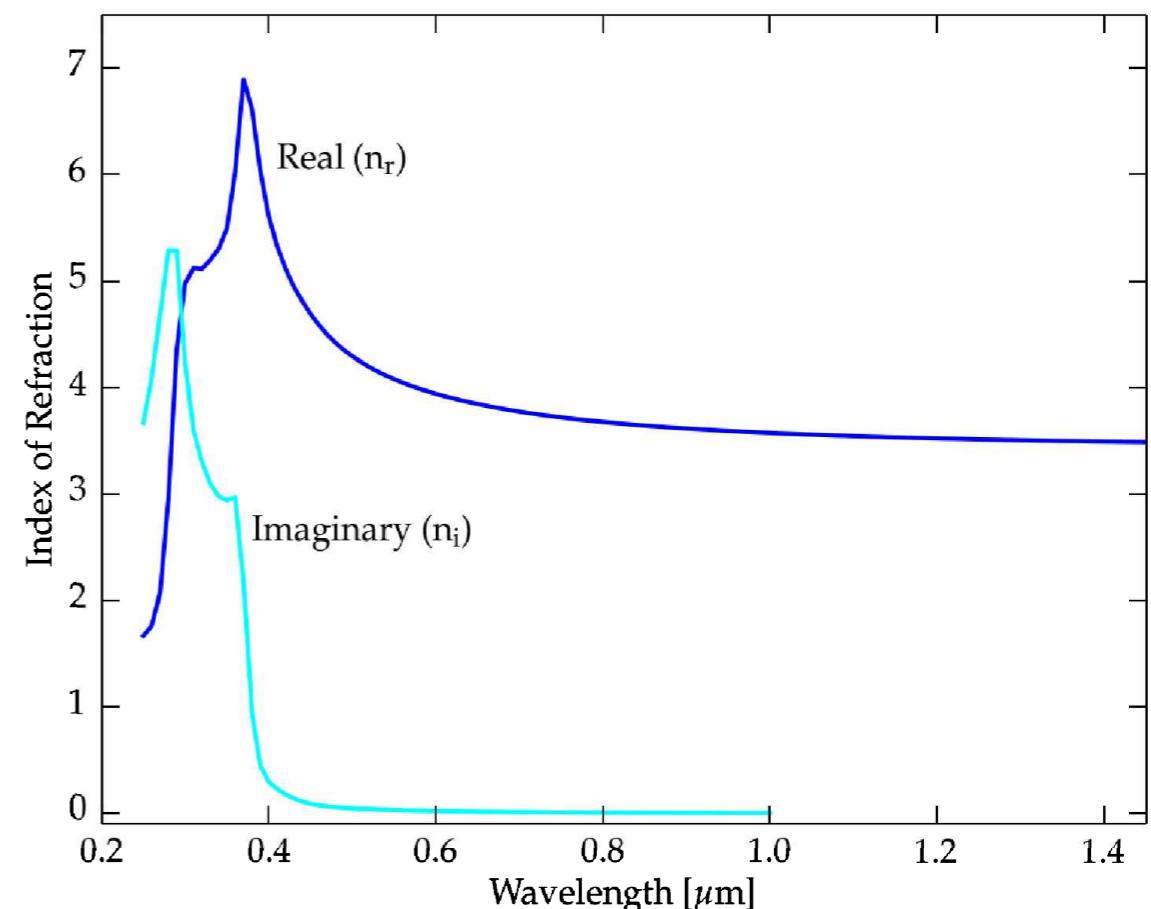
$$m = 1.31 + i(3.1 \times 10^{-9}) \quad \text{pure water ice, } \lambda = 5500\text{\AA}$$

- ▶ 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:

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

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

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

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

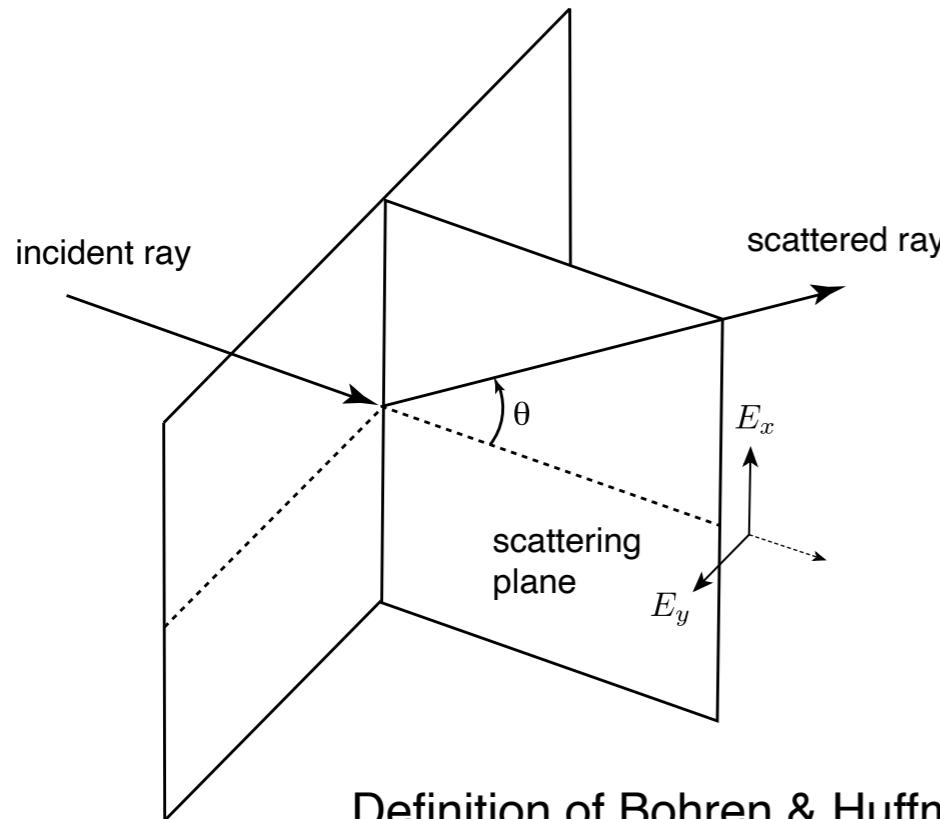
$$y_0(x) = -\frac{\cos x}{x}$$

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

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>).

Scattering Phase Function

Let's define the scattering geometry as follows:



Definition of Bohren & Huffman

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

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

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

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

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

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

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