

Quantum Concepts (on exam 4)

<u>Who</u>	<u>When</u>	<u>What</u>	<u>Equation</u>
1. Planck	1905	Quantization of Energy	$\Delta E = h\nu$
2. Einstein	1905	Particle Nature of Light	$p = h/\lambda$
3. DeBroglie	~1920	Wave Nature of Particles	$\lambda = h/p$
4. Bohr	~1920	Quantization of Angular Momentum	$L^2 = l(l+1) (h/2\pi)^2 ;$ $L_z = m (h/2\pi)$ 2L+1 m values from -L to +L
5. Heisenberg	~1925	Uncertainty Principle	$\Delta p_x \Delta x \cong h$

or: **ZERO POINT ENERGY: confinement causes kinetic energy**

or: "why the electron does not fall into the nucleus"

THEN CAME THE Schrödinger Equation (1926)
which says all of the above

This equation was **DISCOVERED**, not derived

$$H\Psi = E \Psi$$

Energy operator x wavefunction = Energy x wavefunction

Schrodinger **did not know what to make of Ψ** when he published his equation. Everyone knew it was important because the equation gave all the correct energies for the “well behaved” solutions.

Also was immediately shown that Newton's Laws could be derived from the Schrodinger Eq.
(but not the other way around!)

1926 Schrodinger's Equation:

A simple equation that was discovered (not derived)

Classical Mechanics

Kinetic Energy + Potential Energy = Total Energy

Quantum Mechanics (Schrodinger's Equation without time) translated into English:

$-\hbar^2/8\pi^2\text{mass} \times \text{Curvature of Wavefunction} + \text{Potential Energy} \times \text{Wavefunction} = \text{Energy} \times \text{Wavefunction}$

Kinetic energy is the ONLY thing that is wierd about quantum mechanics

curvature operation
(2nd derivative)

$h/2\pi$

$$: -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi = E\psi$$

mass

Kinetic energy

potential energy (SAME as classical mechanics)

Total energy

****This for 1 particle
in only 1 dimension
and $\Psi = \Psi(x)$**

Time independent Schrodinger Equation for many particles in 3 D

$$-\frac{\hbar^2}{8\pi^2} \times \sum_{\text{all particles } j} \left(\frac{\partial^2}{\partial x_j^2} + \frac{\partial^2}{\partial y_j^2} + \frac{\partial^2}{\partial z_j^2} \right) \Psi + \text{potential } E \times \Psi = \text{total } E \times \Psi$$

or : kinetic energy operator $\times \Psi$ + classical potential energy $\times \Psi$
= total energy $\times \Psi$

$H\Psi = E\Psi$, where H = Hamiltonian = total energy operator

$\Psi^* \Psi$ = probability per unit volume for finding all particle locations at once

Ψ^* is the complex conjugate . i.e., change all $i \rightarrow -i$

where $i = \sqrt{-1}$

Potential energy is EXACTLY the same as in Classical mechanics

Three things are different from Classical mechanics:

1) The **wavefunction (orbitals)**

(Schrödinger *did not know* what its physical meaning was at the time he published).
Later the consensus was reached that the absolute square of the wavefunction gives the **probability density** for finding the particle.)

2) **Kinetic energy**

is represented by the **CURVATURE** of the **Wavefunction**.

In calculus, that is the 2nd derivative (i.e., the slope of the slope of the function)

3) **h** , Planck's constant, which was empirically adjusted so that the Schrödinger Equation gives agreement with experiment.

This simple equation embodies the 5 seemingly distinct new "quantum concepts"

More on **zero point energy** and uncertainty principle

Zero point kinetic energy is $\cong h^2 / (m \Delta x^2)$, where h = Planck's constant, m = mass, and Δx is the length of the region to which the particle is **confined**.

All energy level equations have $h^2 / (m \Delta x^2)$.

Small mass and small space give the quantum energy levels.

For example, as a nucleus pulls an electron close, the zero-point energy increases and **the electron will not fall to the nucleus**. (It is as if the small things like electrons "refuse" to be localized.)

Note: $h^2 = \text{J}^2 \text{s}^2 = \text{kg}^2 \text{m}^4 \text{s}^{-4} \text{s}^2$, so $h^2 / (m \Delta x^2) = \text{kg}^2 \text{m}^4 \text{s}^{-2} / (\text{kgm}^2) = \text{kg m}^2 \text{s}^{-2} = \text{J}$

Heisenberg Uncertainty: $\Delta x \Delta p \cong h$, i.e., product of uncertainty in x and uncertainty in momentum is about $= h$.

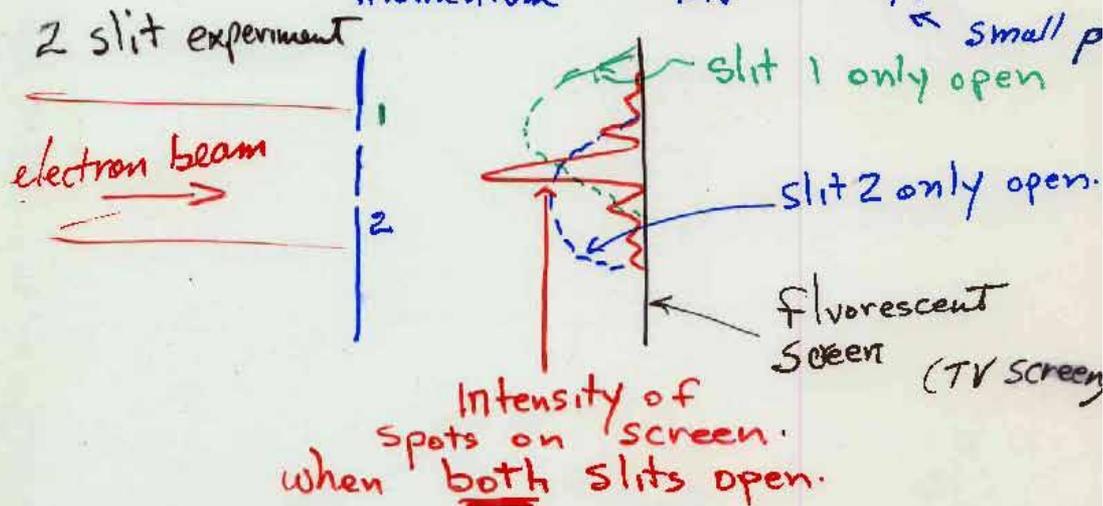
ΔH of chemical reactions is equal to the **change in quantum zero point energy** at 0 Kelvin, and is only slightly different at room temperature due to heat capacity differences.

The mysterious "**DARK ENERGY**" that is apparently causing the acceleration of expansion of the Universe is most discussed as **quantum zero point energy** (of gravity, for which there is no quantum theory yet.)

3. WAVE NATURE OF PARTICLES

de Broglie ~ 1920

$$\lambda = \frac{h}{\text{momentum}} = \frac{h}{mv} \equiv \frac{h}{p} \quad \leftarrow \text{small } p$$



TIME EXPOSURE (1 particle per second)

GIVES EXACTLY SAME RESULT !!!

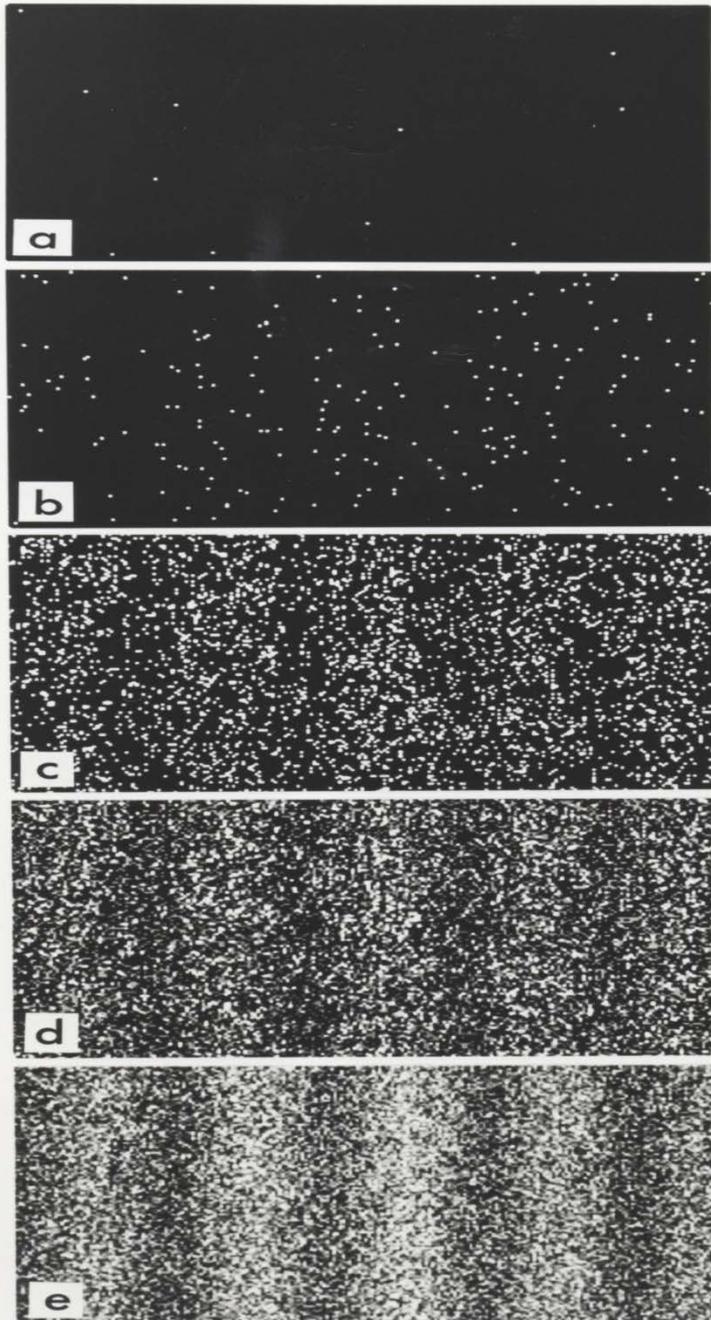
SAME FOR PHOTONS !!!

Interference is a SINGLE PARTICLE phenomenon! (one particle or photon does not interfere with another)

This phenomenon captures the essential mystery of quantum behavior

Results of a [double-slit-experiment](#) performed by Dr. A. Tonomura showing the build-up of an interference pattern of **single electrons**. Numbers of electrons are 10 (a), 200 (b), 6000 (c), 40000 (d), 140000 (e).
(Provided with kind permission of Dr. Akira Tonomura.)





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Electron or photon interference is a single particle phenomenon!

Movies available at:
<http://www.hitachi.com/rd/research/em/movie.html>

Time dependent Schrödinger Equation

$$\frac{\partial \Psi(r,t)}{\partial t} = -i \frac{H}{\hbar} \Psi(r,t)$$

i simply means
90 degrees out of phase

$H\Psi = E\Psi$, where H = Hamiltonian = total energy operator

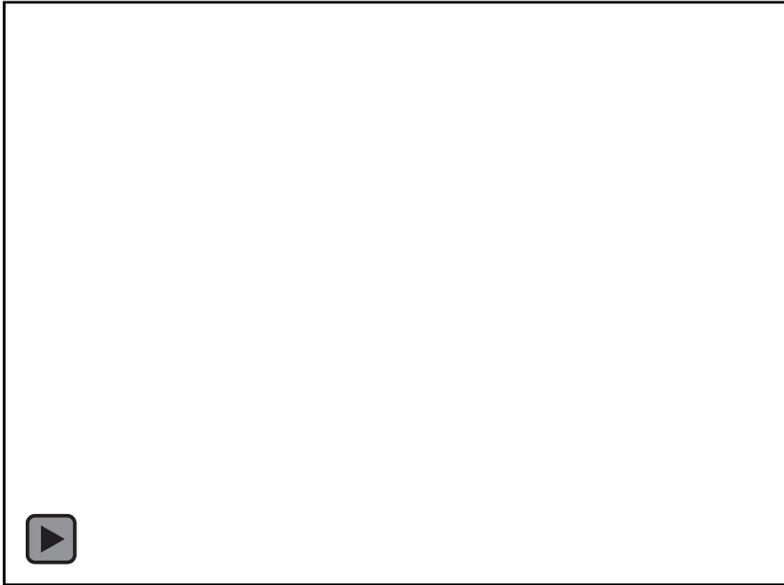
It says by inspection that the **future** of a quantum state is predicted, IF one knows the wavefunction at a given time.

(we never do, except for very simple experiments)

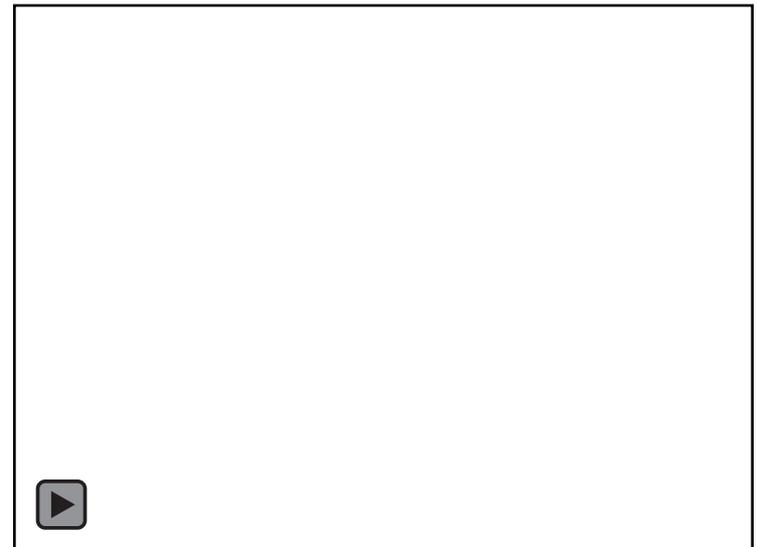
All (non-relativistic) dynamics in nature are in principle described by this simple equation! Only limited by computer size and power.

Below are videos of time dependent quantum computations of an electron moving through a double slit.

Single slits: 3 different widths (confinements!)



Single particle (photon or electron) diffraction from exact solutions of time dependent Schrodinger Equation.



<http://msc.phys.rug.nl/quantummechanics/diffint.htm>

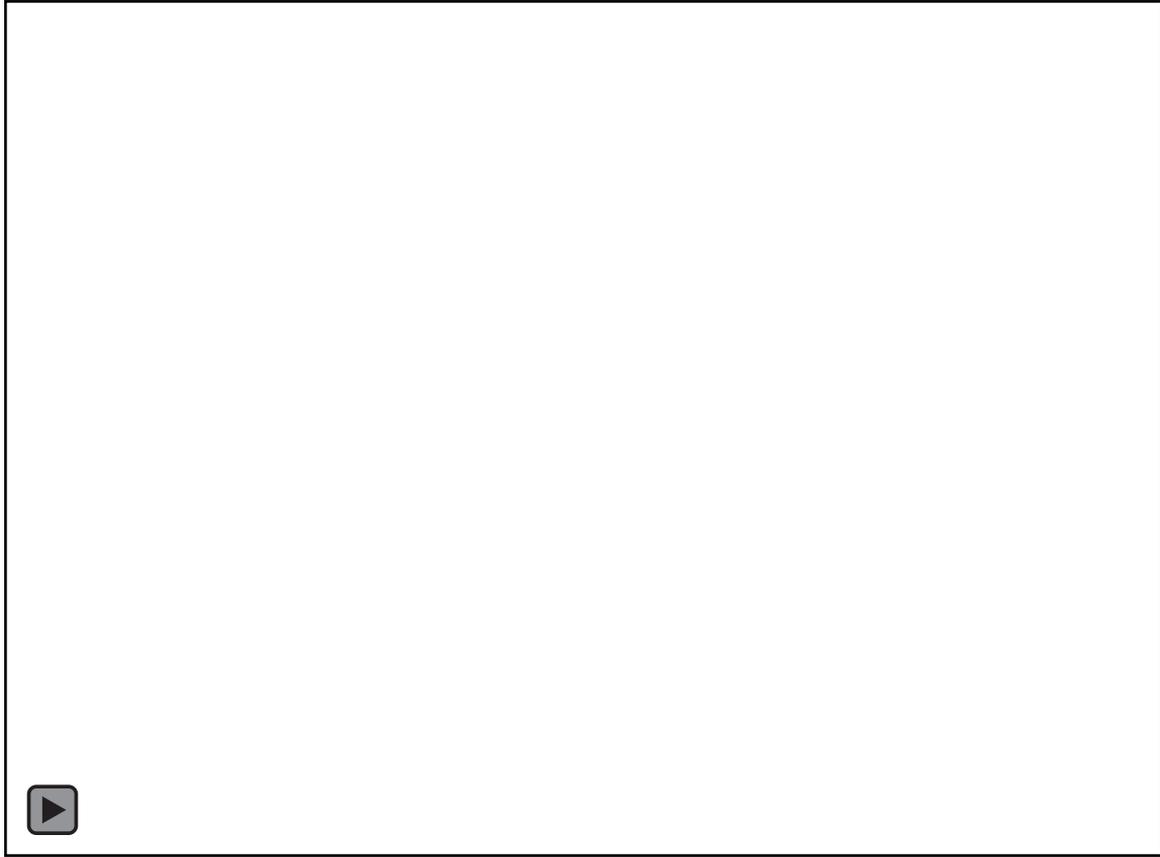
[Materials Science Group, University of Groningen](#)

Two slit interference

Single particle (photon or electron) diffraction from exact solutions of time dependent Schrodinger Equation.

Particle wavefunction squared moving toward two slits in a solid plate. The particle is partially reflected backwards from plate and partially passed through the two slits. Peaks of the interference pattern are as predicted for Bragg's Law.



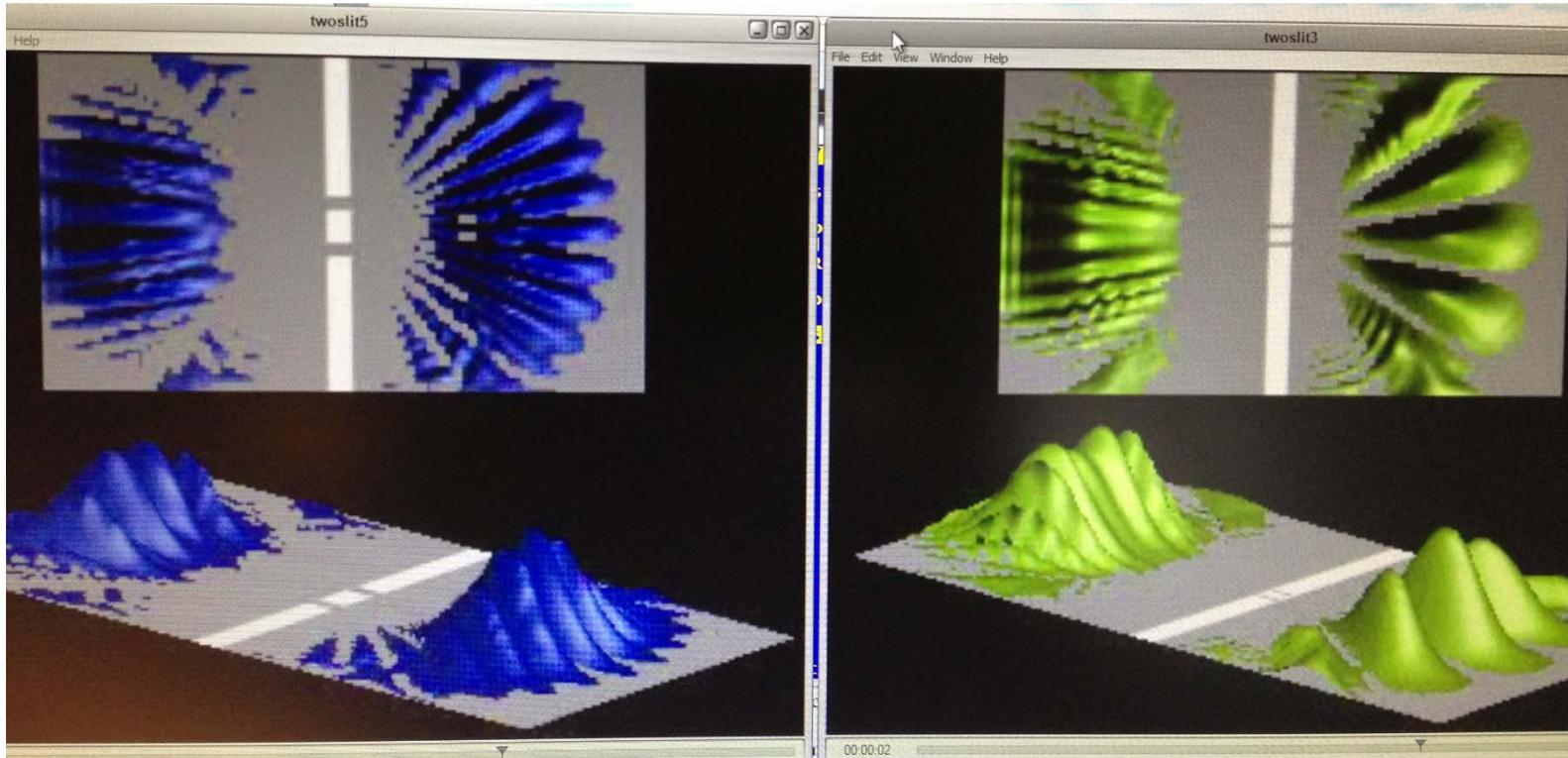


Illustrates Braggs Law of interference:

$$\sin \theta = n \text{ wavelength} / (\text{twice the distance between slits})$$

Slits far apart \rightarrow Many peaks

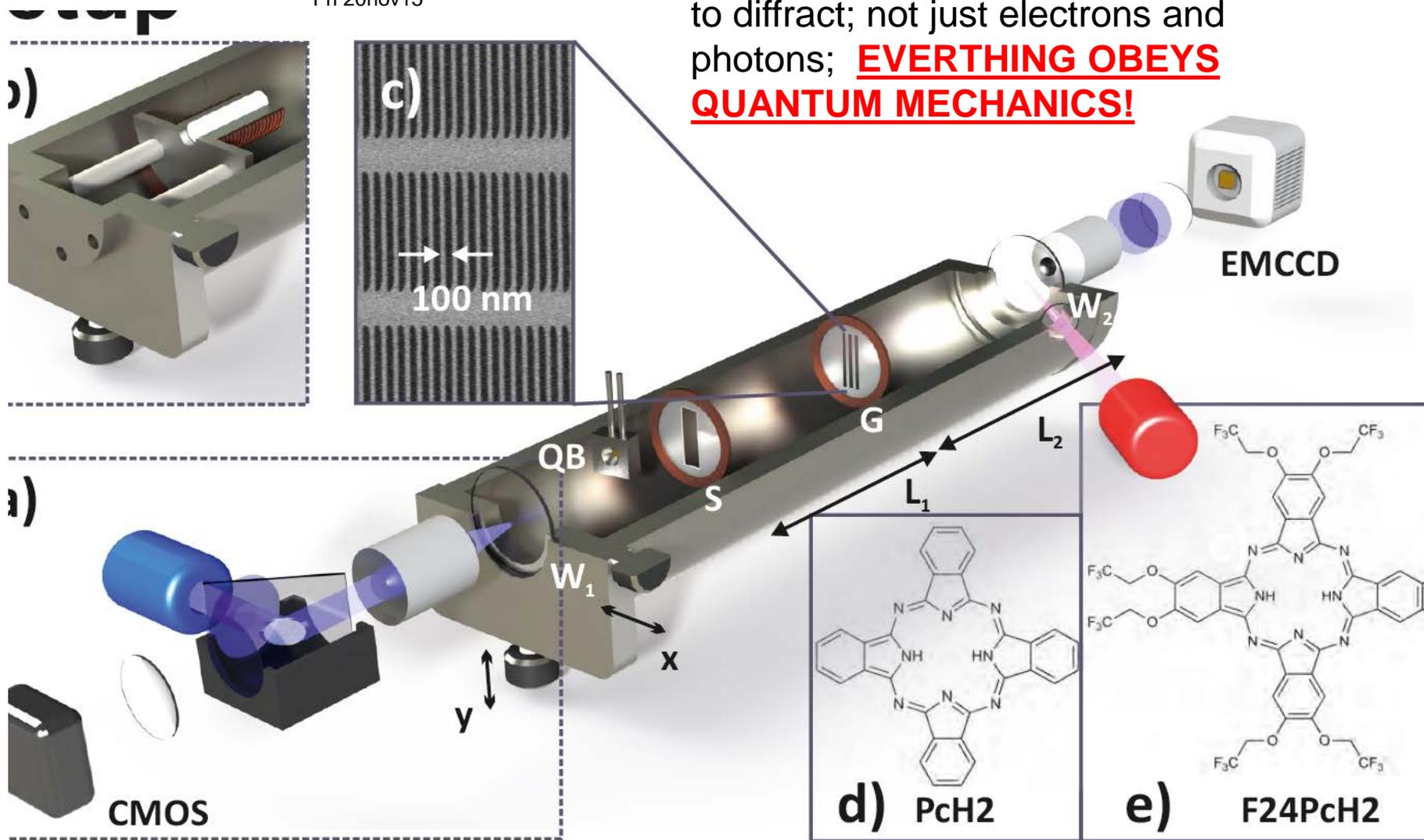
Slits far apart \rightarrow Few peaks



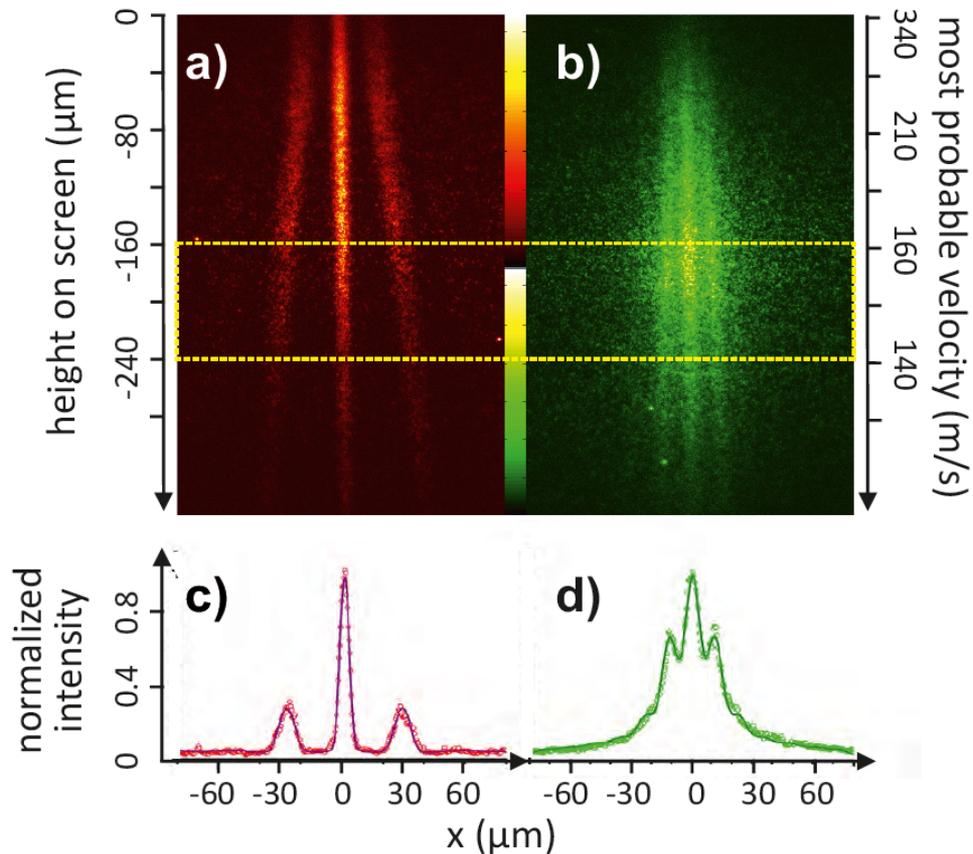
This is exactly what happens with x-rays, electrons and neutrons when directed on a molecular crystal.

The structure of the molecule may be computed from the diffraction pattern

Large dye molecules also observed to diffract; not just electrons and photons; **EVERYTHING OBEYS QUANTUM MECHANICS!**



Phthalocyanine derivatives



Far-field diffraction of larger molecules [2,4]

- Phthalocyanine P_cH₂ (red):
Highly fluorescent dye, thermally stable
- Perfluoro-alkylated phthalocyanines (green):
Higher masses, high volatility,
optical properties similar to P_cH₂.

http://www-lpl.univ-paris13.fr/icap2012/docs/Juffmann_poster.pdf

http://www.youtube.com/watch?v=NUS6_S1KzC8



The Final Topic: Physical Chemistry of Climate

Light emitted by all objects not at 0 Kelvin.

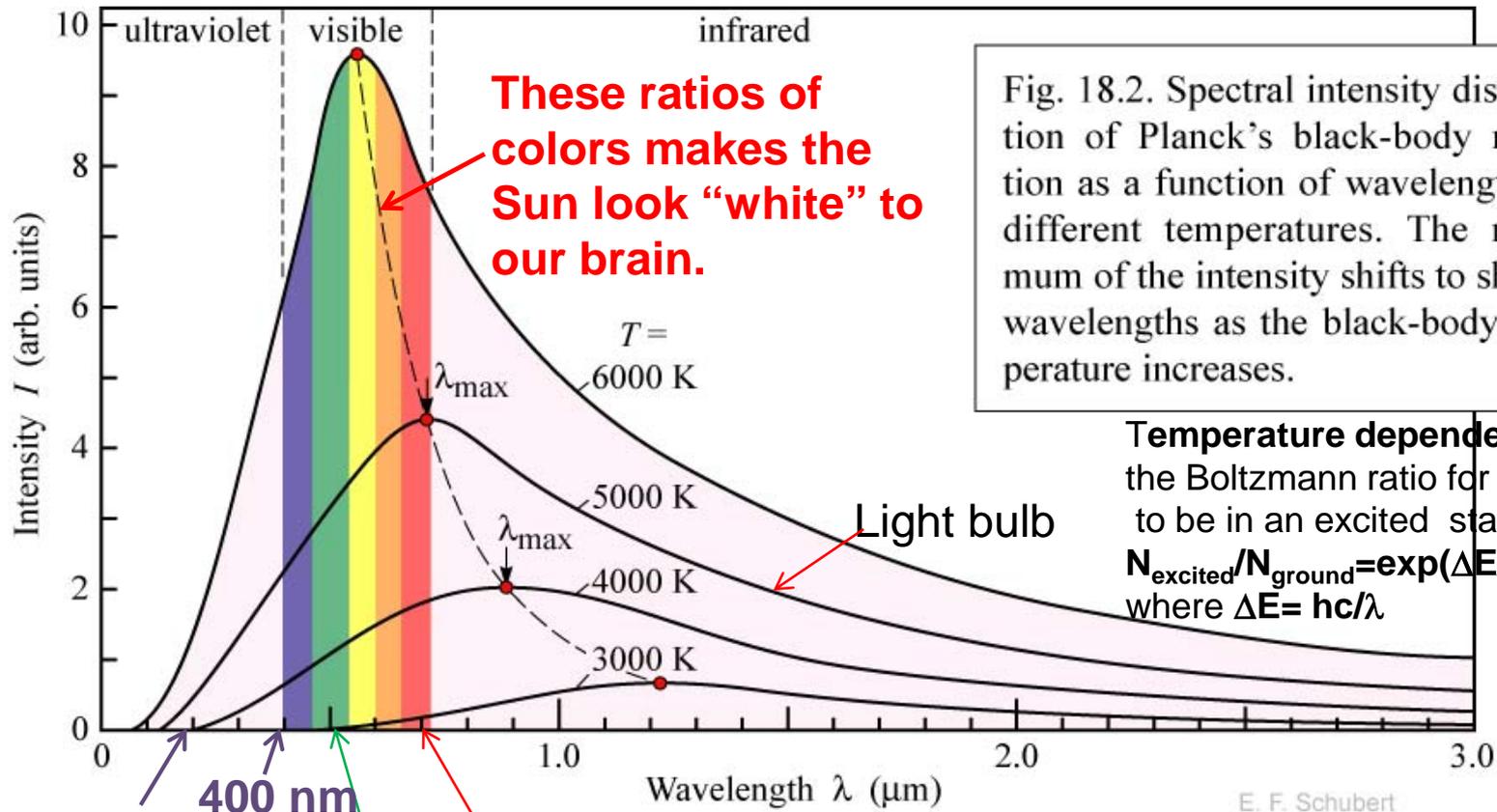


Fig. 18.2. Spectral intensity distribution of Planck's black-body radiation as a function of wavelength for different temperatures. The maximum of the intensity shifts to shorter wavelengths as the black-body temperature increases.

These ratios of colors makes the Sun look "white" to our brain.

Temperature dependence is from the Boltzmann ratio for probability to be in an excited state:

$$N_{\text{excited}}/N_{\text{ground}} = \exp(\Delta E/k_B T)$$
 where $\Delta E = hc/\lambda$

200 nm
 Where N_2 and O_2
 start to absorb

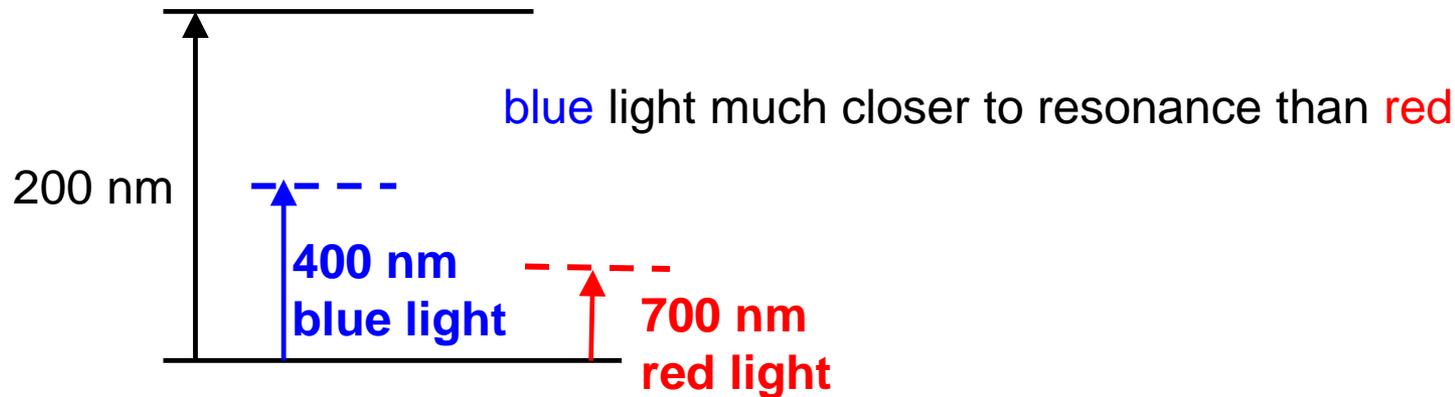
400 nm
500 nm
700 nm

E. F. Schubert
 Light-Emitting Diodes (Cambridge Univ. Press)
 www.LightEmittingDiodes.org

Why is the sky **BLUE**, but sunsets are **RED**?

This question may be on the Final Exam (demo with pendulums)

N₂ and **O₂** are small. Therefore quantum electron energy levels are spaced far apart: They absorb at 200 nm, far in UV



Rayleigh scattering efficiency increases as λ^{-4}

$$(700/400)^4 = 9.4$$

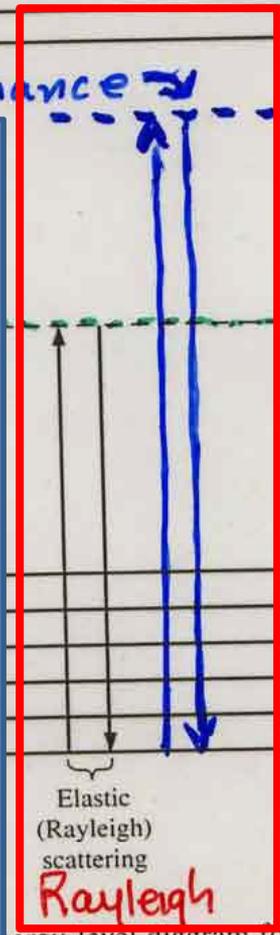
so blue light scatters far more than red;

The scattered sunlight is **greatly enriched in blue**

FIG 10.27

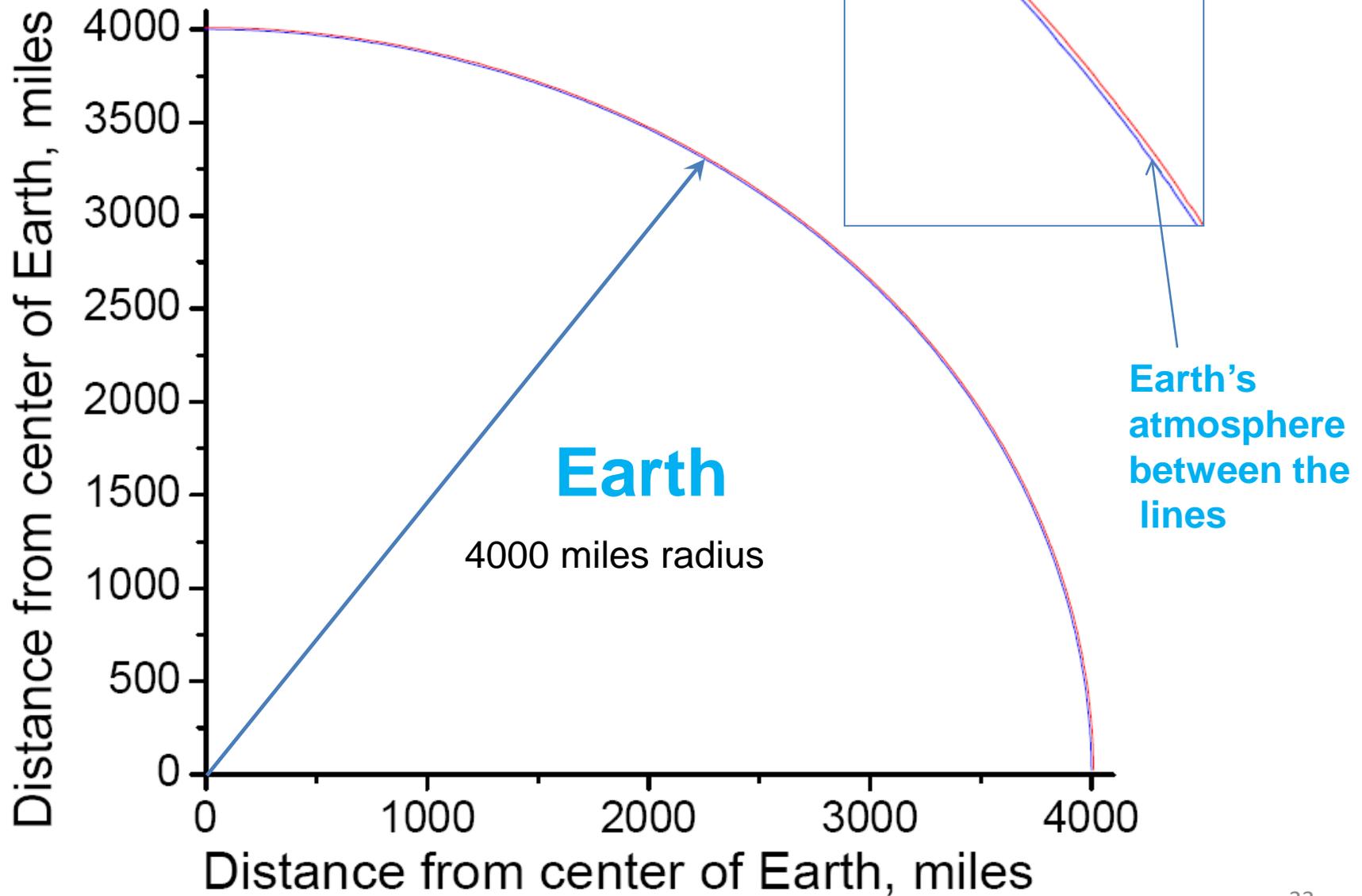
scattering

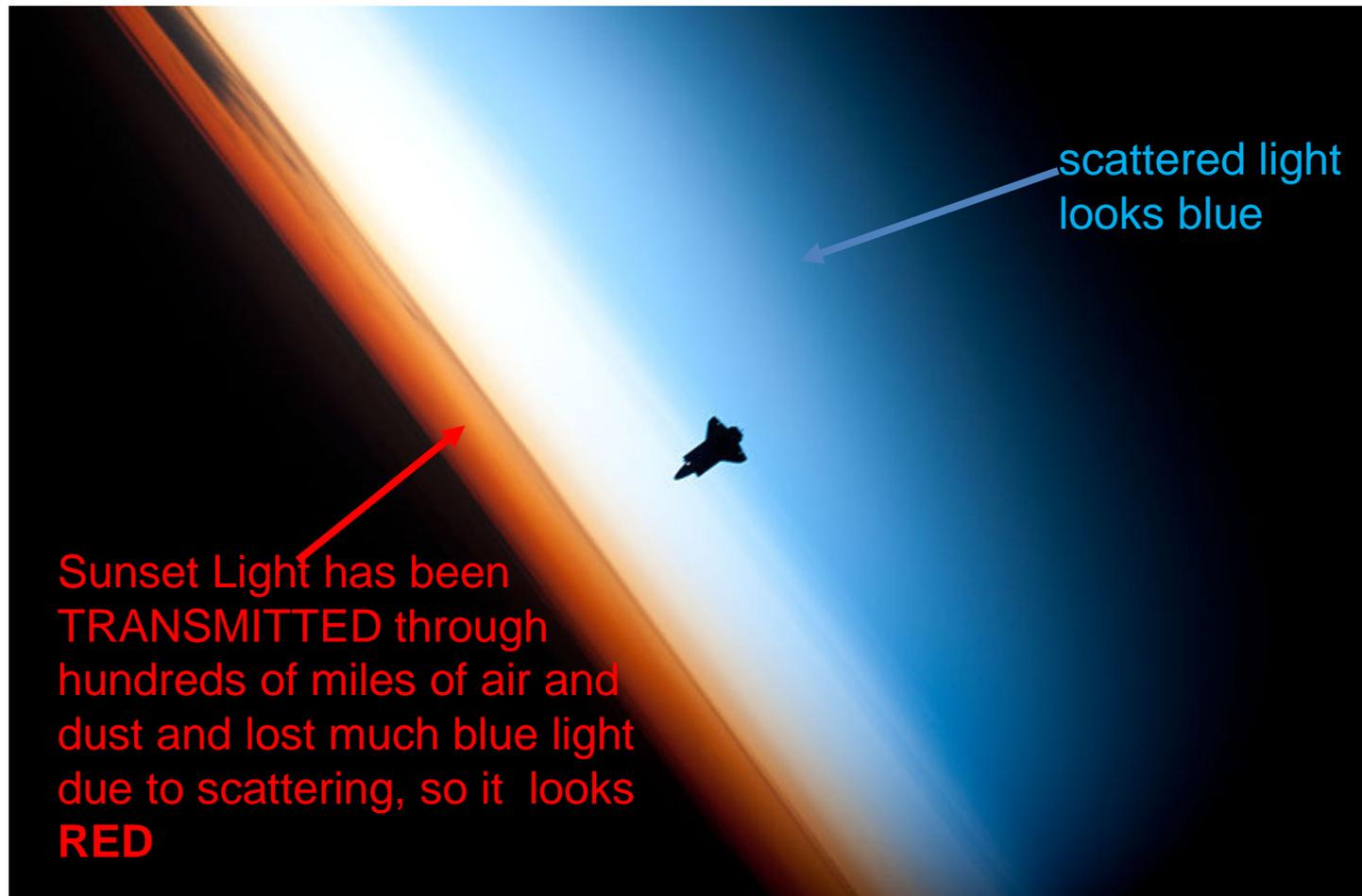
Closer to resonance



energy-level diagram for
inelastic (Raman) scatter
the ground electronic state
transitions are allowed. For elastic scattering
equal to the frequency of the scattered
frequency of the scattered light is different
initial state shown can have any energy; t
of the spectrum.

1. The *pertinent* atmosphere is very thin (from here to Belgrade)





[Space Shuttle Endeavour](#) appearing to straddle the stratosphere and mesosphere. The orange layer is the [troposphere](#), which gives way to the whitish [stratosphere](#) and then the blue [mesosphere](#).^[14] (Why is the troposphere reddish?)