

## 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  $\Delta x$  is the length of the region to which the particle is confined. 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.)

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

$\Delta H$  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.)

# 1925 Schrodinger's Equation:

A simple equation that was **discovered** (not derived), **whose simple solutions contain all the quantum concepts listed above, and much more!**

## Classical Mechanics

Kinetic Energy + Potential Energy = Total Energy

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

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

curvature operation  
(2<sup>nd</sup> derivative)

The diagram shows the Schrodinger equation with various parts annotated by arrows:

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

- An arrow from  $h/2\pi$  points to  $\hbar$ .
- An arrow from "curvature operation (2<sup>nd</sup> derivative)" points to  $\partial^2 \psi / \partial x^2$ .
- An arrow from "mass" points to  $m$ .
- An arrow from "Kinetic energy" points to the entire first term  $-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}$ .
- An arrow from "potential energy" points to  $V(x)$ .
- An arrow from "wavefunction" points to  $\psi$  in  $V(x)\psi$ .
- An arrow from "Total energy" points to  $E$ .

Time independent Schrodinger Equation :

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

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 density for finding particle locations

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

$$i = \sqrt{-1}$$

Potential energy EXACTLY same as in Classical mechanics

Three things are different from Classical mechanics:

1) The **wavefunction** (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"**

# Understanding Quantum Mechanics?

Richard Feynman lecturing to a lay audience at  
Cornell, *circa*. 1965:

“There was a time when the newspapers said that only twelve men understood the theory of relativity. I do not believe there ever was such a time... After they read the paper, quite a lot of people understood the theory of relativity... On the other hand, I think it is safe to say that *no one* “*understands*” *quantum mechanics*... Do not keep saying to your self “But how can it be like that?”, because you will get “down the drain” into a blind alley from whihc nobody has yet escaped. **NOBODY KNOWS HOW IT CAN BE LIKE THAT.** “

--Richard P. Feynman

Chapter 6, *The Character of Physical Law*

23<sup>rd</sup> Printing, 1998

**Feynman, from *Lectures on Physics III* :**

**Quantum Mechanics exactly describes the behavior electrons and light.**

**“Electrons and light do not behave like anything we have ever seen.”**

**“There is one lucky break, however—electrons behave just like light”**

**[FIG 10.27]**

*scattering*

**Excited Electronic State**

*Closer to resonance*

*Different Vibs*

**Virtual state**

**Light is not absorbed**

*Vibrational energy levels & states*

*Abs.*

**Ground Electronic State**

Infrared absorption

Elastic (Rayleigh) scattering

Inelastic (Raman) scattering

Resonance Raman scattering

**IR**

**Rayleigh**

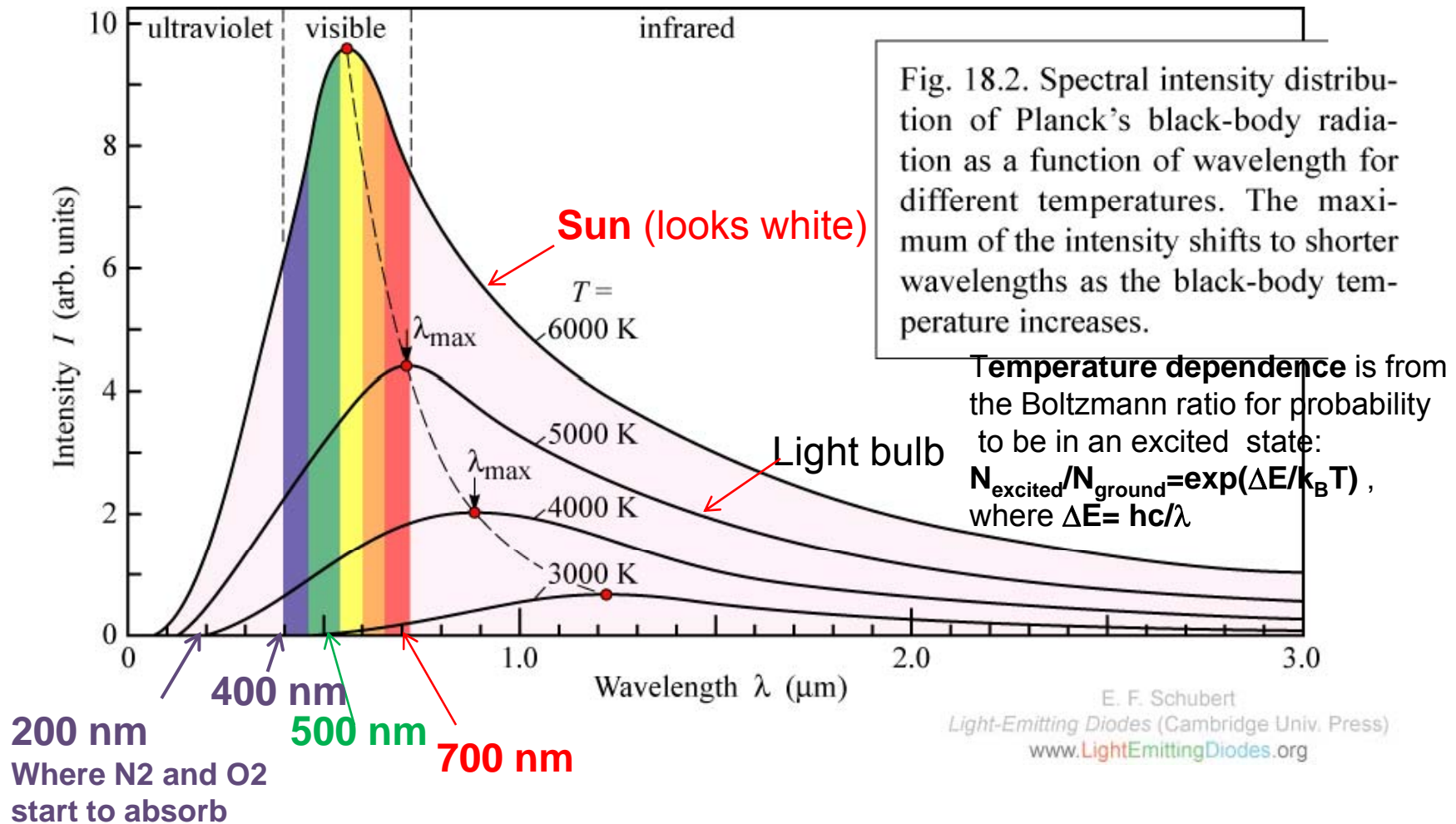
**Raman**

**Resonance Raman**

**Fig. 10.41** Energy-level diagram for infrared absorption, elastic (Rayleigh) scattering, and inelastic (Raman) scattering. Transitions between vibrational energy levels of the ground electronic state absorb infrared radiation; not all transitions are allowed. For elastic scattering the frequency of the incident light is equal to the frequency of the scattered light. For inelastic scattering the frequency of the scattered light is different from that of the incident light. The virtual state shown can have any energy; the scattering of light occurs in any region of the spectrum.

*~ 1000 times enhanced.*

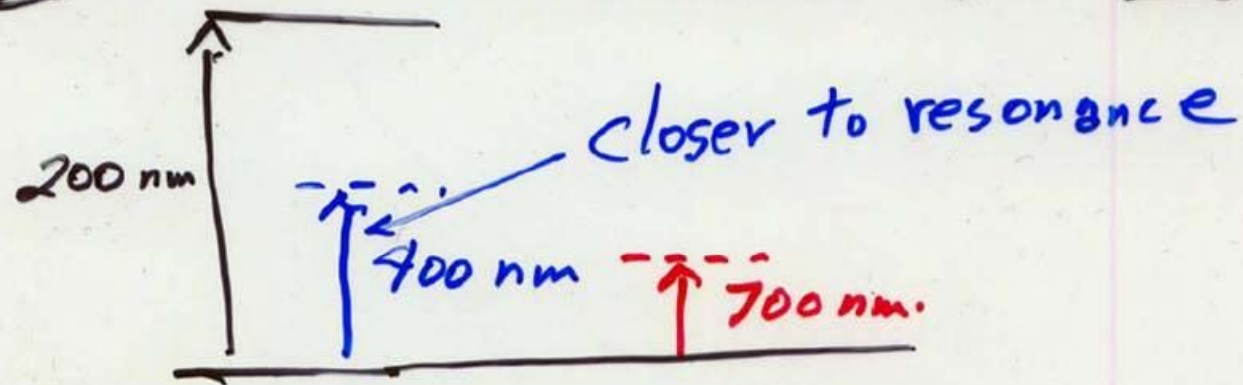
Light emitted by all objects not at 0 Kelvin.





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

$N_2$  &  $O_2$  resonance at  $\sim 200$  nm

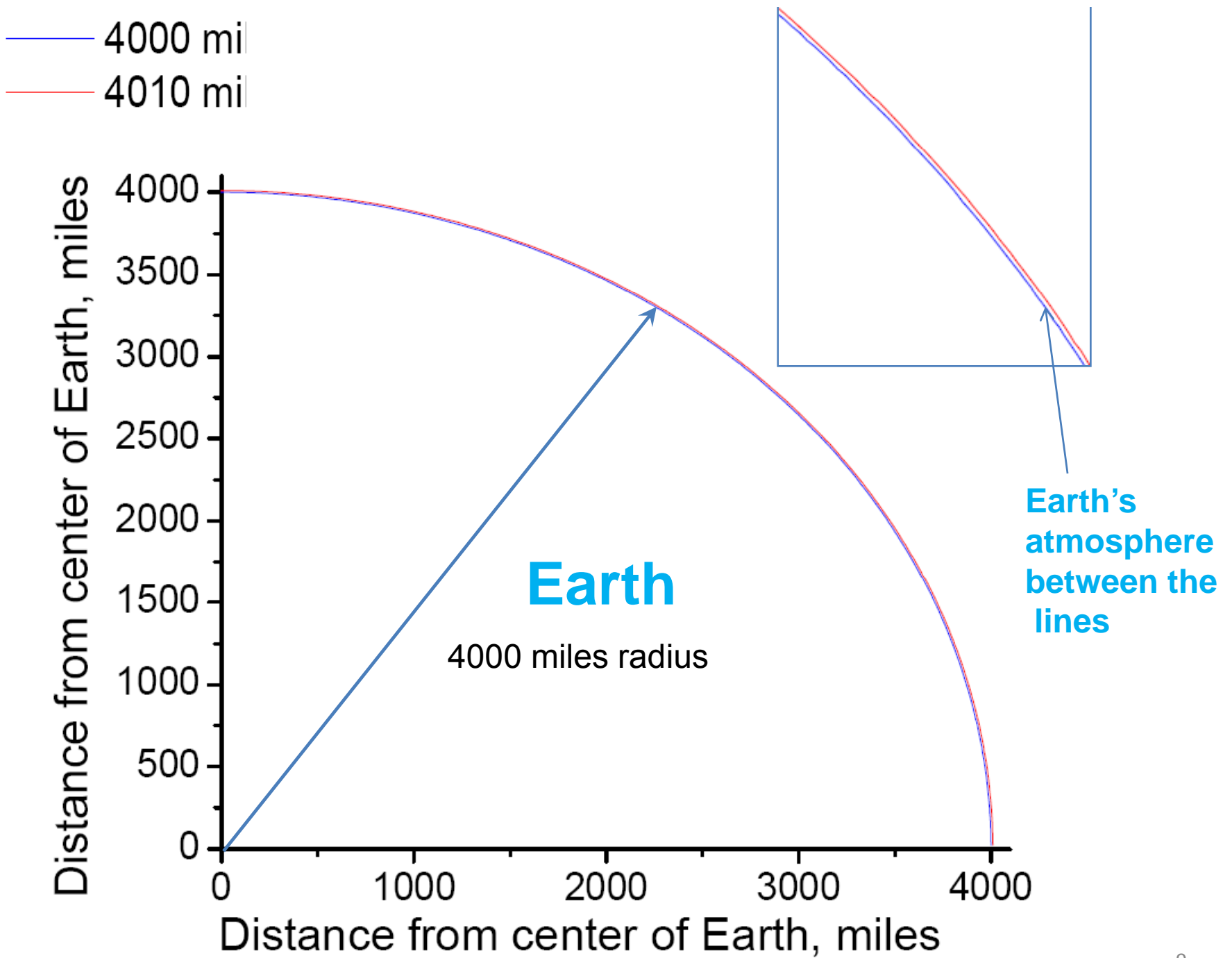


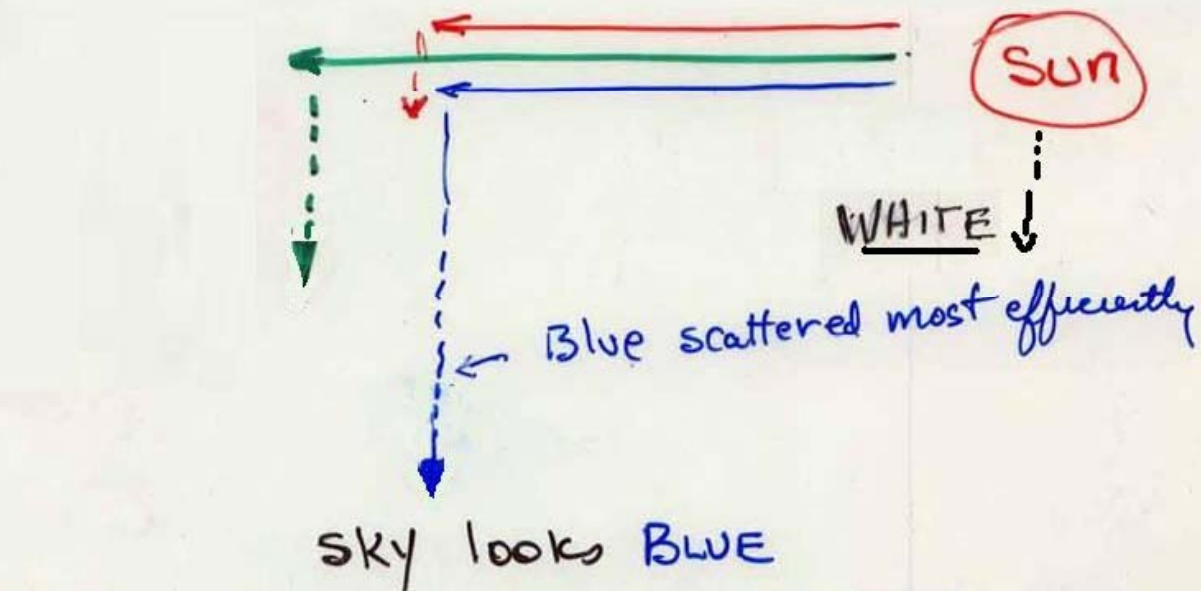
Rayleigh scattering efficiency increases

as  $\frac{1}{\lambda^4}$

$$\left(\frac{7}{4}\right)^4 \approx 9$$







WHAT IS TRANSMITTED ?



LOOKS REDDISH at SUNSET, but..

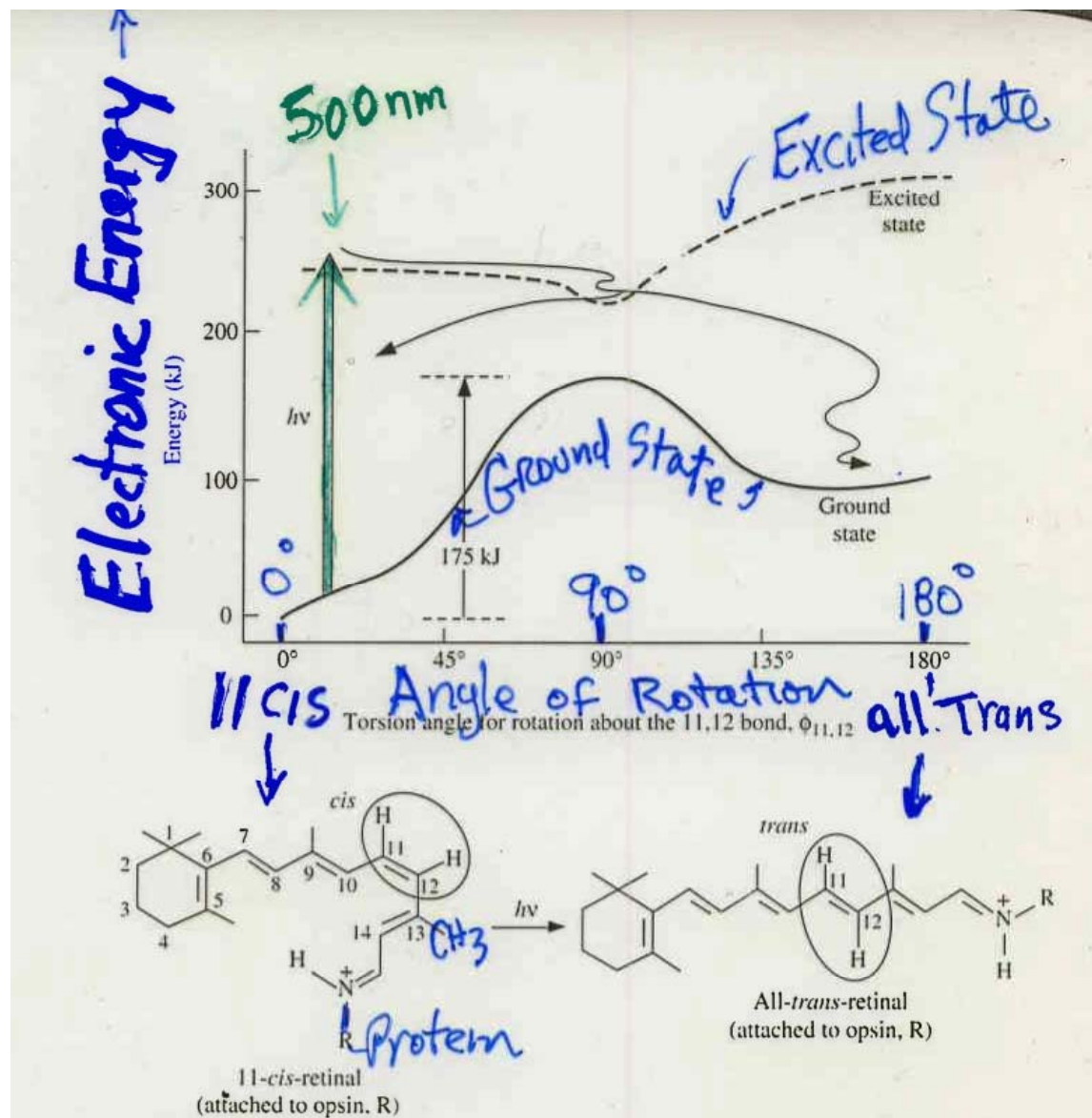
why does Sun look white at noon?

Why is steam white, but smoke, and viruses are blue?

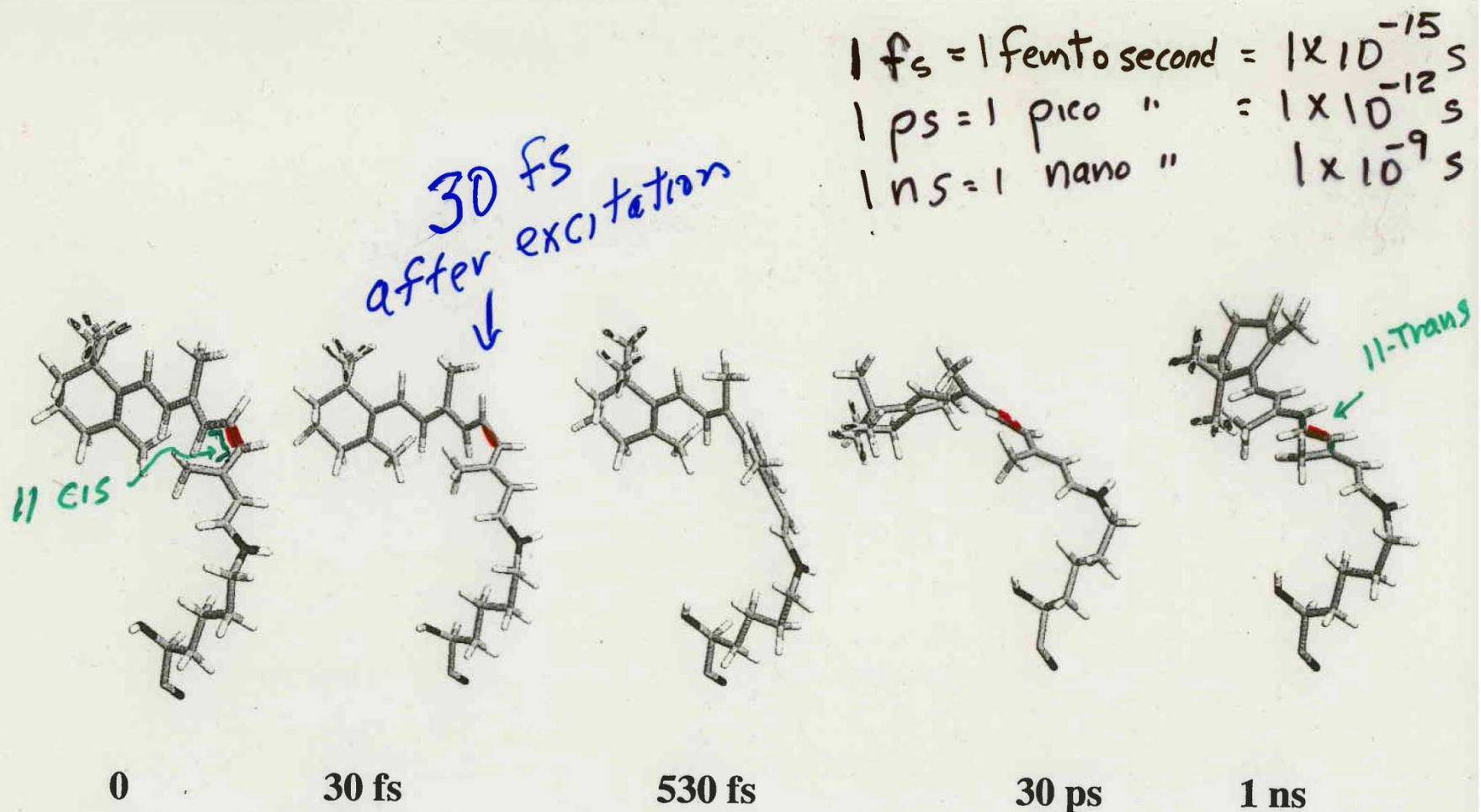
- G-Protein-Coupled receptors have emerged over the last 20 years as a MAJOR biological signaling motif--constituting perhaps 10% of the human genome, and the target of 60% of commercial drug research .

- Examples:

<u>Receptor</u>	<u>Mediates</u>	<u>Drug/Hormone (ligand)</u>
Adrenergic	hypertension	beta blockers/adrenaline
Cannabinoid	lots of things	marijuana
..... dozens more		
Rhodopsin	vision	retinal Schiff base + light



**Fig. 9.1** Light-driven isomerization of 11-*cis*-retinal attached to opsin (R) by a Schiff's base linkage. Theoretical calculations of the energy of both the ground state and an excited electronic state suggest a possible path whereby absorption of a photon will lead to conversion from the *cis* to the *trans* configuration about 60% of the time. The angle of rotation about the 11,12-double bond is plotted as the horizontal axis.



**Snapshots of simulated isomerization of retinal Schiff base of rhodopsin (1hxx)**

(Sterling Paramore\* and Patrik Callis, unpublished results)

\* Research Experience for Undergraduates (REU) student, summer 2000