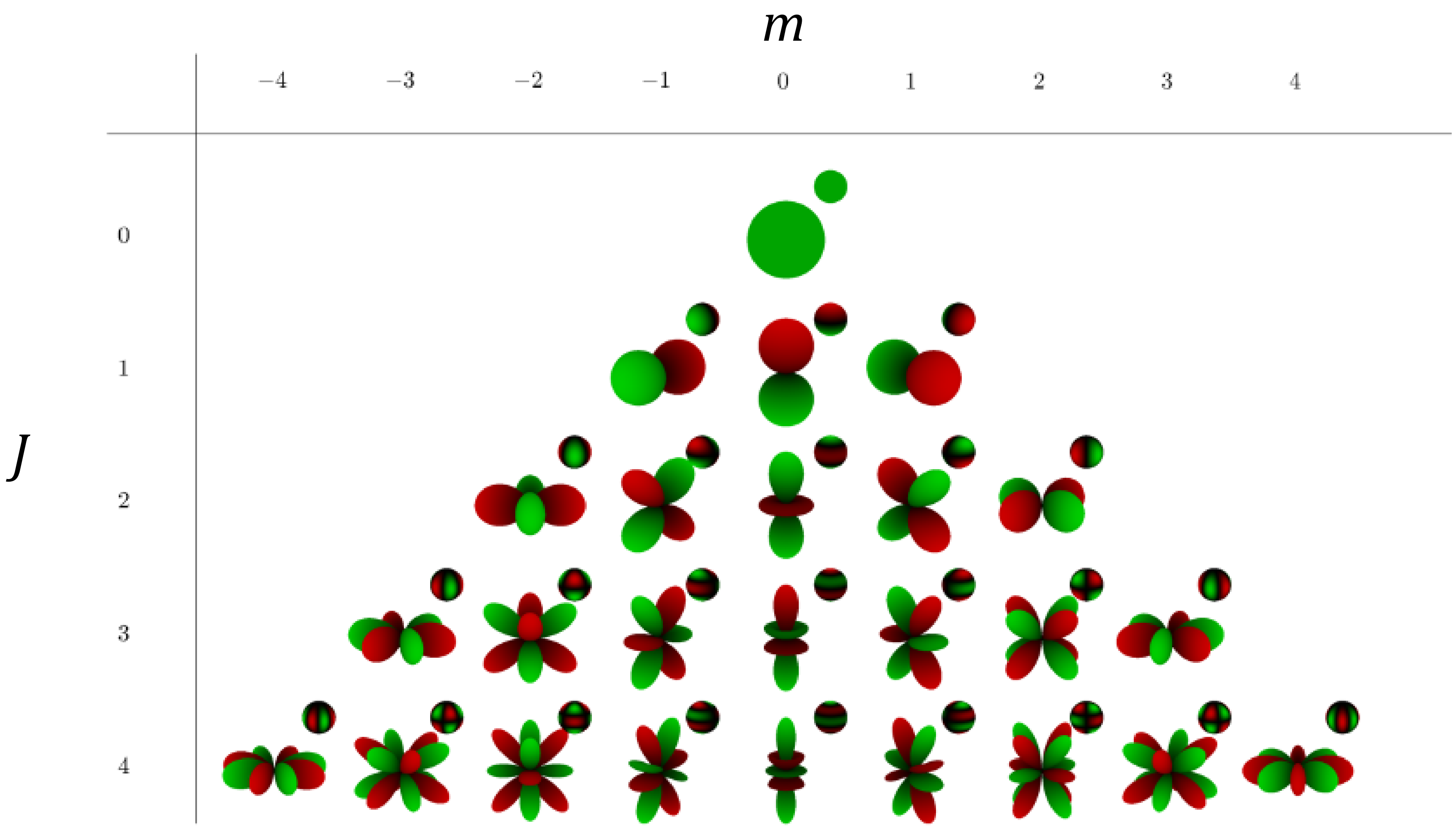
Take another look at the spatial distributions of the wavefunction solutions to the rigid rotor Hamiltonian - the spherical harmonics.

A. What information does the quantum number J encode?

B. What information does the quantum number m encode?

$$Y_J^m(\theta, \phi)$$



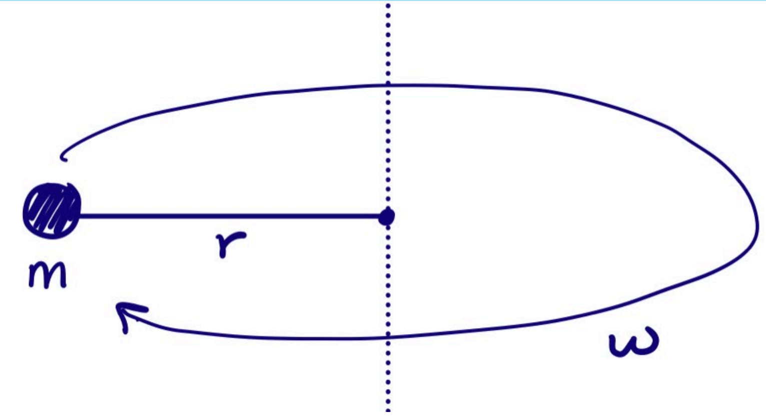
CHM 305 The Quantum World

Lecture 11: Molecular Spectroscopy

McQuarrie Ch. 5, 6

Last time we talked about: angular momentum

- Lay out definitions for classical circular motion and angular momentum



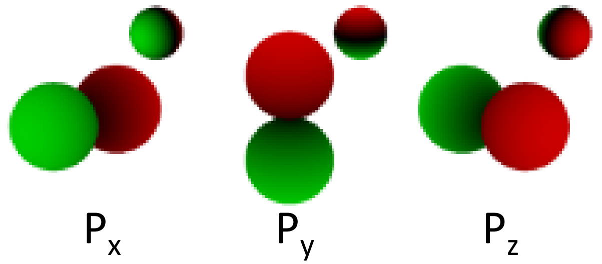
- Discuss rotations of classical and quantum mechanical rigid bodies

- Write down the Schrodinger equation and its solutions for the quantum rigid rotor in spherical coordinates

$$\hat{H} = -\frac{\hbar^2}{2\mu}\nabla^2$$

$$\hat{H}\psi(\theta,\phi) = E\psi(\theta,\phi)$$

- Make connections to rotations of diatomic molecules and the hydrogen atom



Road map for today's lecture

Overall goal: use harmonic oscillator and rigid rotor to model the frequencies of light that molecules absorb

1. Harmonic oscillator ↔ vibrational/infrared spectroscopy
   transition energies, selection rules
   beyond the HO approximation (anharmonicity)

2. Rigid rotor ↔ rotational/microwave spectroscopy
   transition energies, selection rules
   beyond the rigid rotor approximation (centrifugal distortion)

2. Harmonic oscillator-rigid rotor ↔ rovibrational spectroscopy
   and rotation-vibration interaction

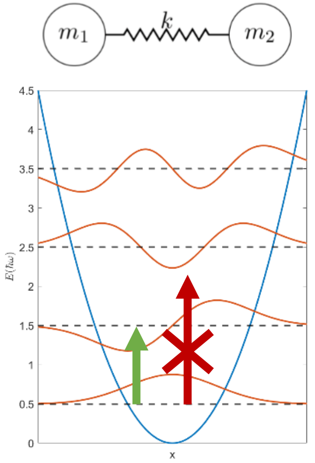
The basic principle of absorption spectroscopy

source of
light with tunable
energy

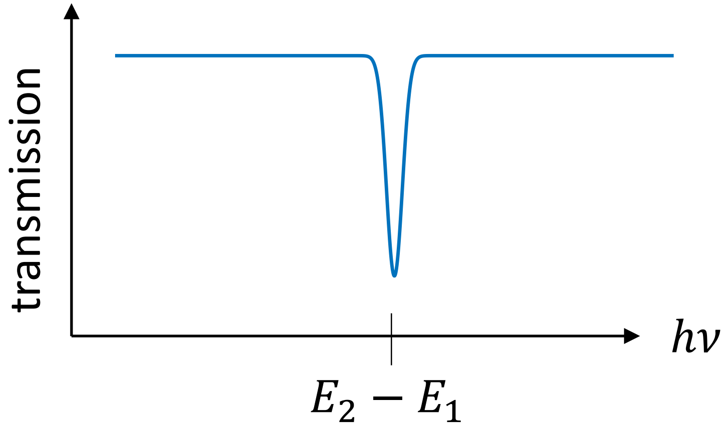
$$E = h\nu$$

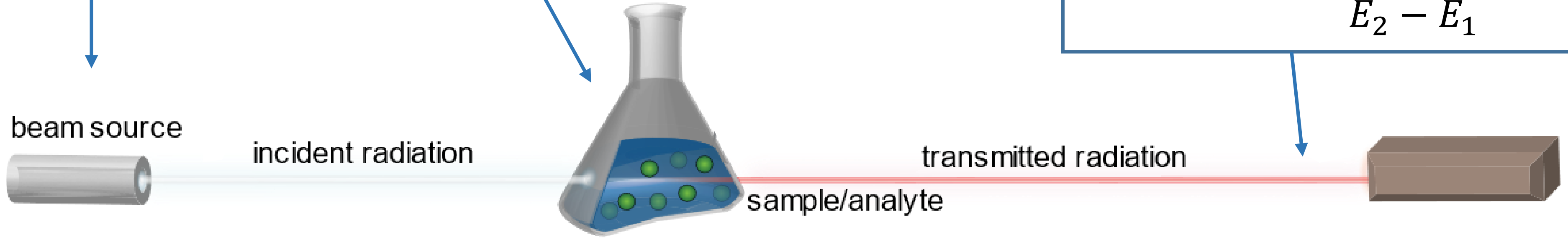
light can drive a transition between states 1 and 2 if

$$E_2 - E_1 = h\nu$$



scan the frequency of light to record an absorption spectrum

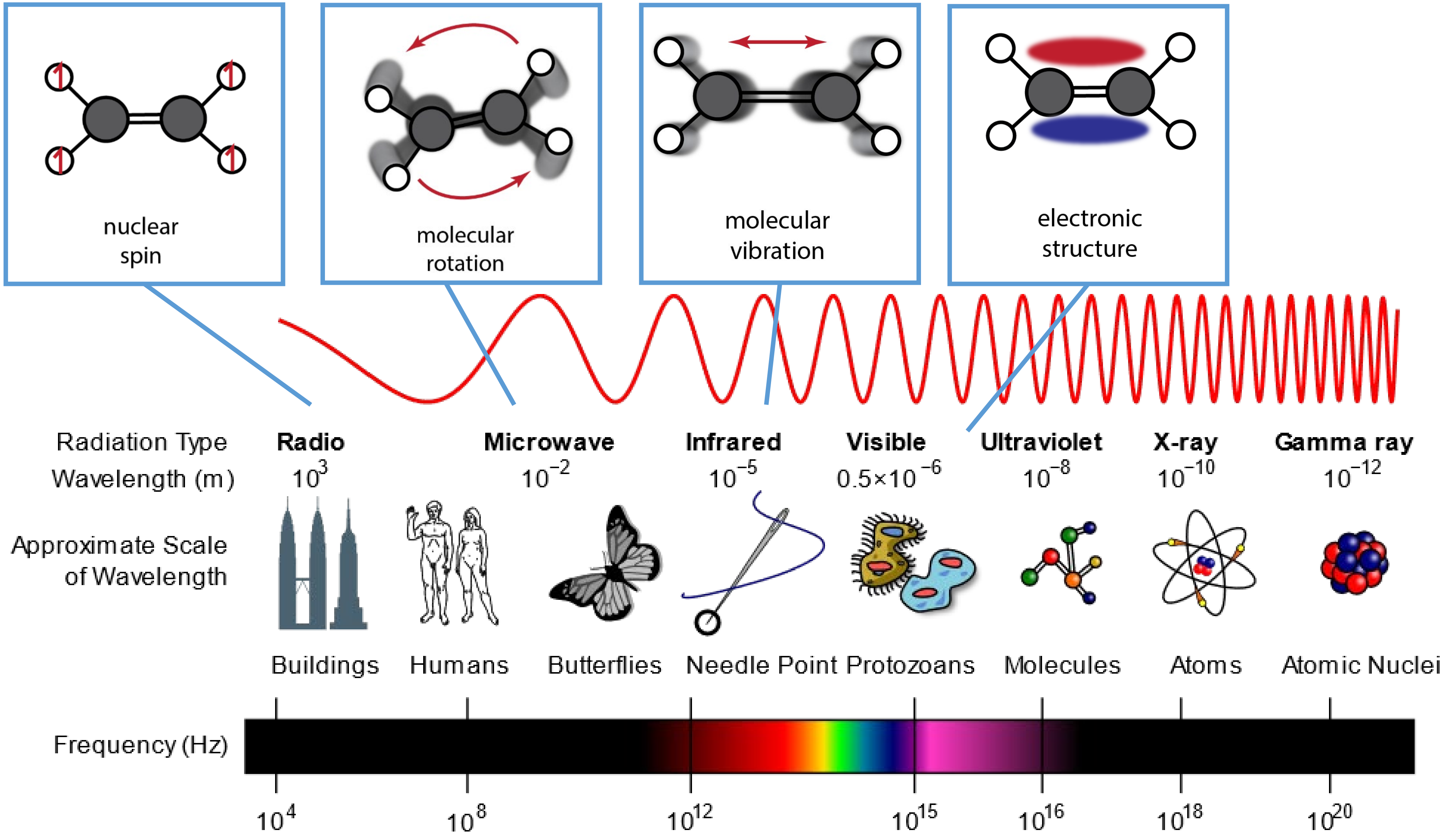




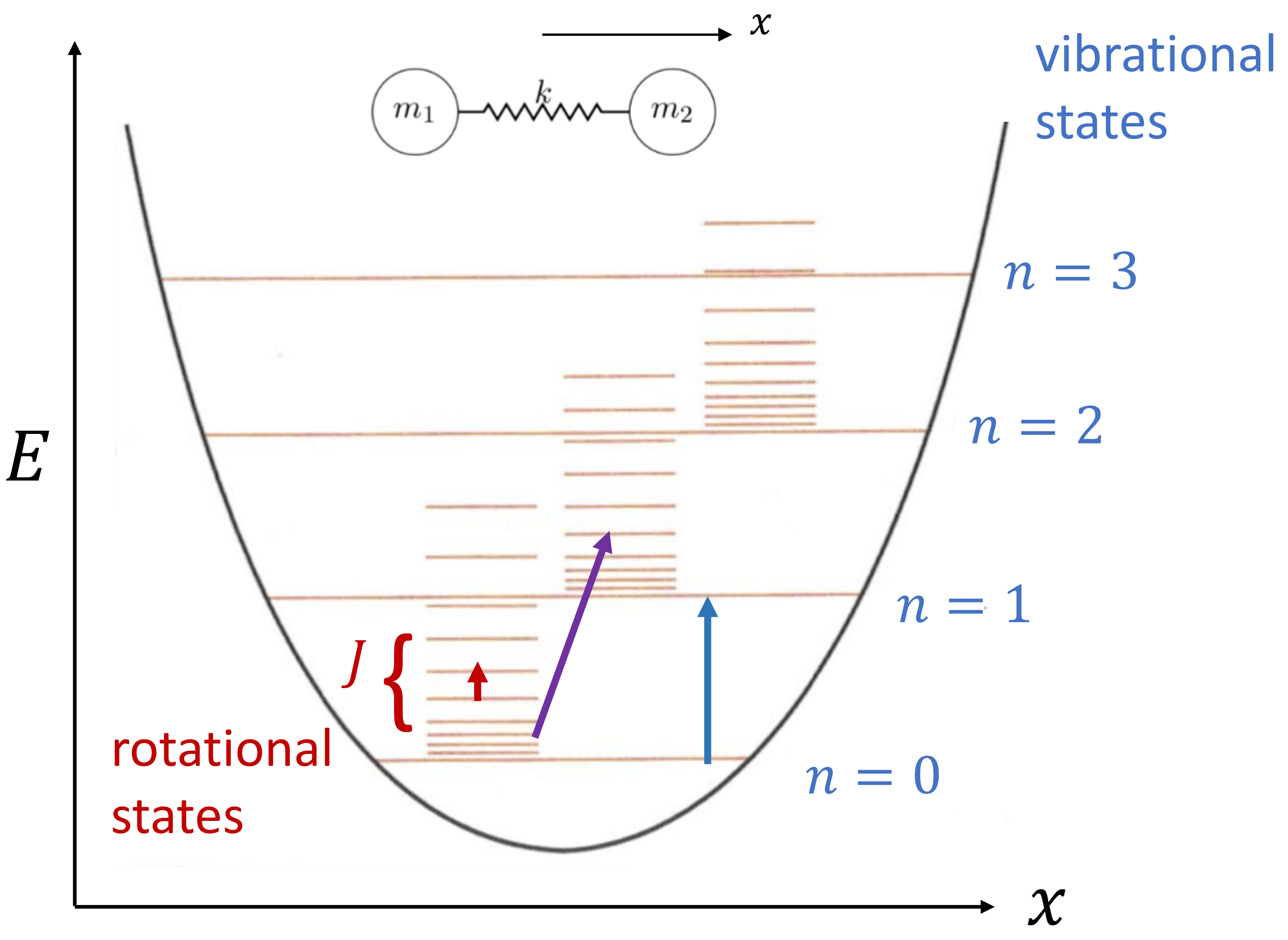
Emission **Absorption** **Transmission** **Detection**

https://commons.wikimedia.org/w/index.php?curid=12659294

Different frequencies of light drive different molecular transitions



Rovibrational transitions



Vibrations

- Harmonic oscillator model
- Transitions driven by infrared light = IR spectroscopy

Rotations

- Rigid rotor model
- Transitions driven by microwave light = microwave spectroscopy

Can also drive “rovibrational” transitions that change both n and J quantum numbers