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?
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
- 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

[Diagram showing emission, absorption, transmission, and detection processes]
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