Selection Rules:

Selection Rules

- Each of the spectroscopies have associated selection rules.
- Selection rules originate from the quantum mechanical description of electromagnetic radiation interaction with matter.
- Use time-dependent perturbation theory to derive probability of excitation between two states.
- Consider a two-level system

General Properties

- Wavefunctions are
- Wavefunctions are eigenstates of a specific operator

Iclicker: Eigenstates

- Which of the following functions are eigenstates of the hamiltonian, $\hat{H}_o = d/dx$
  - A - $\Psi = x$
  - B - $\Psi = x^2$
  - C - $\Psi = e^x$
  - D - $\Psi = e^{x^2}$

Perturbative Hamiltonian

- Apply perturbation theory
- $\hat{H}_o$ is independent of time.
- Separated time and spatial parts
- Interaction with radiation is represented by perturbative component
- $\hat{H}_1$ depends on time and radiation.

Total wavefunction

- Total wavefunction a linear combination of eigenstates
- Probability of finding system in state 2 at time t is given by

Excitation Probability (1)

- Evaluate time-dependent Schrodinger equation to determine excitation probability

Excitation Probability (2)

- Evaluate time-dependent Schrodinger equation to determine excitation probability

Excitation Probability (3)

- Evaluate time-dependent Schrodinger equation to determine excitation probability

Rotational Selection Rules (1)

- Selection rule comes from

Rotational Selection Rules (2)

- Selection rule comes from

- Summary

Harmonic Oscillator Selection Rules (1)

- Selection rule comes from

Harmonic Oscillator Selection Rules (2)

- Selection rule comes from

- Summary