# Nuclear Magnetic Resonance

# Transition Moment Integral

- Probability of an excitation
- Hamiltonian $\hat{H}_1$ defined as

# Selection Rules

- Selection rules developed using perturbation theory as before (rotations and vibrations)

- Assume field lies along each direction and determine excitation probability

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# Ladder Operators

- a and b are eigenstates of $I^2$ and $I_z$ but not $I_x$ and $I_y$.
- Rewrite in terms of raising and lowering operators.

- Redefine $I_x$.

# Transition Moment Integral

- Use ladder operator to evaluate integral.

- Ladder operator results.

# Transition Moment Integral

- Evaluate integral.

- Selection Rules

# Shielding

- NMR spectroscopy is useful based on sensitivity to “local” chemical environment.
- Consider benzene molecule

- Introduce the concept of a chemical shift

# Chemical Shift

- Desire to compare data from machines with different magnetic fields.
- Calibrate spectra in ppm relative to standard reference

- Chemical shift scale

- Chemical shift example

# Chemical Shift

- Difference between chemical shifts is independent of field strength

- NMR difference example

# Representative Chemical Shifts

- Different types of chemical environments show different chemical shifts (Table 14.3 from book).

| Compound | Proton | Example | d |
|---|---|---|---|
| Alkane | $R_2CH_2$ | $(CH_3)_2C\underline{H}_2$ | 1.2 – 1.4 |
| Aromatic | ArH | Benzene | 6.0 – 8.5 |
| Chloroalkane | $RCH_2Cl$ | $CH_3C\underline{H}_2Cl$ | 3.4 – 3.8 |
| Ether | $ROCH_2R$ | $CH_3OC\underline{H}_2CH_3$ | 3.3 – 3.9 |