Physics 224
The Interstellar Medium

Lecture #4

- Part I: Order of Magnitude Atomic/Molecular Energy Levels

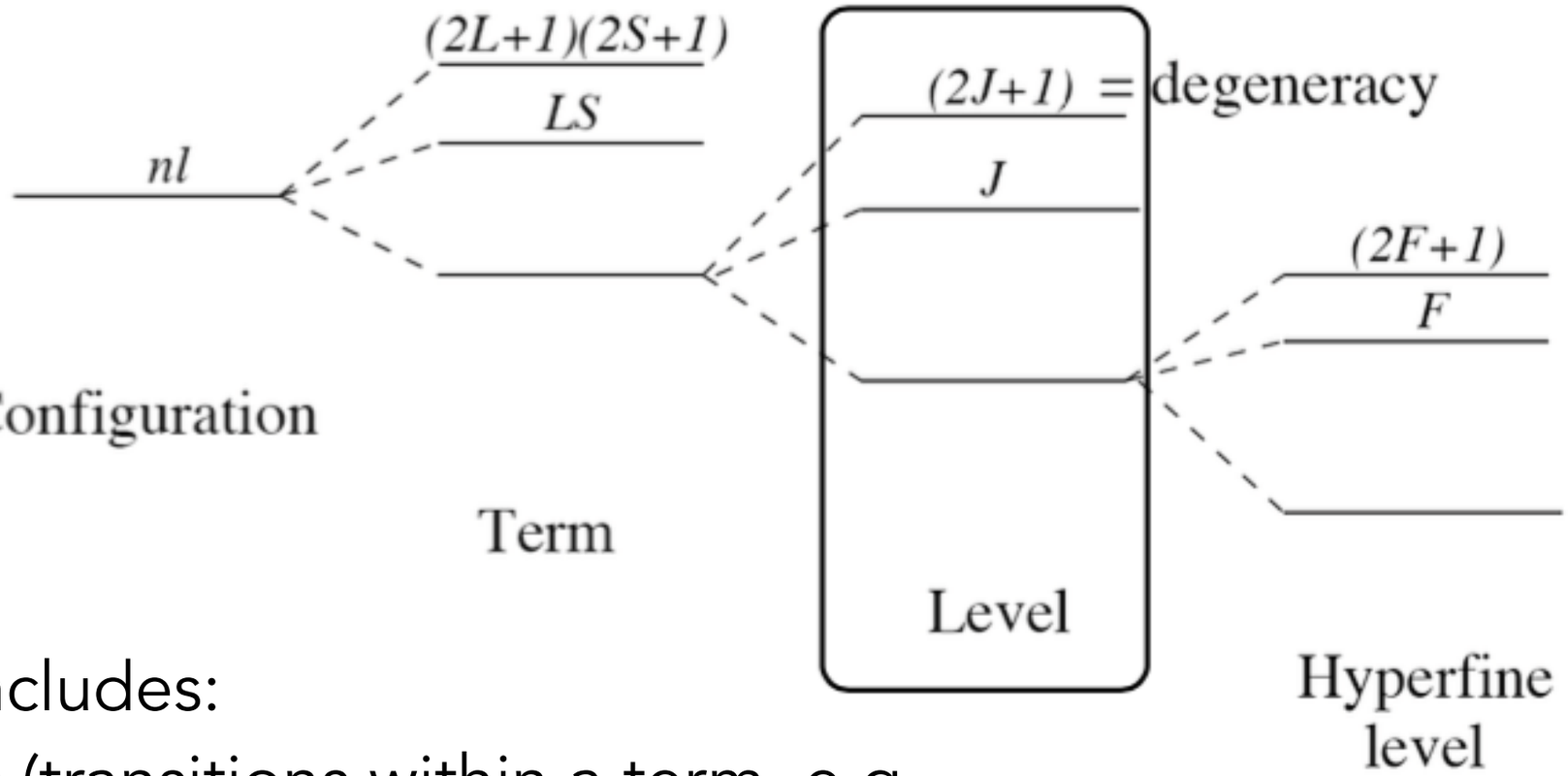
- Part II: Transitions between Energy Levels

- Part III: Line Profiles

Type	Mechanism	Rules
“allowed"	electric dipole	1) Parity must change 2) ΔL = 0, ±1 3) ΔJ = 0, ±1 but not J=0→0 4) only one e- wavefunction $\boldsymbol{nl}$ changes with $\Delta\boldsymbol{l}$ = ±1 5) ΔS = 0
“semi-forbidden”	electric dipole but with ΔS ≠ 0 from configuration mixing due to relativistic effects	same as “allowed” except violates #5
“forbidden"	magnetic dipole or electric quadrupole	violates at least one other selection rule other than #5

Fine and Hyperfine Structure Transitions

Fine & Hyperfine are "forbidden"



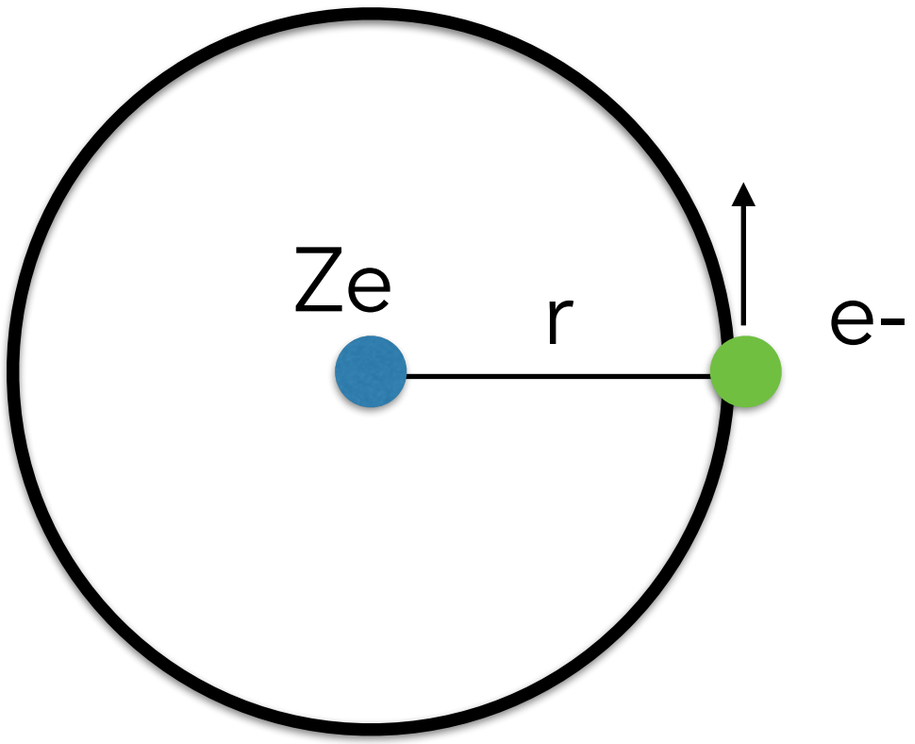
Includes:

-fine structure transitions (transitions within a term, e.g. $^2P_{1/2}$ - $^2P_{3/2}$ 158μm line of [CII] within ^2P term)

-hyperfine structure transitions (transitions within a given level of a term caused by splitting due to interaction of electron & nuclear spin, e.g. HI 21 cm spin-flip transition)

Order of Magnitude Energy Levels

Classical non-relativistic atom



First
"allowed transitions"

Coulomb interactions
between e- and nucleus

Order of Magnitude Energy Levels

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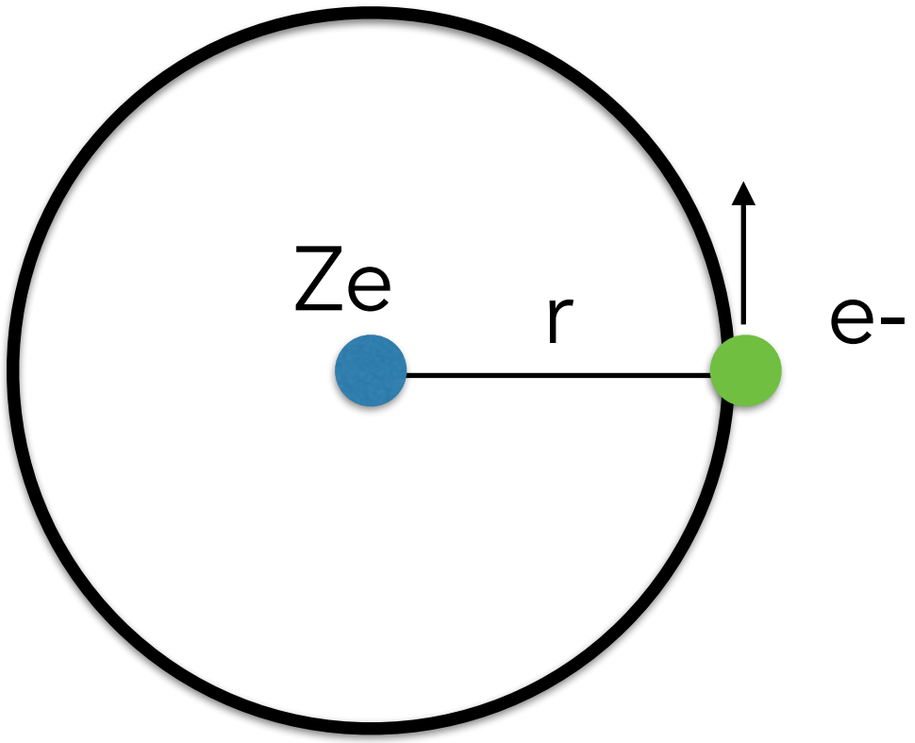

First
"allowed transitions"

Coulomb interactions between e- and nucleus

$E \sim 13.6\ eV\ (Z^2/n^2)$

Order of Magnitude Energy Levels

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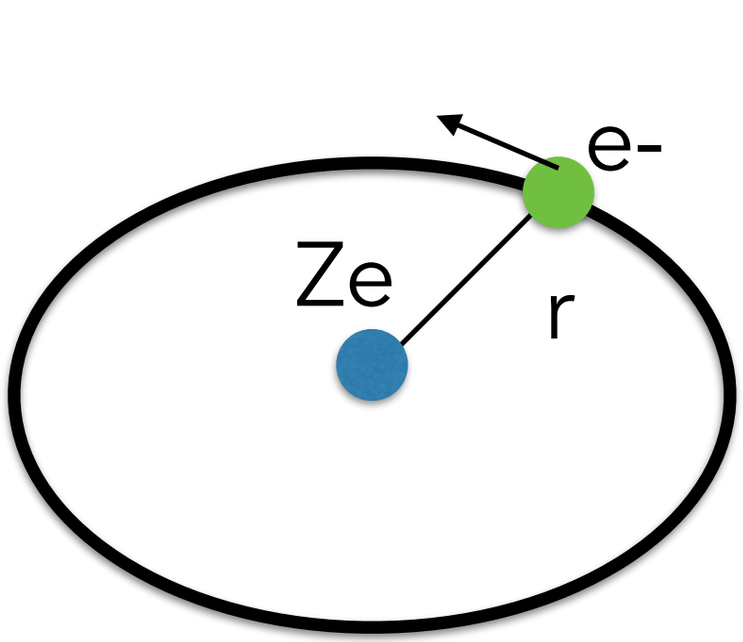
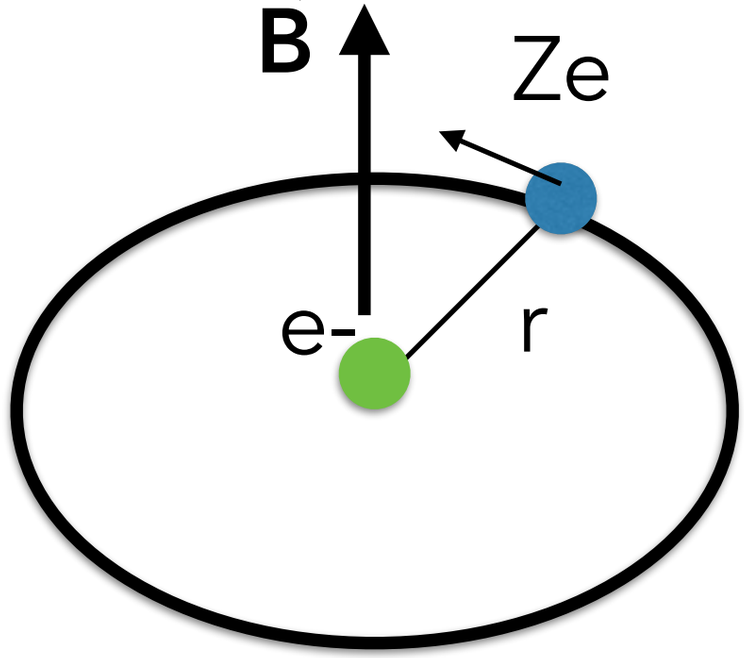


from nucleus's point of view

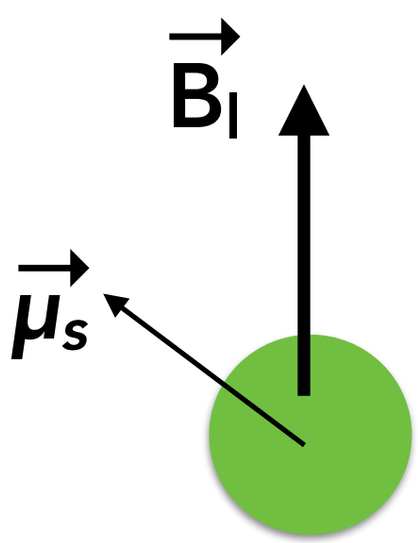
→



from e- point of view
orbiting proton generates B-field

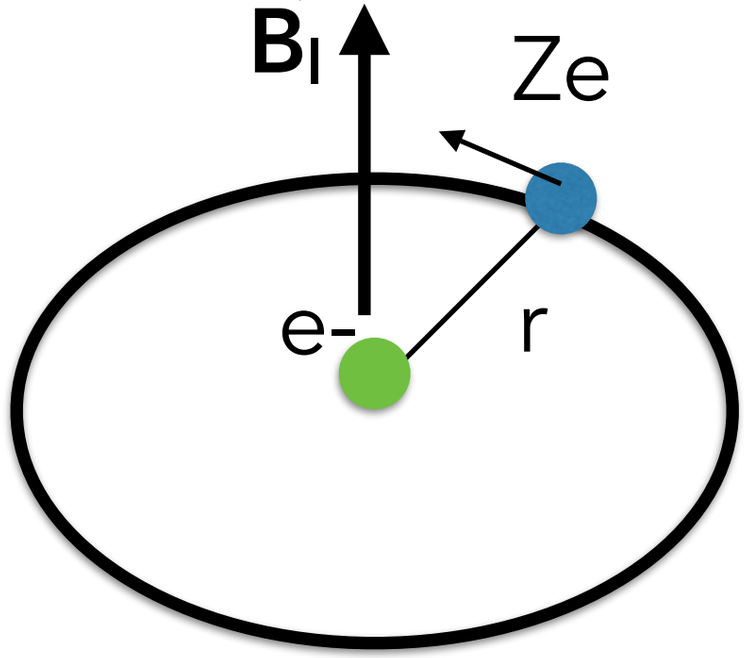
Order of Magnitude Energy Levels

Classical non-relativistic atom



spin magnetic moment of electron interacts with orbit B-field

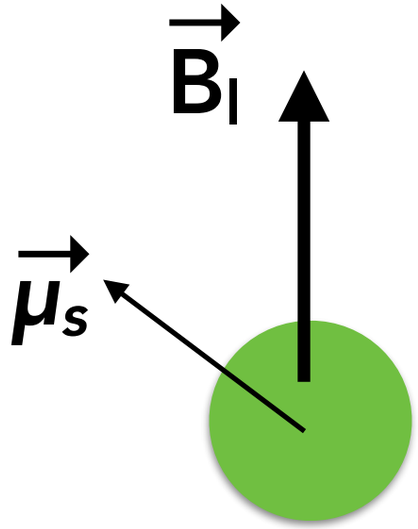
Spin-Orbit coupling!



from e- point of view orbiting proton generates B-field

Order of Magnitude Energy Levels

Classical non-relativistic atom



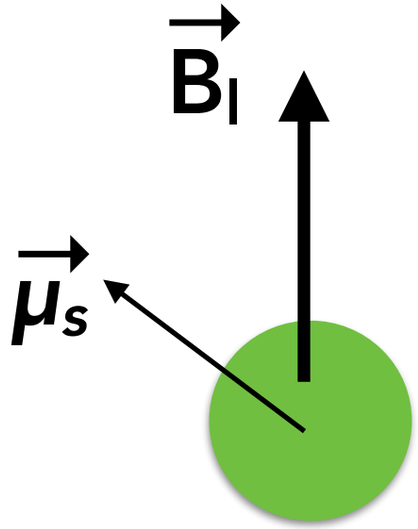
spin magnetic moment of electron interacts with orbit B-field

"fine structure" transitions

interaction between spin and angular momentum of e-

Order of Magnitude Energy Levels

Classical non-relativistic atom



spin magnetic moment of electron interacts with orbit B-field

"fine structure" transitions

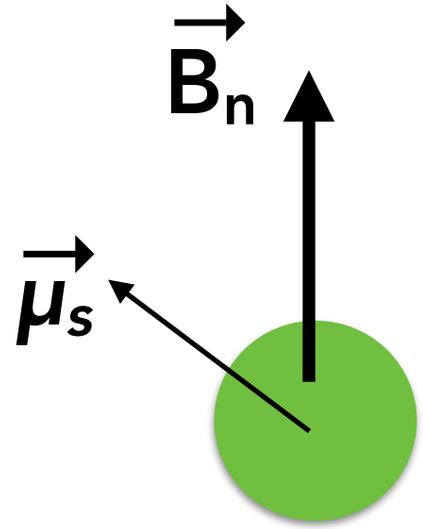
interaction between spin and angular momentum of e-

E ~ 13.6 eV ($\alpha^2 Z^4/n^5$)

Order of Magnitude Energy Levels

Classical non-relativistic atom

→



spin magnetic moment of electron interacts with B-field from nuclear spin

"hyperfine structure" transitions

interaction between magnetic moments of nucleus and e-

Order of Magnitude Energy Levels

Classical non-relativistic atom

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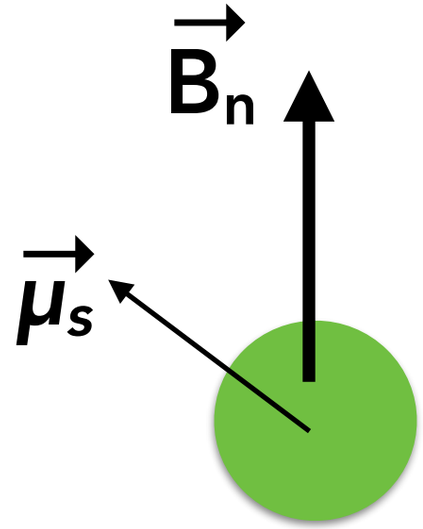


spin magnetic moment of electron interacts with B-field from nuclear spin

"hyperfine structure" transitions

interaction between magnetic moments of nucleus and e-

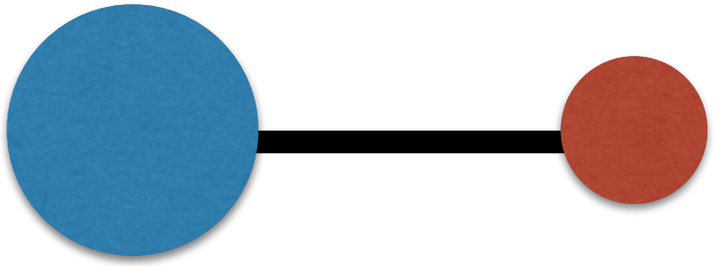
$E \sim 13.6\ eV\ (m_e/m_n)(\alpha^2 Z^4/n^5)$

Order of Magnitude Energy Levels

"Allowed" Electric Dipole	E ~ 13.6 eV (Z^2/n^2)
"Forbidden" Fine Structure	E ~ 13.6 eV ($\alpha^2 Z^4/n^5$)
"Forbidden" Hyperfine Structure	E ~ 13.6 eV (m_e/m_n)($\alpha^2 Z^4/n^5$)

Order of Magnitude Molecular Energy Levels

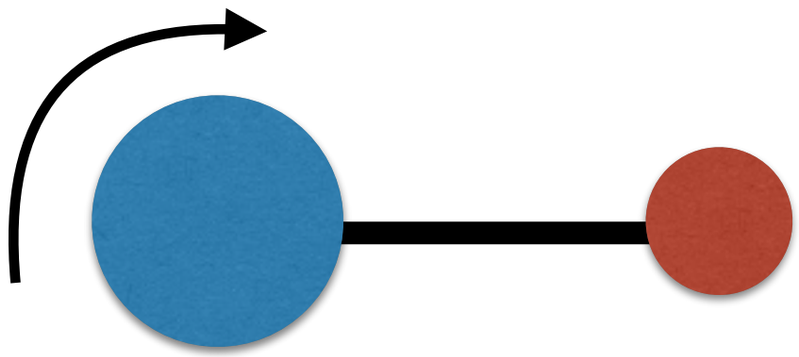
Cover diatomic molecules, read Draine ch 5 for more detailed info.



1) Electronic Transitions of e-

Order of Magnitude Molecular Energy Levels

Cover diatomic molecules, read Draine ch 5 for more detailed info.

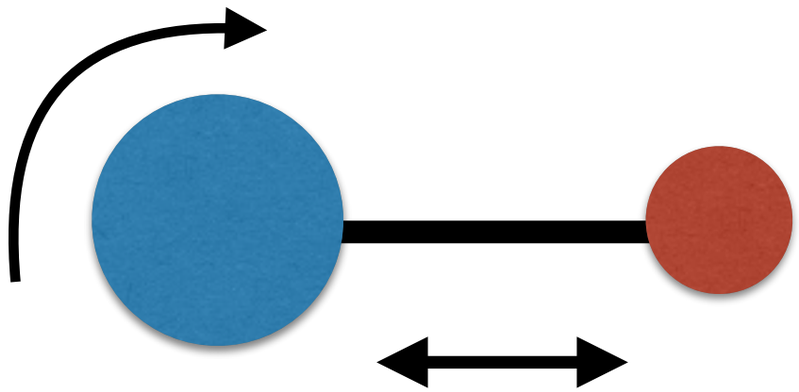


1) Electronic Transitions of e-

2) Rotational Transitions

Order of Magnitude Molecular Energy Levels

Cover diatomic molecules, read Draine ch 5 for more detailed info.



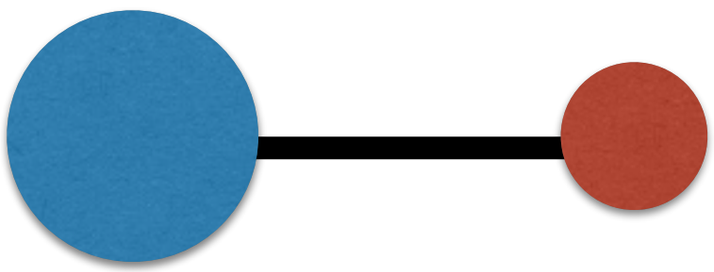
1) Electronic Transitions of e-

2) Rotational Transitions

3) Vibrational Transitions

Order of Magnitude
Molecular Energy Levels

Typical energies

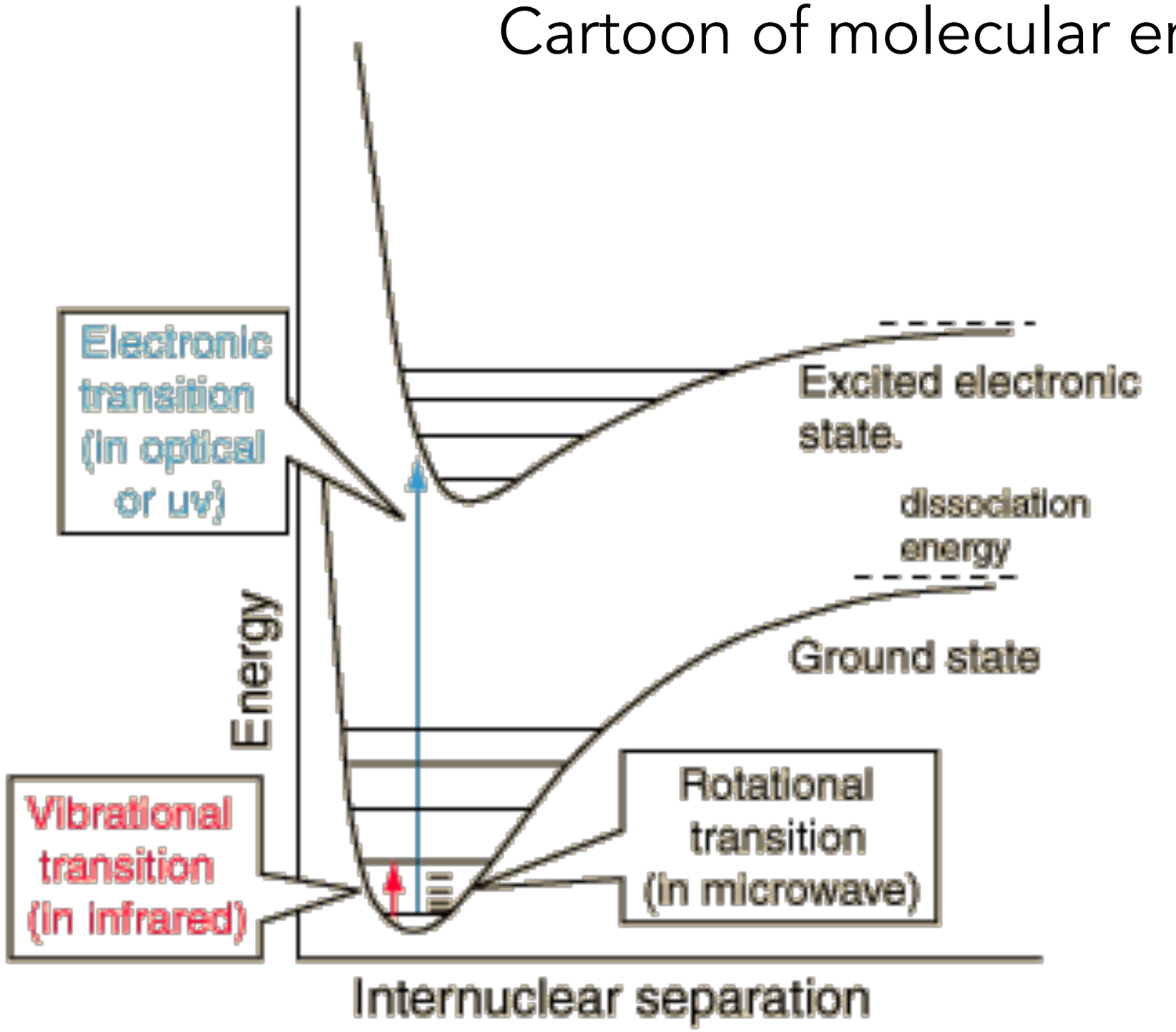


$$E \sim E_{rot} + E_{vib} + E_{el}$$

10^{-3}-10^{-2} eV 10^{-2}-10^{-1} eV 1-10 eV

Electrons move much more quickly than nuclei
so for rotation/vibration calculations we can average over
the electron transitions (Born-Oppenheimer approximation)

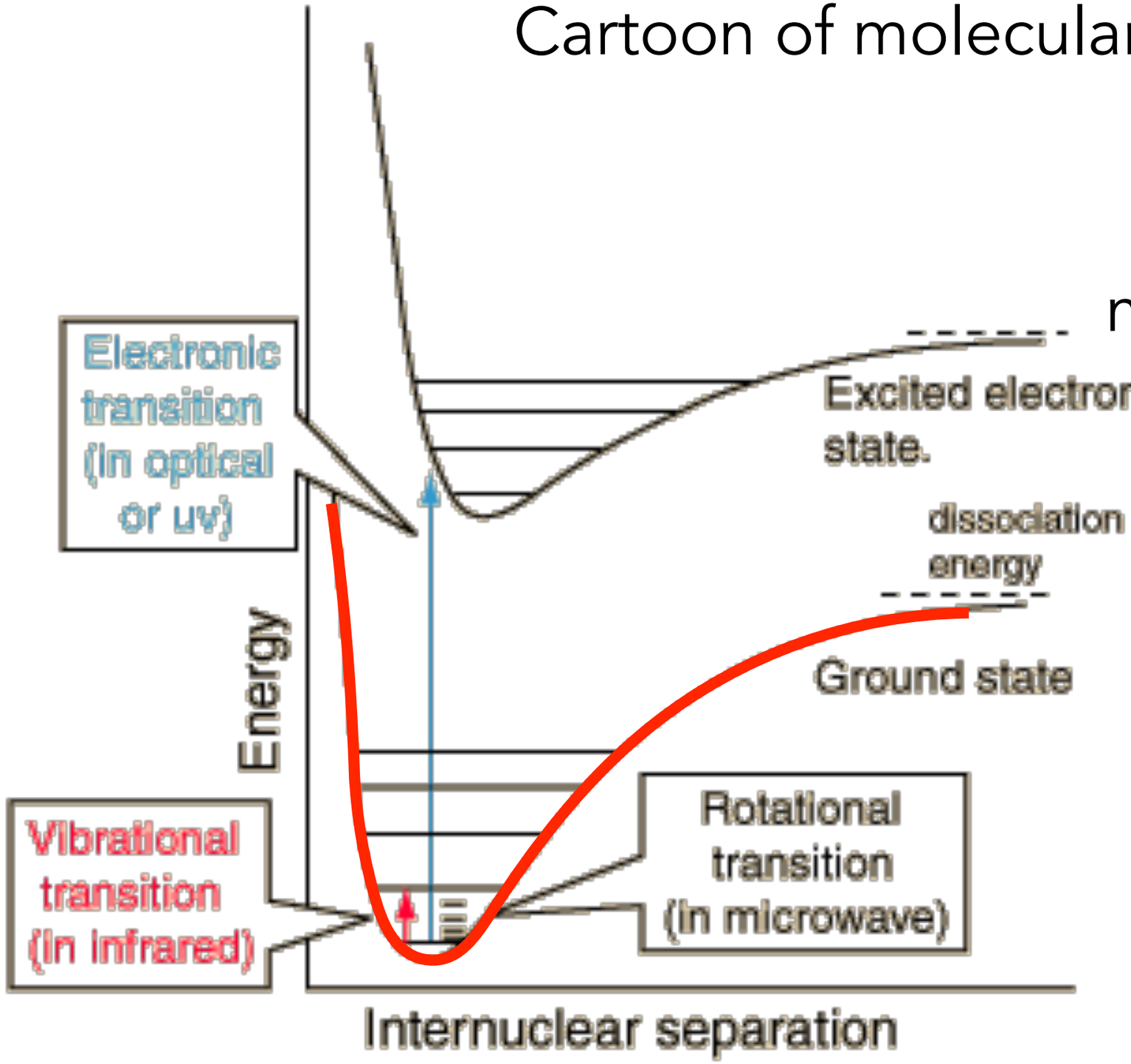
Cartoon of molecular energy levels



http://hyperphysics.phy-astr.gsu.edu/hbase/molecule/molec.html

Cartoon of molecular energy levels

Basic structure of molecule sets this curve



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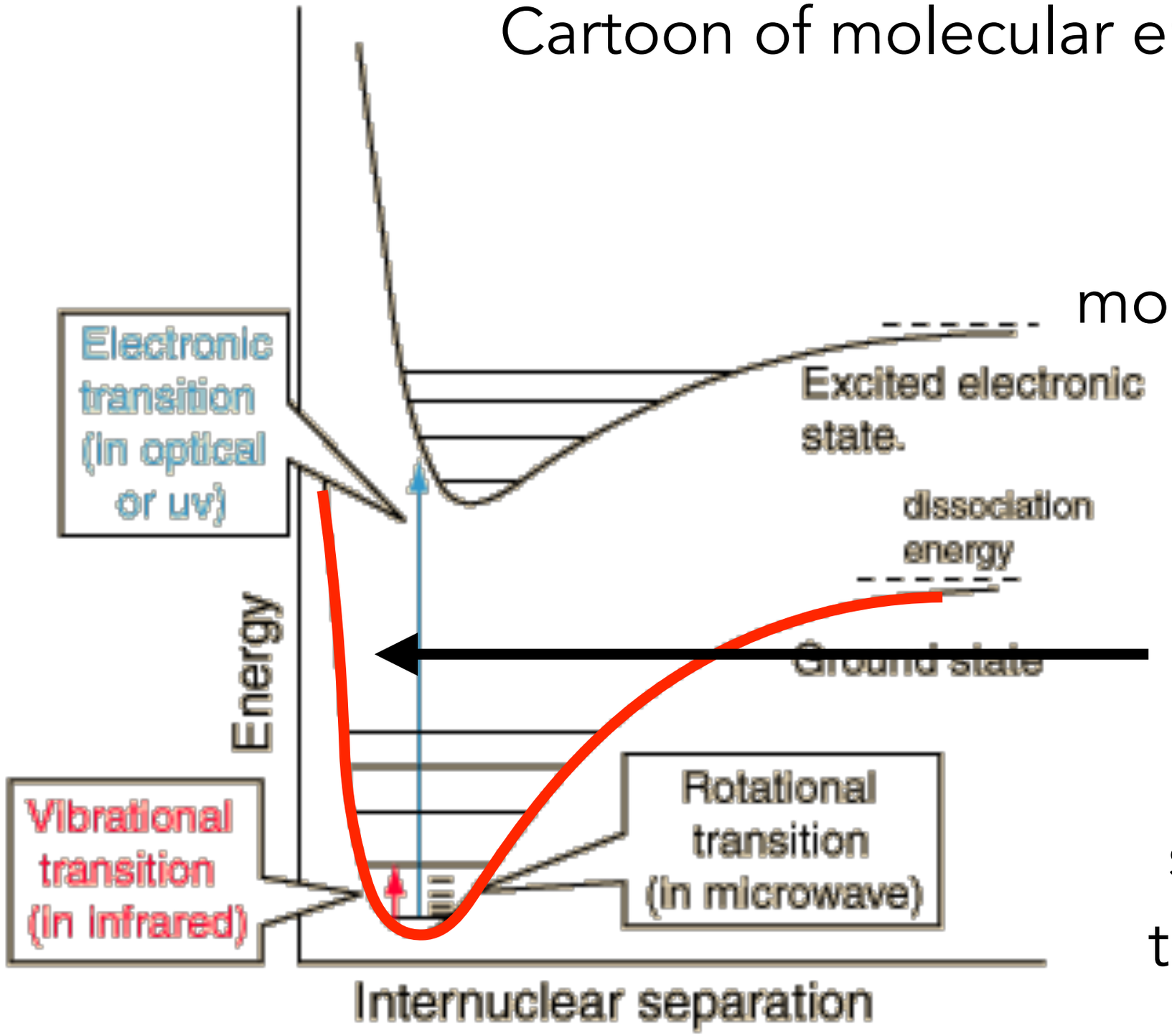
Cartoon of molecular energy levels



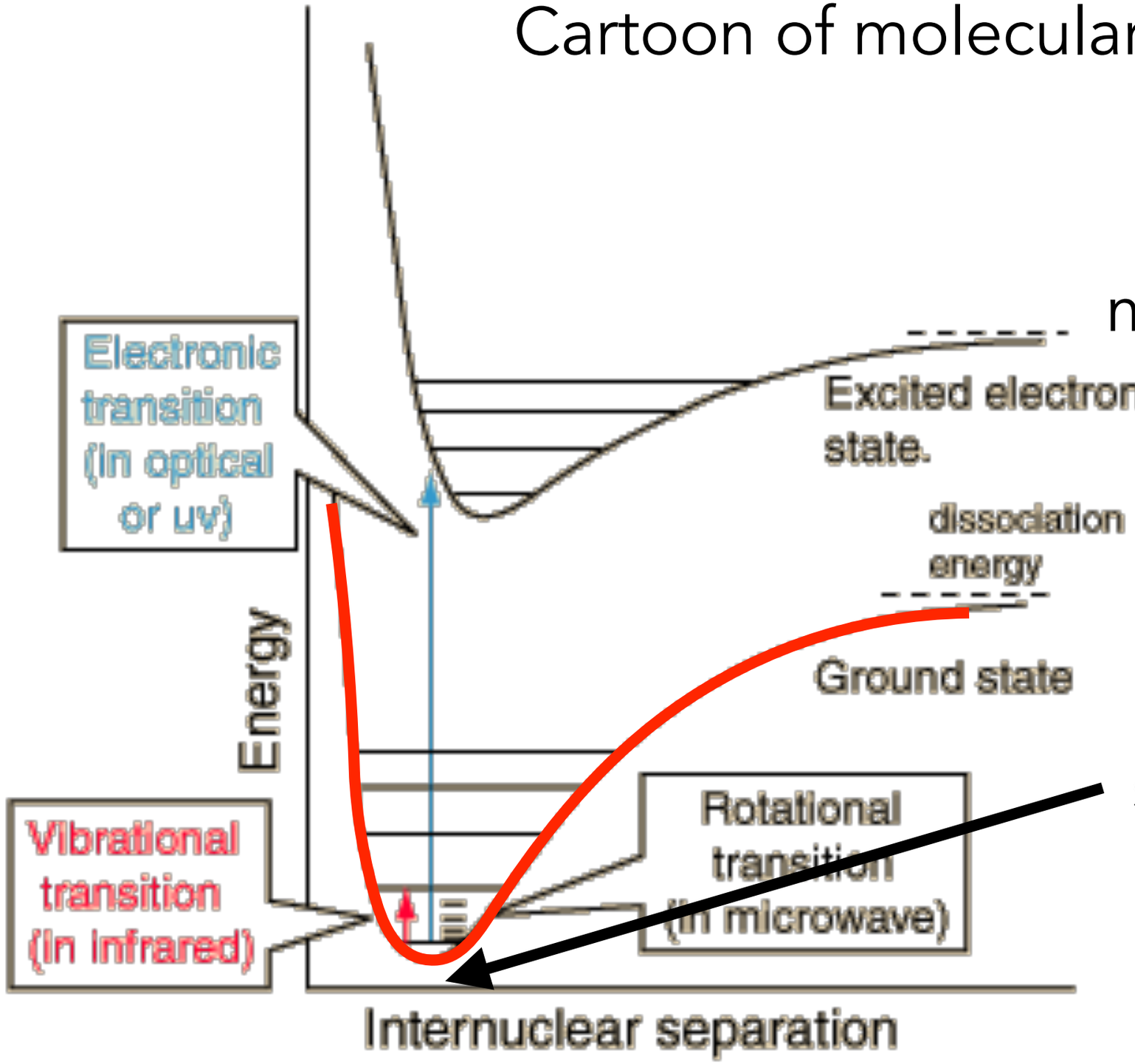
Basic structure of molecule sets this curve

If nuclei get too close together the repel each other, so energy required to make to get R->0 is large.

http://hyperphysics.phy-astr.gsu.edu/hbase/molecule/molec.html

Cartoon of molecular energy levels

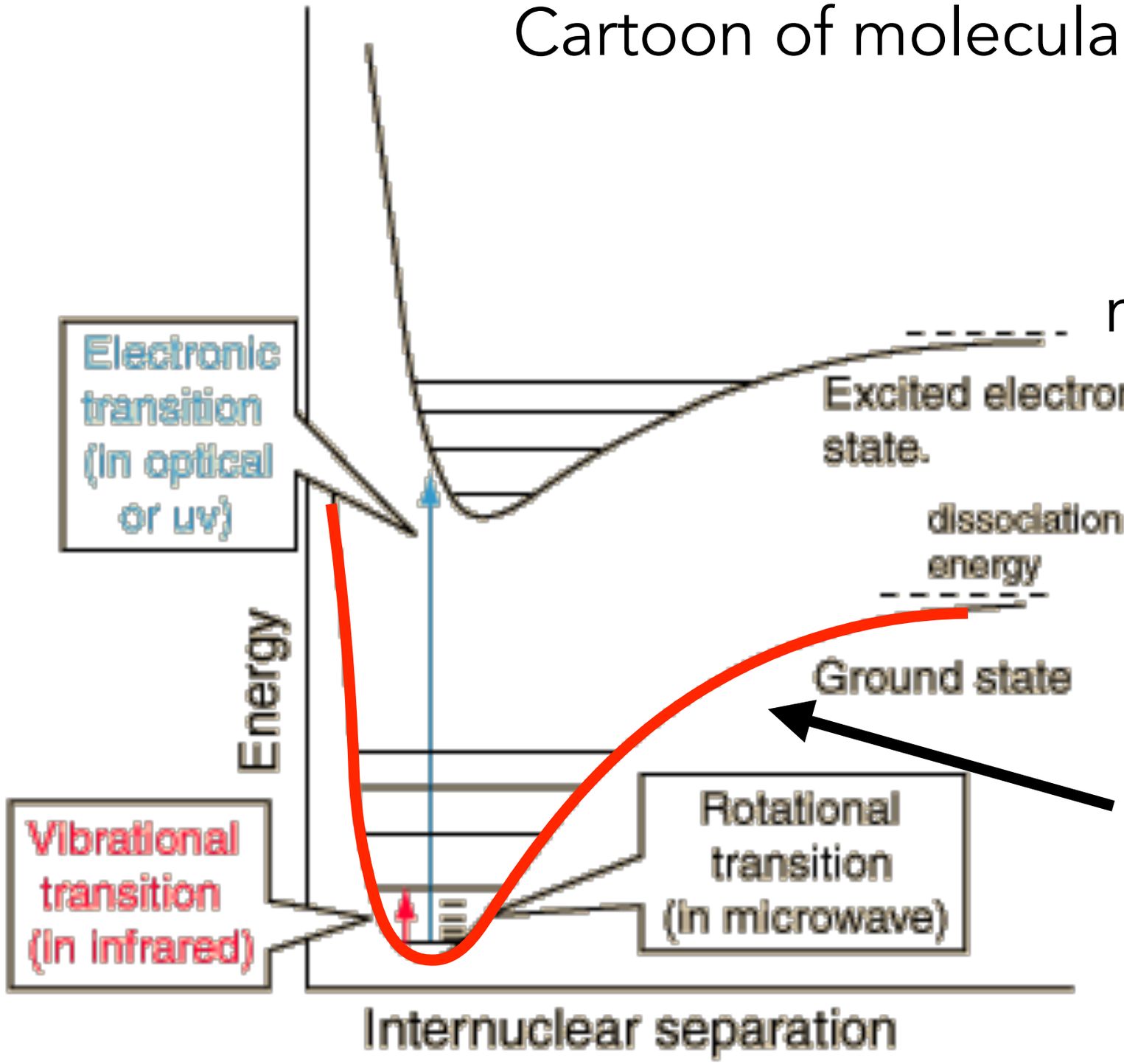
Basic structure of molecule sets this curve



Minimum separation set by the properties of the specific molecular bond.

http://hyperphysics.phy-astr.gsu.edu/hbase/molecule/molec.html

Cartoon of molecular energy levels

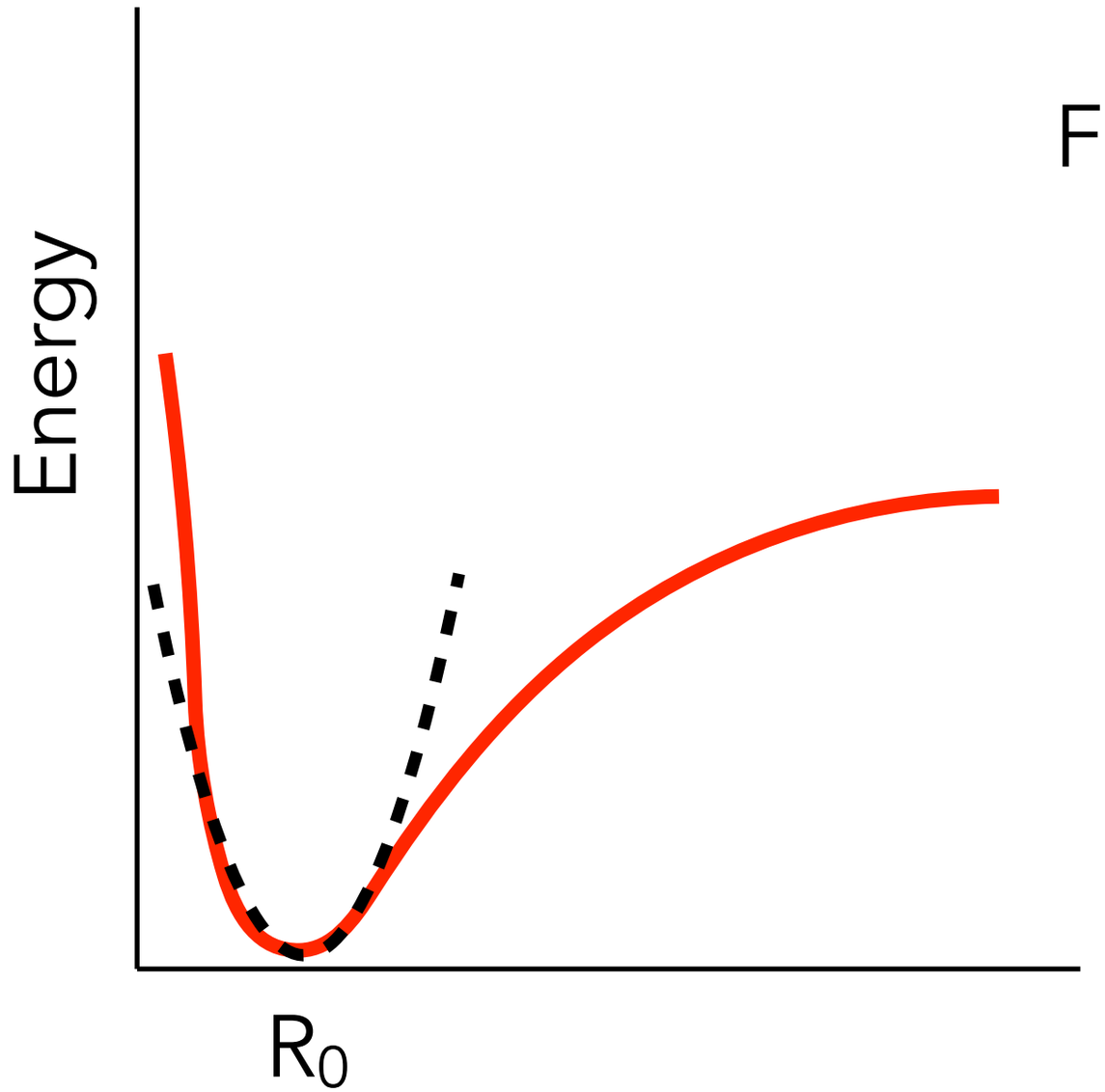


Basic structure of molecule sets this curve

R^{-6} long range attraction from van der Waal's force (fluctuations in electric dipole in one nucleus induces electric dipole in other nucleus)

http://hyperphysics.phy-astr.gsu.edu/hbase/molecule/molec.html

Can be approximated as a simple harmonic oscillator around R_0



Potential energy:

$$V(r) = V(R_0) + 1/2\ k\ (r - R_0)^2$$

k = "spring constant"
related to molecular bond

Fundamental Frequency of oscillator:

$$\omega = (k/m_r)^2$$

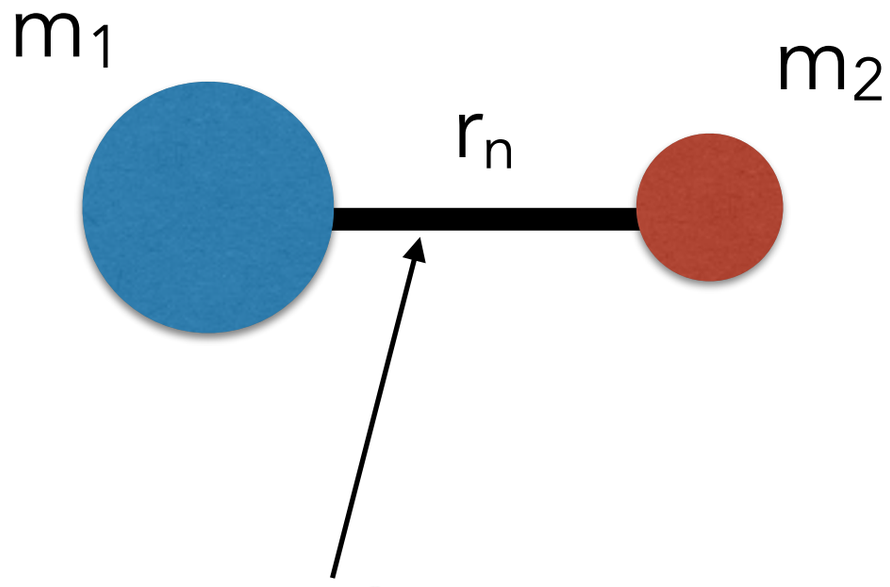
$$m_r = m_1m_2/(m_1+m_2)$$

Vibrational Energy Levels:

$$E_{vib} = \hbar\omega(v + 1/2)$$

v = vibrational quantum number

Rotational Transitions



reduced mass:

$$m_r = m_1 m_2/(m_1+m_2)$$

Moment of intertia:

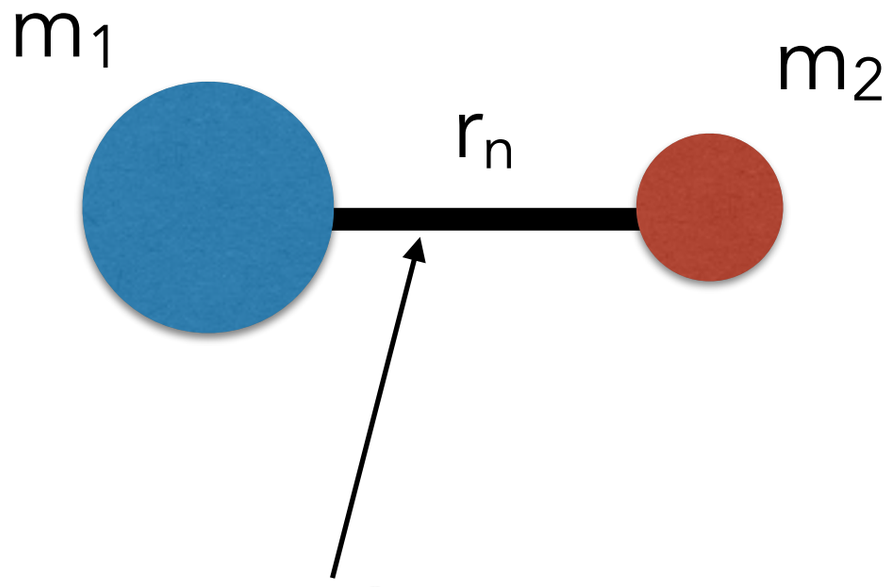
$$I = m_r\, r_n^2$$

Rotational Energy Levels:

$$E_{rot} = \frac{J(J+1)\hbar^2}{2m_r\, r_n^2}$$

J = rotational quantum number

Rotational Transitions



Moment of intertia:

$$I = m_r r_n^2$$

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Rotational Energy Levels:

$$E_{rot} = \frac{J(J+1)\hbar^2}{2m_r r_n^2}$$

J = rotational quantum number

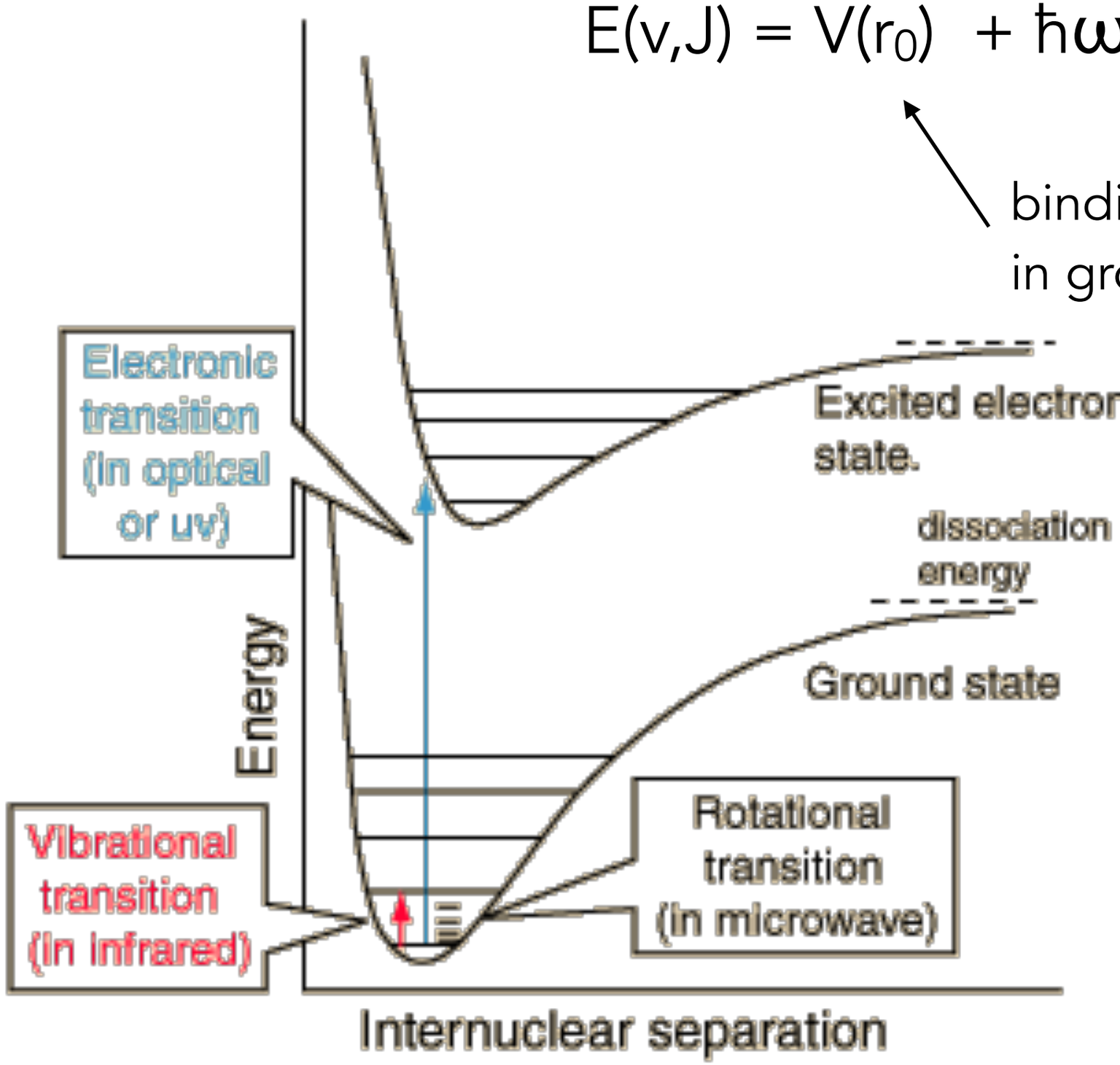
$$\text{Define } B_v = \frac{\hbar^2}{2m_r r_n^2} = 2.1 \times 10^{-3} (m_H/m_r) (1\ \text{Å}/r_n)^2\ \text{eV}$$

"rotational constant"

Total Energy:

$$E(v,J) = V(r_0) + \hbar\omega(v + 1/2) + B_vJ(J+1)$$

binding energy
in ground state



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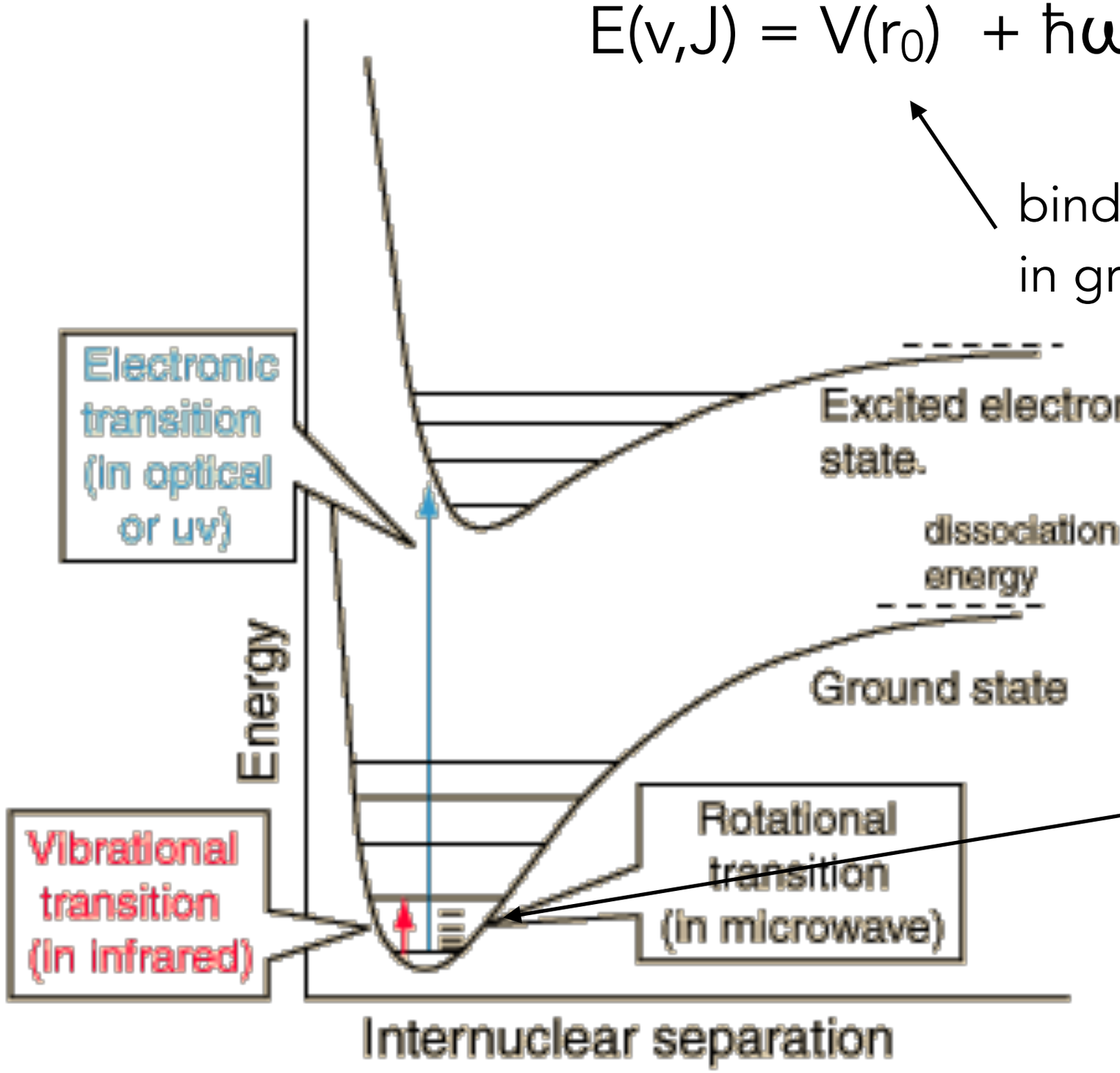
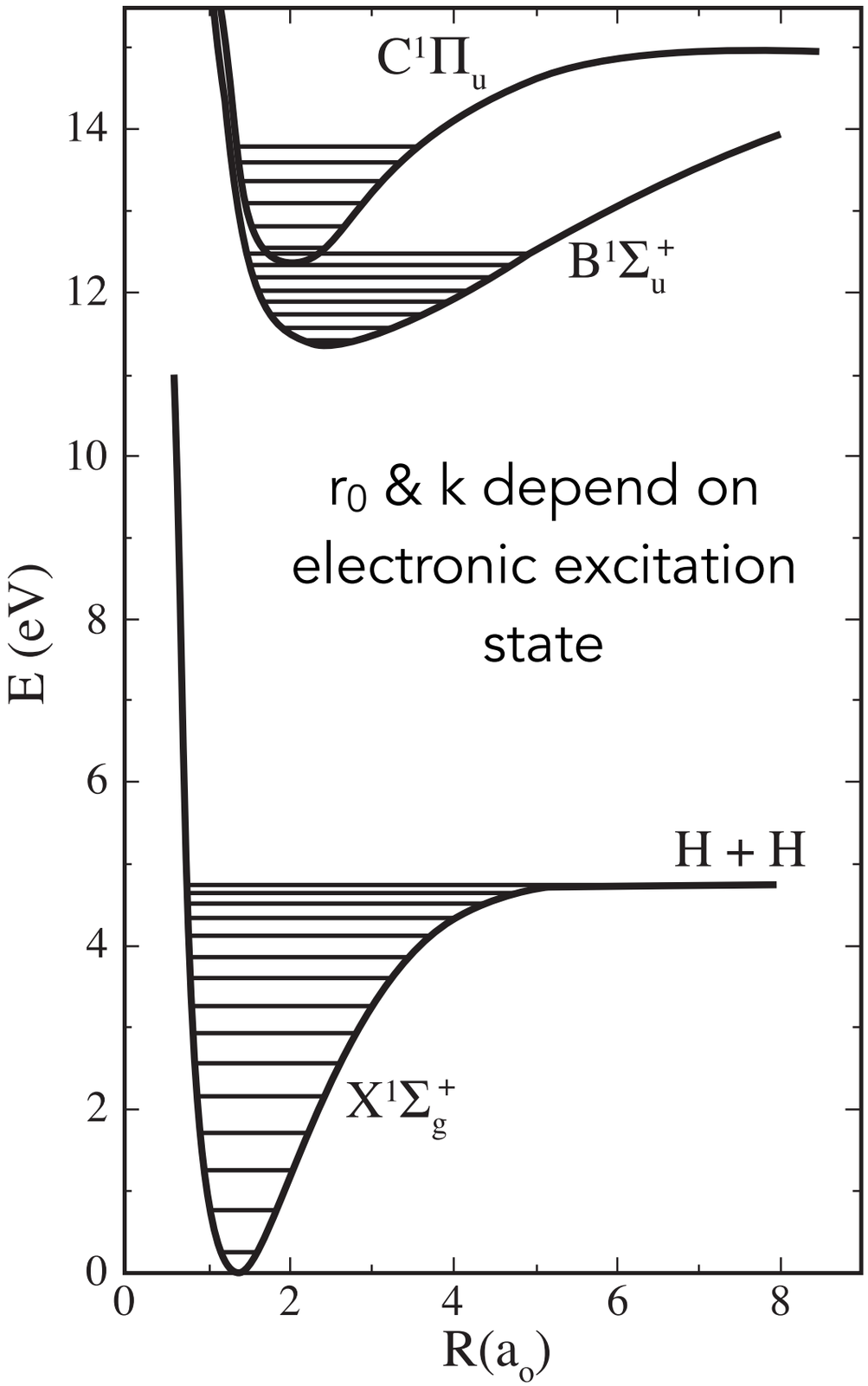


Generally:

$\hbar\omega >> B_v$

so rotational levels are more closely spaced in energy

http://hyperphysics.phy-astr.gsu.edu/hbase/molecule/molec.html



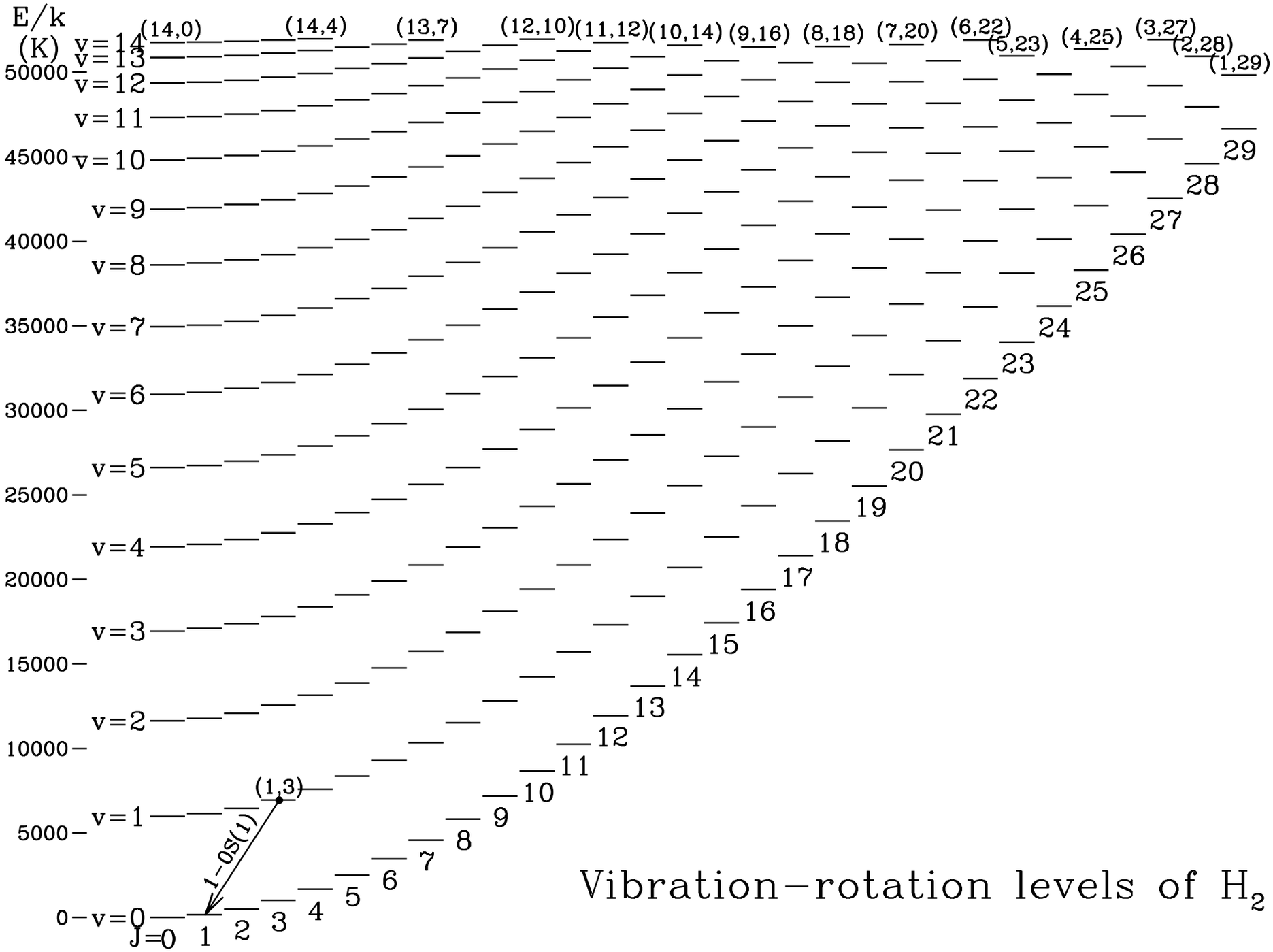
r_0 & k depend on electronic excitation state

H_2 Molecule

Additional wrinkle for H_2: protons, like electrons, can't share same quantum state

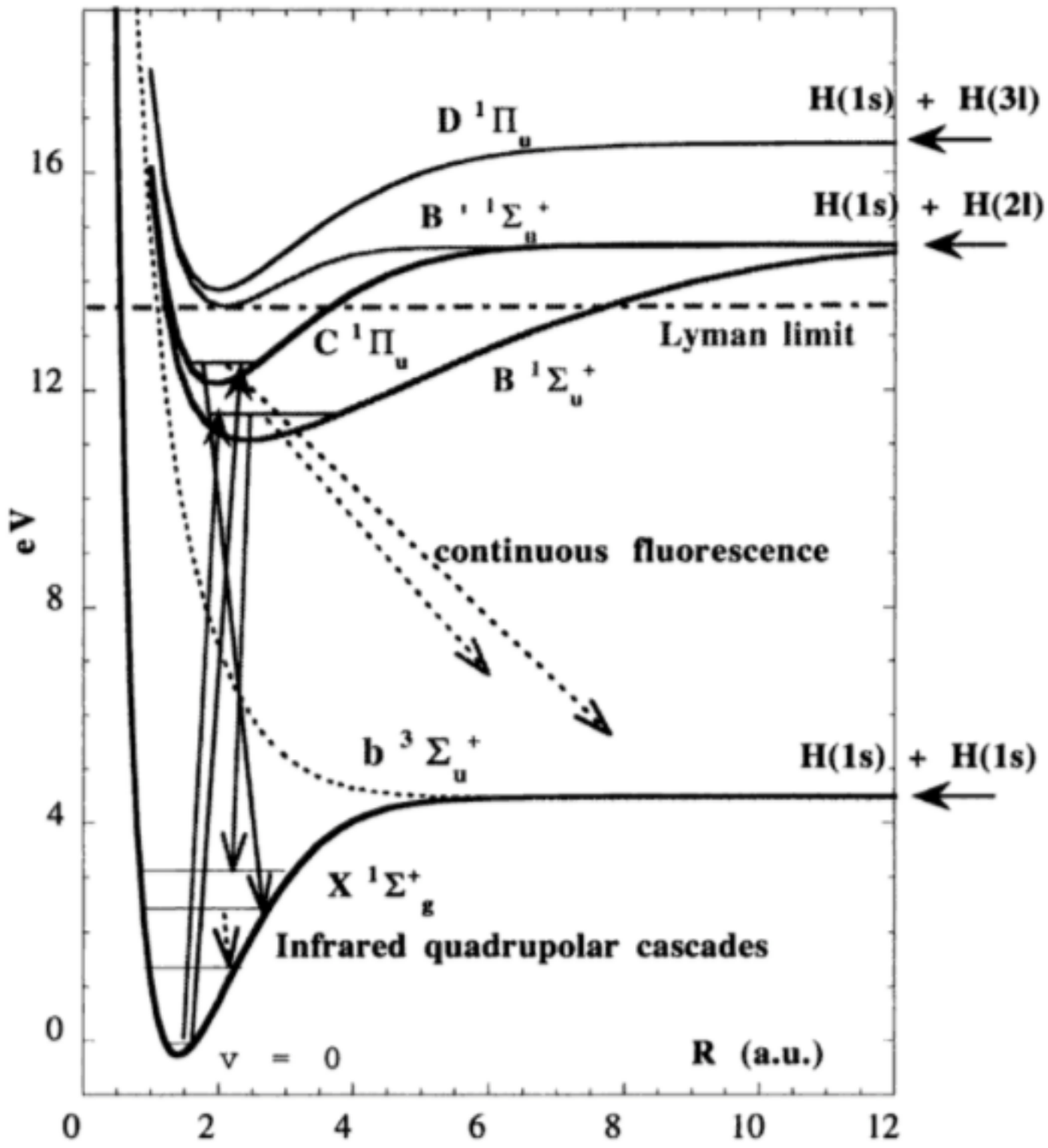
If total proton spin is 1, rotational number J must be even.
-> "para-H_2" J=0,2,4…

If total proton spin is 0 rotational number J must be odd.
-> "ortho-H_2" J=1,3,5…



Vibration−rotation levels of H_2

Only $\Delta J = 0, \pm 2$ are possible to stay para-para or ortho-ortho



Combes & Pineau des-Forets 2000

Lots of interesting ways for H_2 to de-excite after getting into an electronic excited level.

Some involve dissociating some involve rotational cascades.

Will come back to H_2 when we get to molecular gas.

Part II: Two Level System

Interaction of radiation with energy levels of atoms/molecules

Part II: Line Profiles

Line Profile ϕ_ν determined by two processes:

1) Natural Broadening
2) Doppler Broadening

Natural Broadening: from Uncertainty principle $\Delta E \Delta t \geq \hbar$

Δt = lifetime of state

Doppler Broadening: from spread in velocity of particles in the gas

Natural Broadening results in a Lorentz profile (approximately)

$$\phi_\nu \approx \frac{4\gamma_{u\ell}}{16\pi^2(\nu-\nu_{u\ell})^2+\gamma_{u\ell}^2}$$

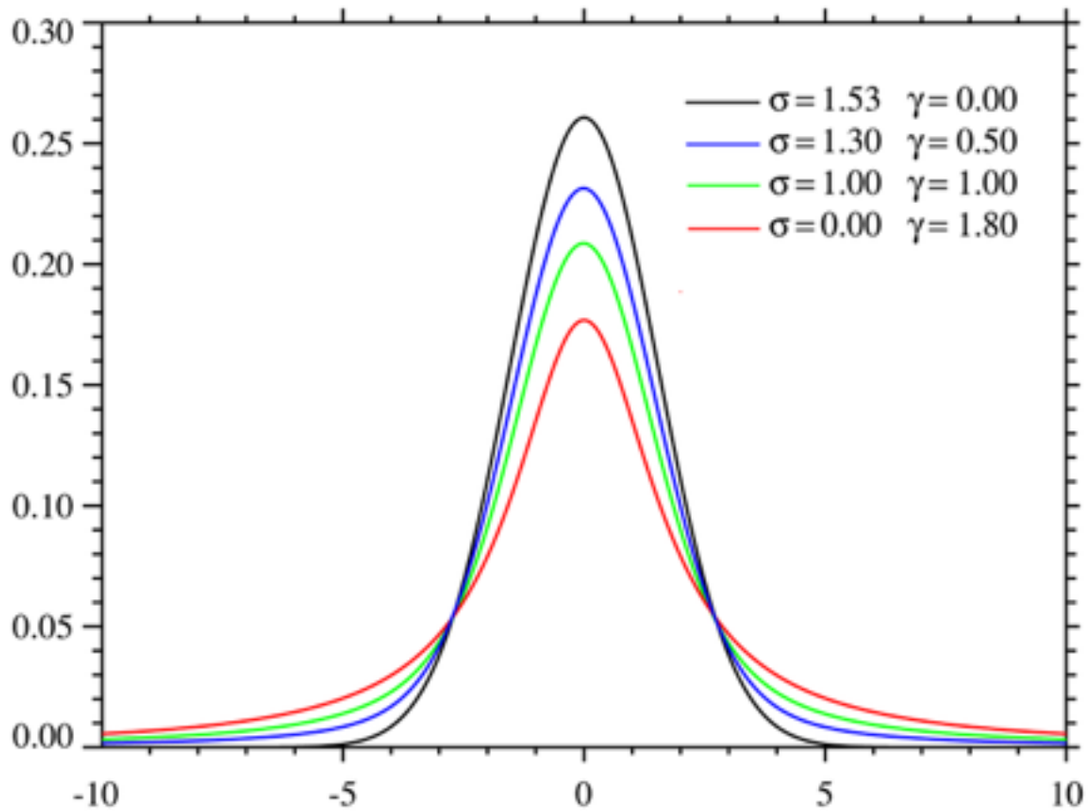
where:

$$\gamma_{u\ell} = \sum_{j<u} A_{uj} + \sum_{j<\ell} A_{\ell j}.$$

Is a sum of all of the relevant lifetimes (~1/A) for the energy levels you are transitioning between.

Doppler Broadening means that
Lorentz profile is convolved with the velocity dispersion
of the gas.

$$\phi_\nu = \frac{1}{\sqrt{2\pi\sigma_v^2}} \int_{-\infty}^{\infty} e^{-v^2/2\sigma_v^2} \frac{4\gamma_{u\ell}}{16\pi^2(\nu - (1 - v/c)\nu_{u\ell})^2 + \gamma_{u\ell}^2} dv$$



This gives you a
"Voigt" profile.