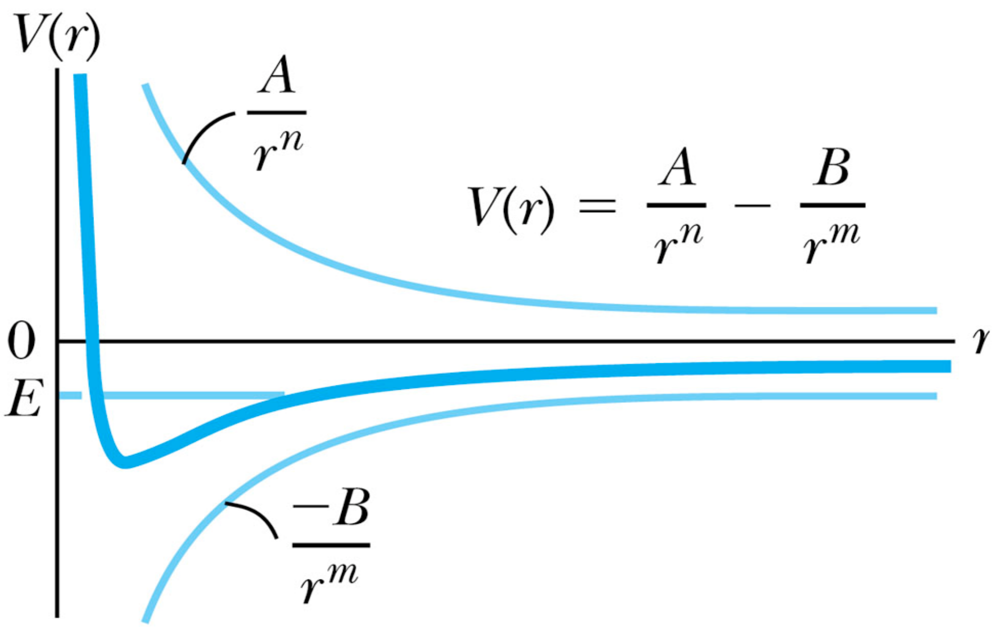
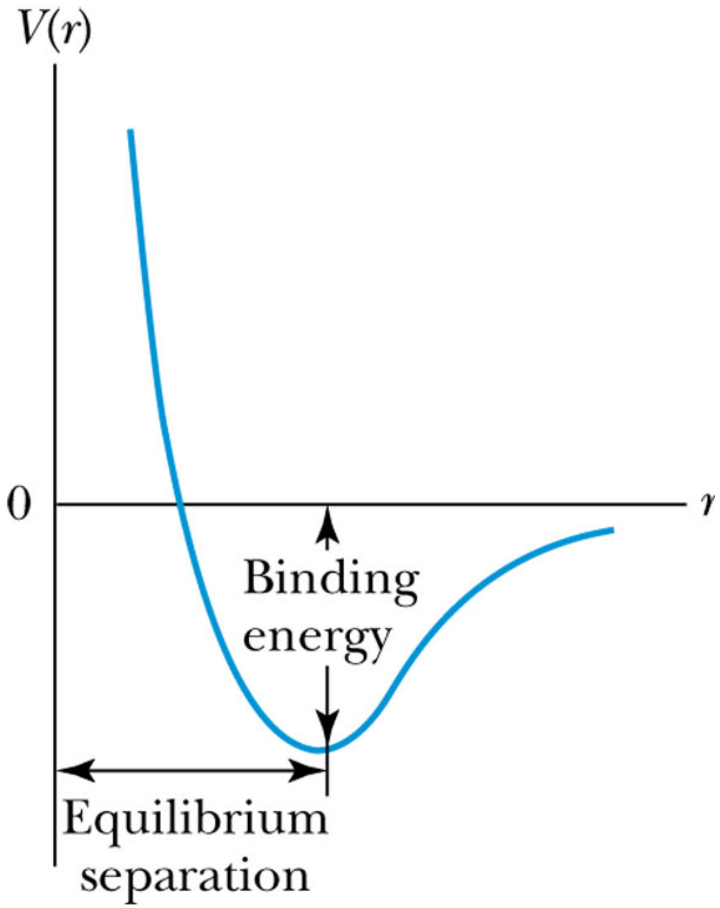
Diatomic Molecules

- Forces holding molecules together are complex combination of attractive and repulsive Coulomb forces – but not simple 1/ r potentials – Lennard-Jones has n = 12, m = 6
- Rem: $F_r = -dV/dr$





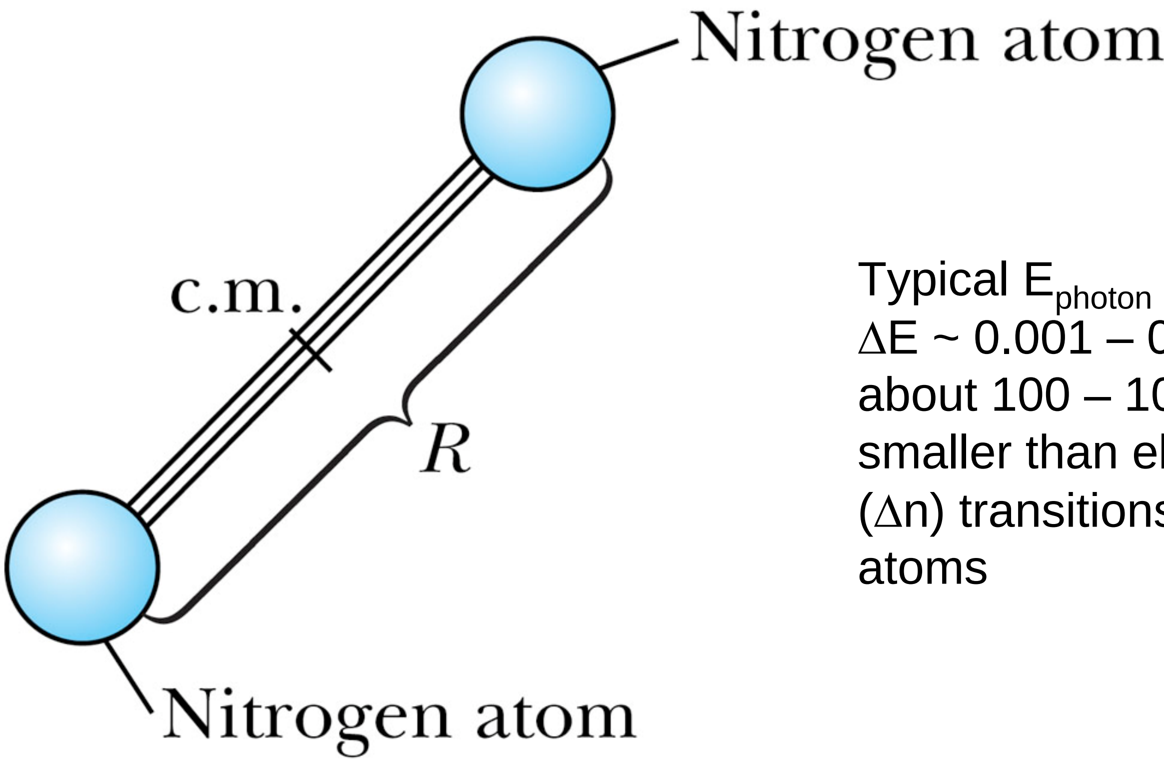
Types of Molecular Bonds

- Ionic bond – between charged ions (Coulomb attraction) – e.g. Na ($1s^2 2s^2 2p^6 3s^1$) ionizes and donates e^- to fill Cl ($1s^2 2s^2 2p^5$)
- Covalent bond – sharing of electrons – larger density of e^- between two atoms and e^- are coupled with opposite spins– e.g. H_2, N_2, O_2
- van der Waals – relatively weak bond – uses dipole-dipole attraction as well as dispersion force
- H- bond – very weak attractive bond – particularly important in biology

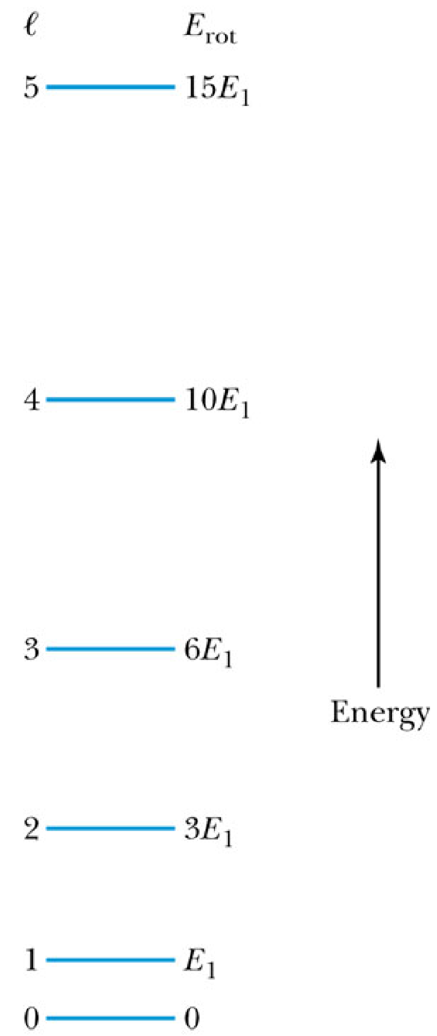
Rotational Energy States

- Rotational energy states

$$E_{rot} = \frac{L^2}{2I} = \frac{\ell(\ell+1)\hbar^2}{2I}$$



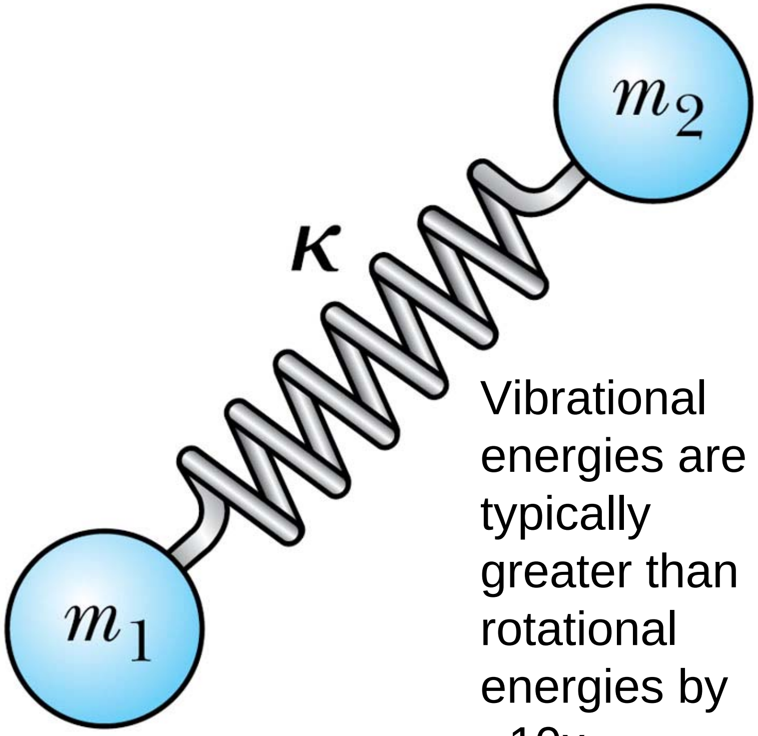
Typical E_{photon} = hf = ΔE ~ 0.001 – 0.01 eV, about 100 – 1000x smaller than electronic (Δn) transitions in atoms



Vibrational Energy States

- Bonds act like springs so there is vibration
- Classically $f = \frac{1}{2\pi}\sqrt{\frac{k}{\mu}}$ while from QM

$$E_{vib} = (n + \tfrac{1}{2})\hbar\omega$$



Vibrational energies are typically greater than rotational energies by ~10x

Table 10.1 Fundamental Vibrational Frequencies and Effective Force Constants for Some Diatomic Molecules

Molecule	Frequency (Hz), $n = 0$ *to* $n = 1$	Force Constant (N/m)
HF	8.72×10^{13}	970
HCl	8.66×10^{13}	480
HBr	7.68×10^{13}	410
HI	6.69×10^{13}	320
CO	6.42×10^{13}	1860
NO	5.63×10^{13}	1530

Spectra from diatomic molecules

- Combined rot and vib spectra:

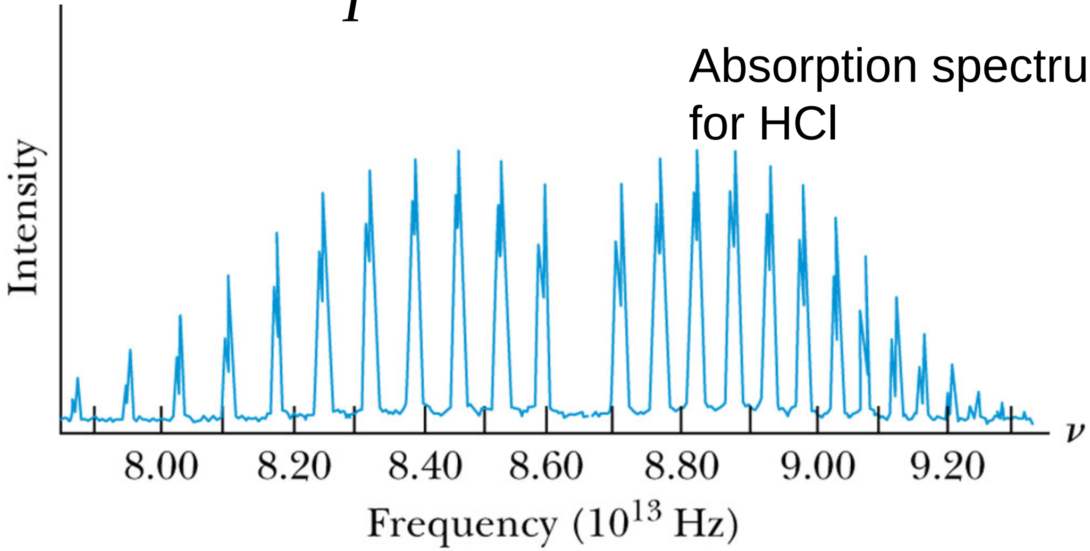
$$E = E_{rot} + E_{vib} = \frac{\hbar^2 \ell(\ell+1)}{2I} + (n + \tfrac{1}{2})\hbar\omega$$

Selection rule is
$\Delta\ell = \pm 1$

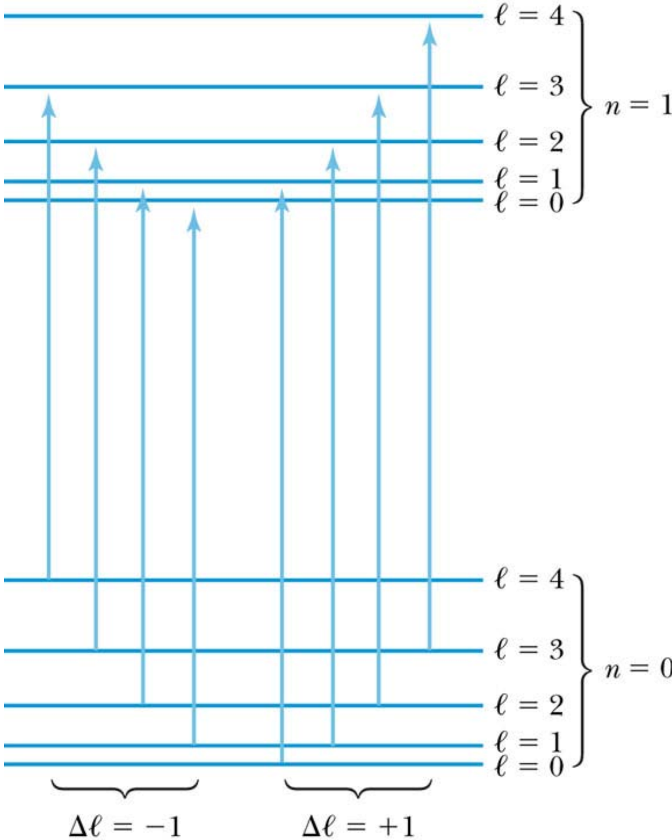
- Photon emitted energies:

$$E_{ph,\Delta n,\ell+1\to\ell} = \Delta n\left(\hbar\omega\right) + \frac{\hbar^2}{2I}\left[(\ell+1)\left(\ell+2\right) - \ell\left(\ell+1\right)\right]$$

$$= \Delta n\left(\hbar\omega\right) + \frac{\hbar^2}{I}(\ell+1)$$

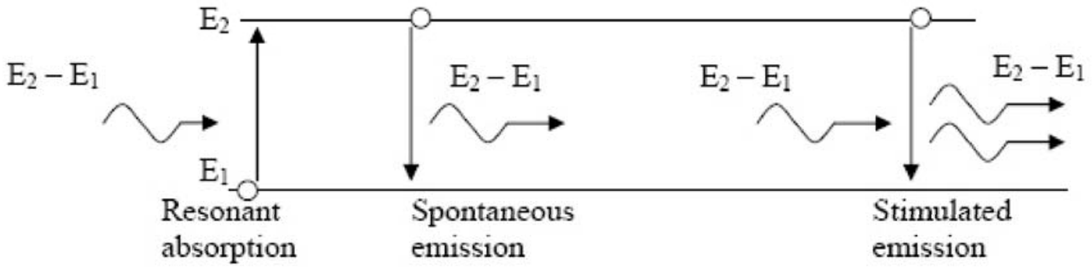


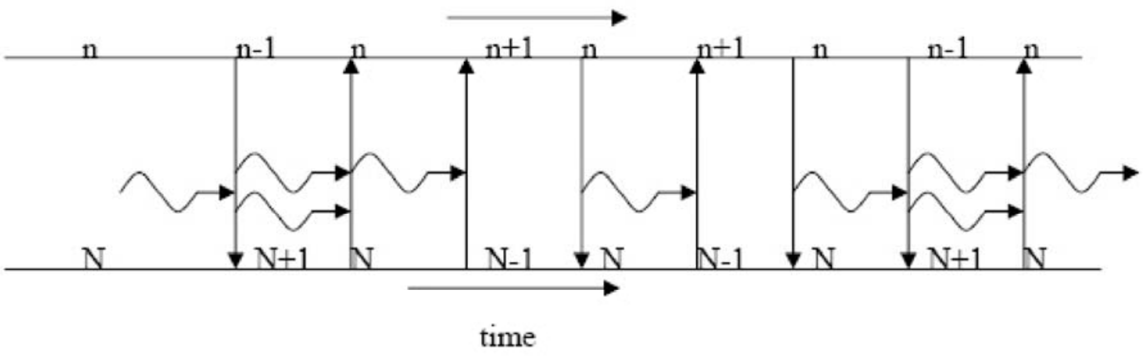
Absorption spectrum for HCl



Lasers -1

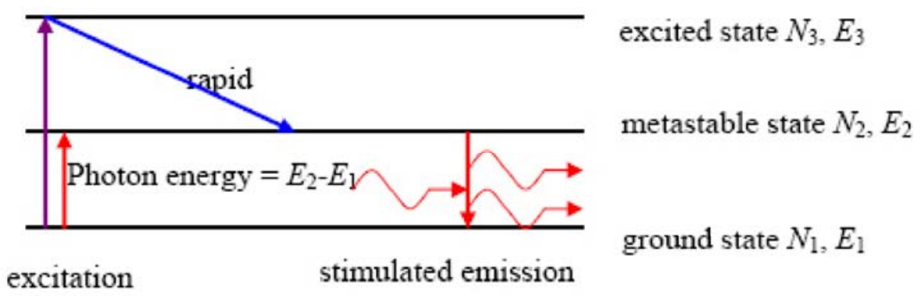
- Light Amplification by the Stimulated Emission of Radiation



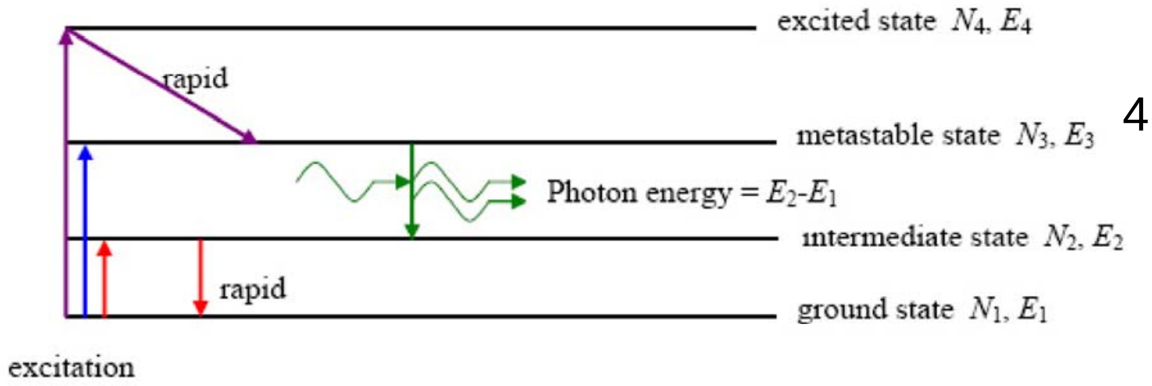


Need population inversion

Lasers - 2

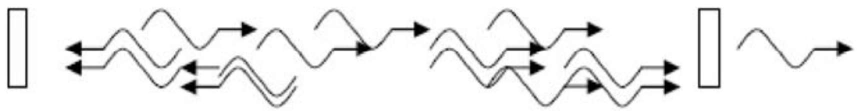


3 – level laser

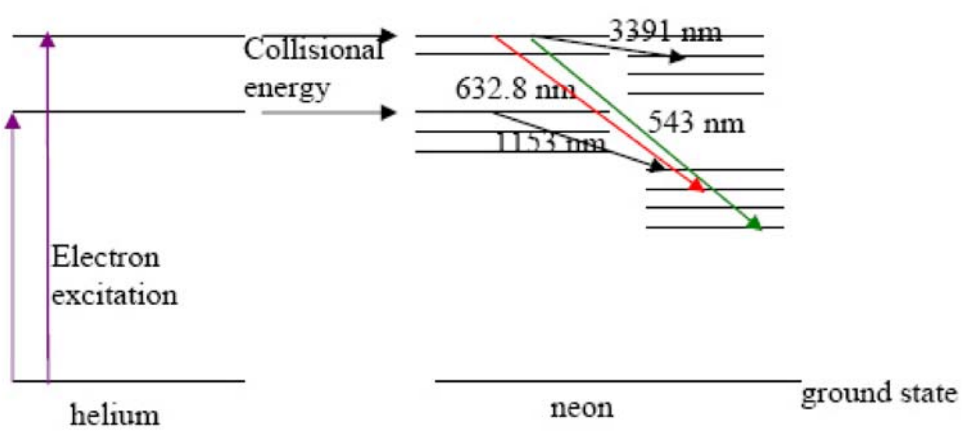


4 level laser

Lasers - 3

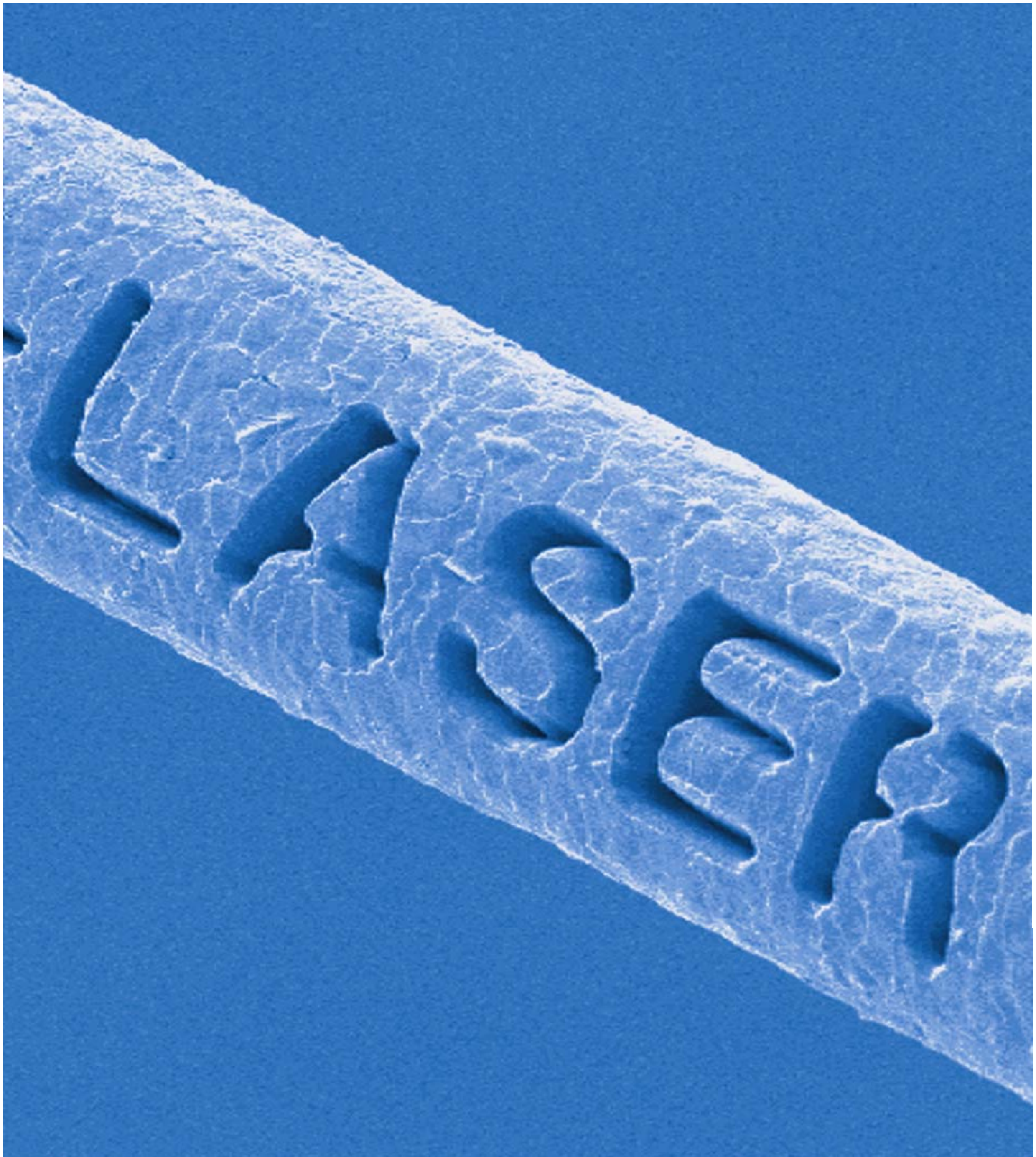


Resonant cavity – making a beam



He-Ne energy levels


CAUTION
Handle with care. Easily damaged by electrostatic discharge.
DANGER
INVISIBLE LASER RADIATION-AVOID DIRECT EXPOSURE TO BEAM
PEAK POWER 5 mW
WAVELENGTH 780 nm
#5
CLASS IIIb LASER PRODUCT
INVISIBLE LASER DIODE
AVOIDE EXPOSURE
—Invisible Laser radiation is emitted as shown.
UNION COLLE


LASER

Laser Tweezers