# Diffraction Gratings, Atomic Spectra

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# Visual Comparisons

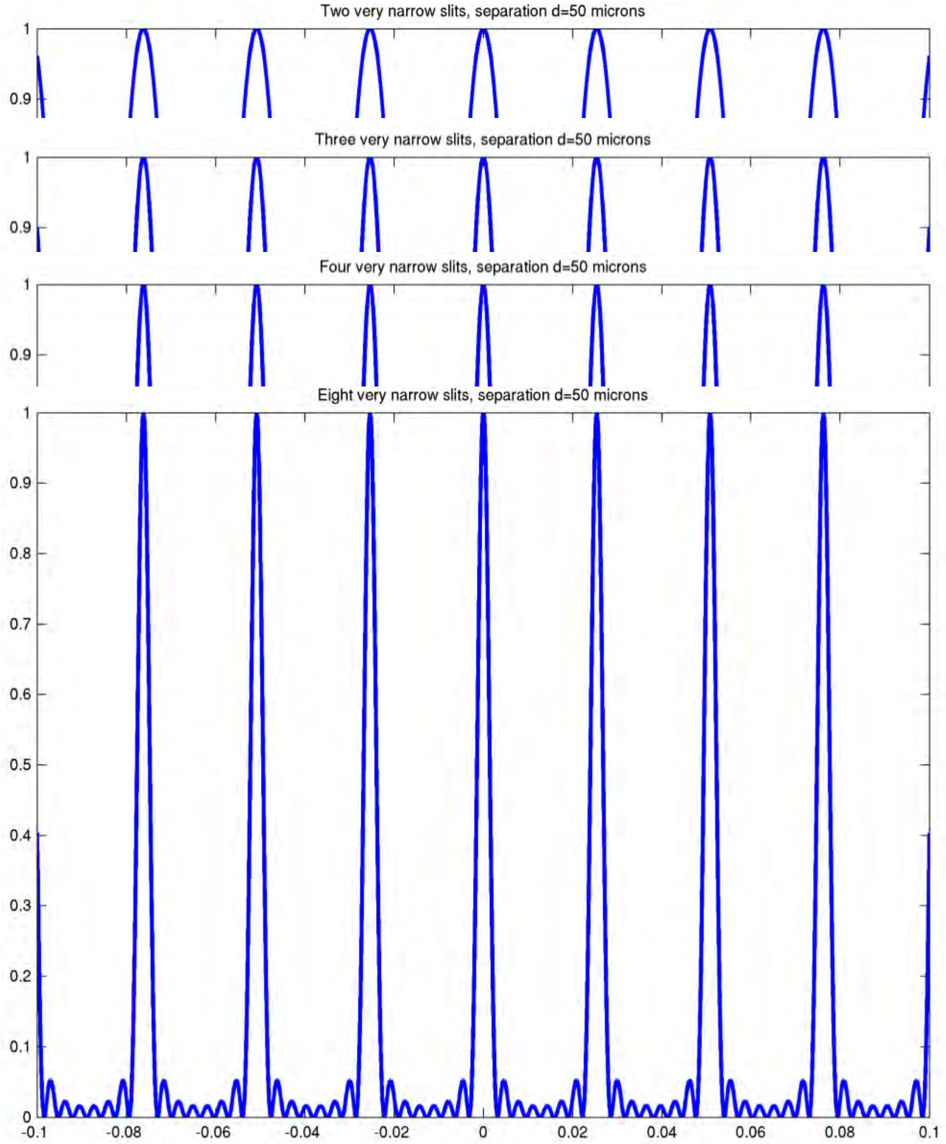
**Increase number of slits:**

**2**

**3**

**4**

**8**



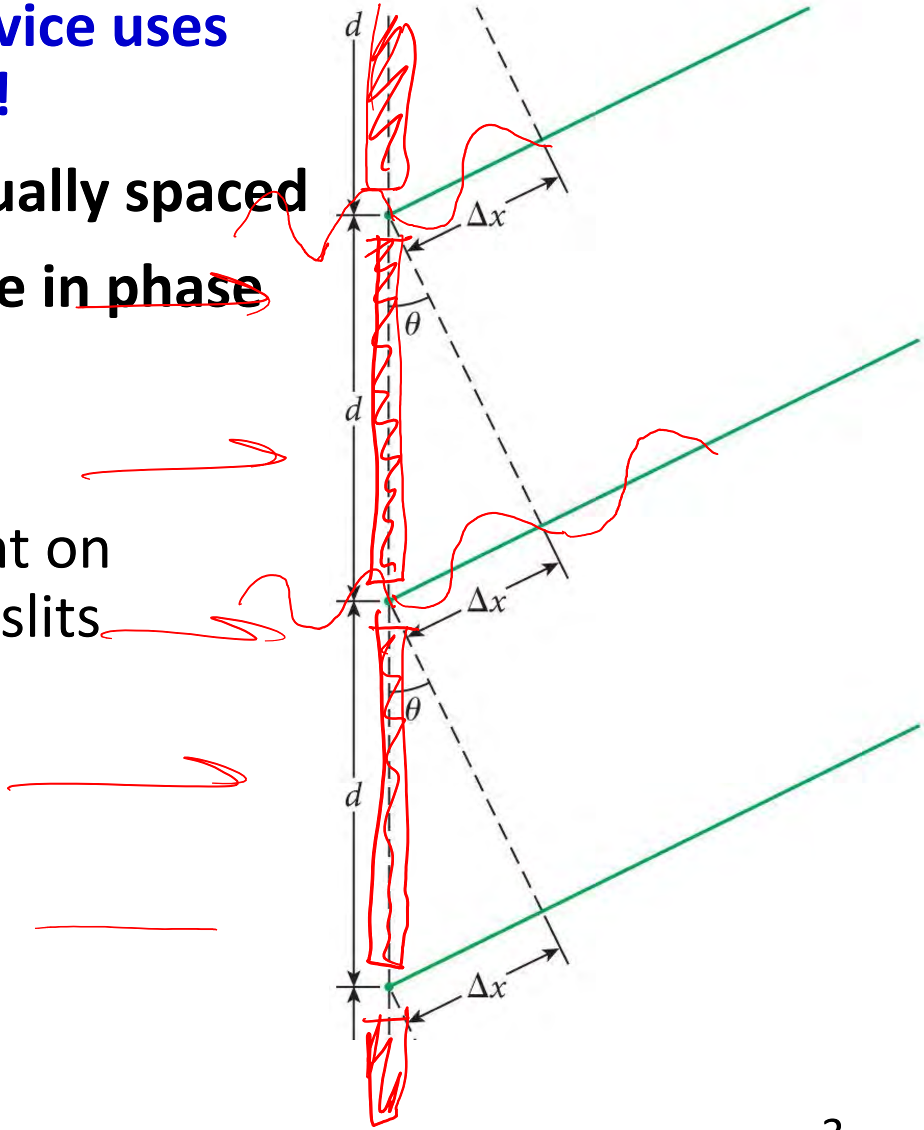
# Diffraction Grating (large $N_{slit}$)

**Note: despite the name, this device uses interference, not diffraction!**

***Many*** **slits (or obstructions), equally spaced**

**Need light from *all* of them to be in phase to get a bright spot**

Ideal picture: plane wave incident on grating, so same phase at all slits



# Pattern from a Diffraction Grating

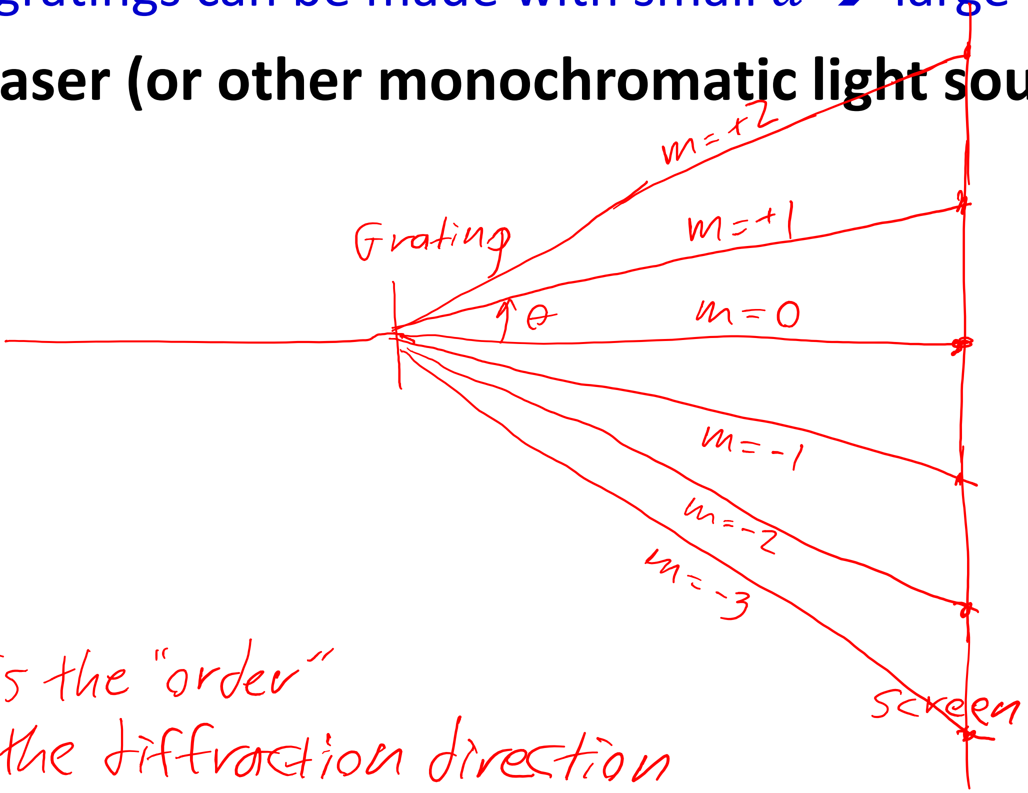
spacing between "slits"

**Constructive interference condition:** $a \sin\theta = m\lambda$

$\sin\theta = m\frac{\lambda}{a}$

Note: gratings can be made with small $a$ ➔ large $\theta$'s

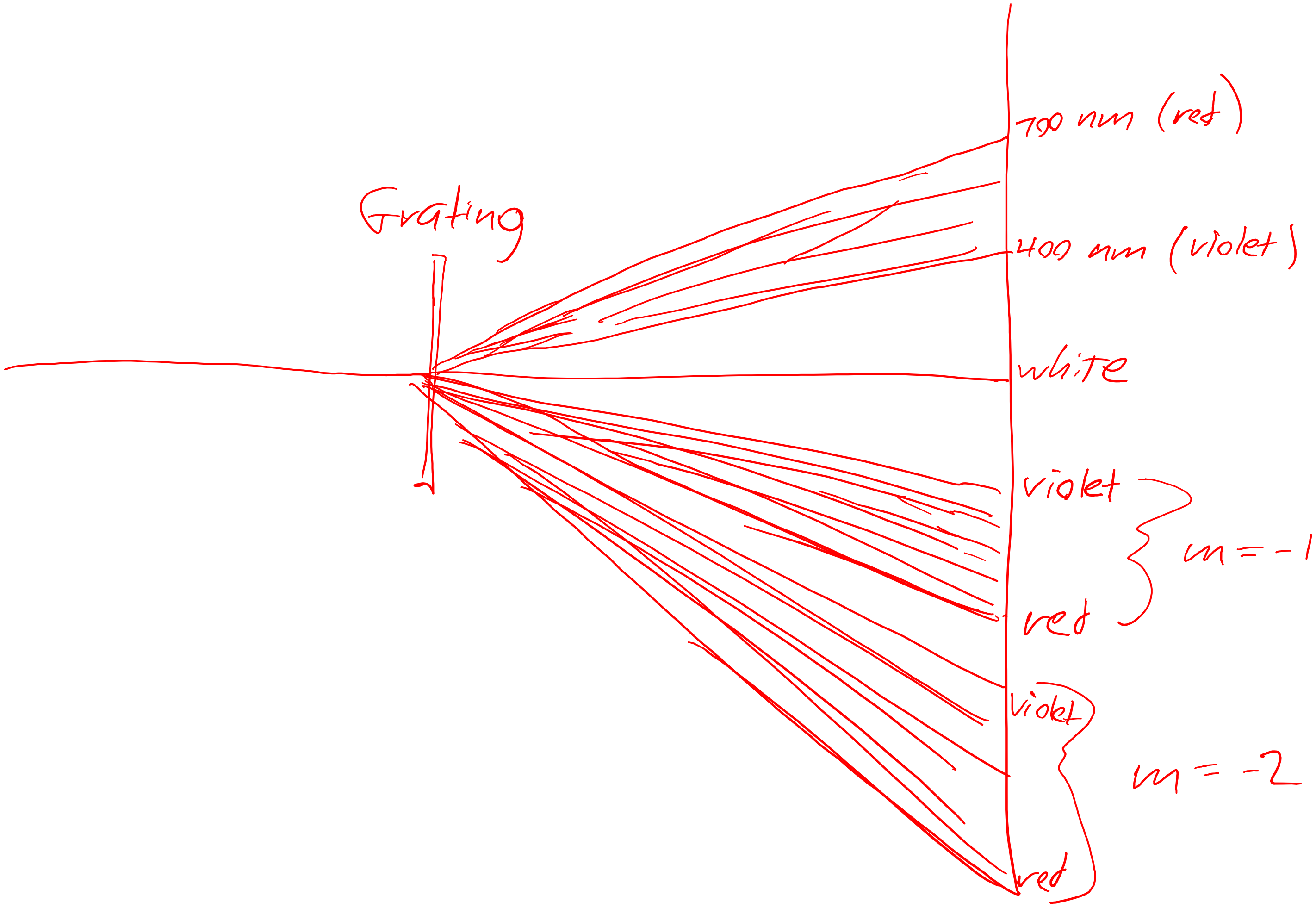
**From a laser (or other monochromatic light source):**



m is the "order" of the diffraction direction

# Pattern from a Diffraction Grating

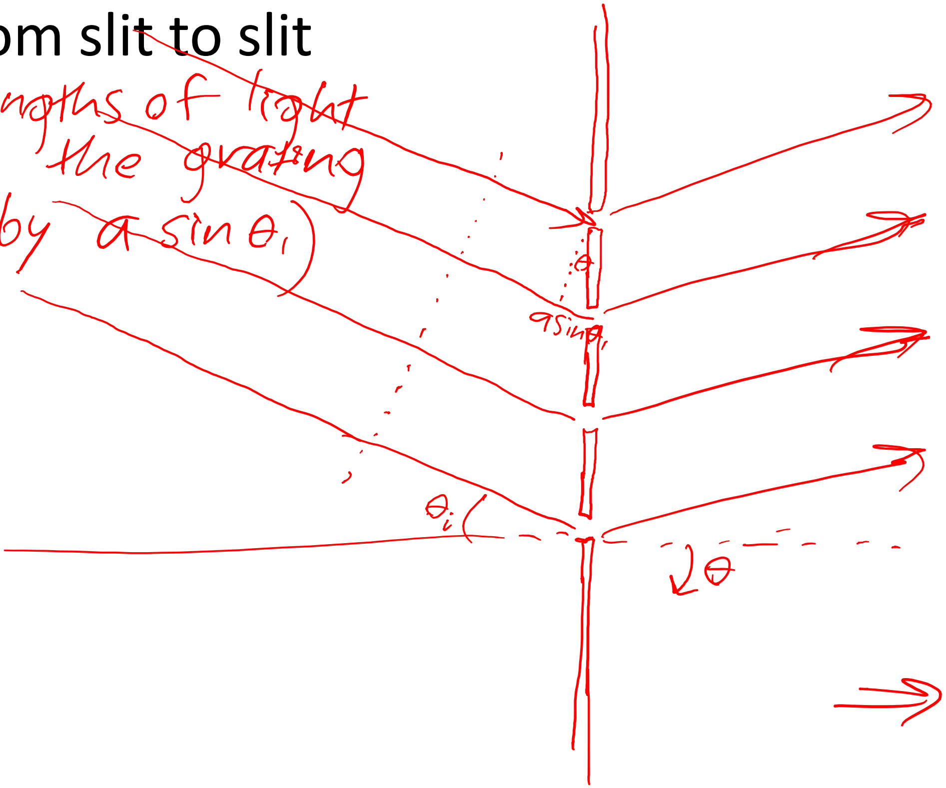
**From a white-light (continuous spectrum) source:**



# What if light is incident on grating at an angle?

Plane wave is now coming in at an angle, so there is a phase shift from slit to slit

(path lengths of light before the grating differ by $a \sin\theta_i$)



→ shift in the bright spot positions, relative to $\theta_i = 0$

Still need outgoing light to all be in phase to get a bright spot, i.e. when $a(\sin\theta_i + \sin\theta) = m\lambda$

# Consequences for your experiment

**Can you count on the grating in your spectrometer to be perfectly aligned, normal to the light beam?** No

**How you can align it:**

Retro-reflect

Adjust so that diffracted lines are at symmetric angles

**How you can take data intelligently to minimize systematic error from mis-alignment:** Measure diffraction in both directions, both positive & negative $\theta$'s, and average

# Transmission vs. Reflection Gratings

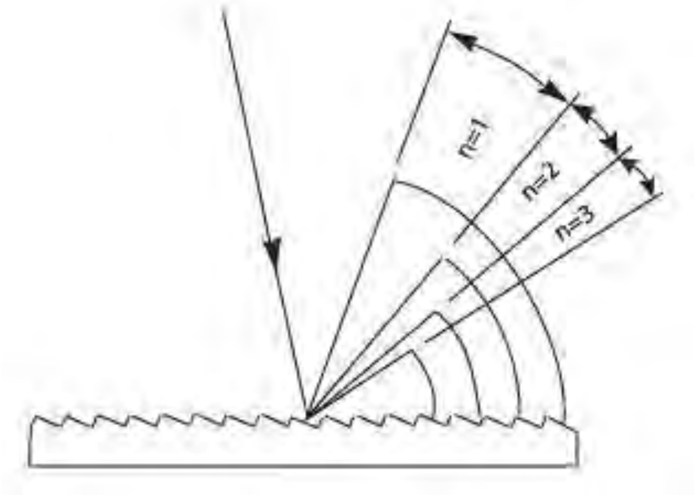
**Transmission: slits, or scratches, or a fine mesh of wires**

**Reflection: Reflective surface with interruptions or surface height changes**

**Note: angles of diffracted beams are typically not small, so you can’t make the approximation $\sin\theta \approx \theta$**

**Tuned reflective surface:**

To improve the “efficiency” for a certain refraction order

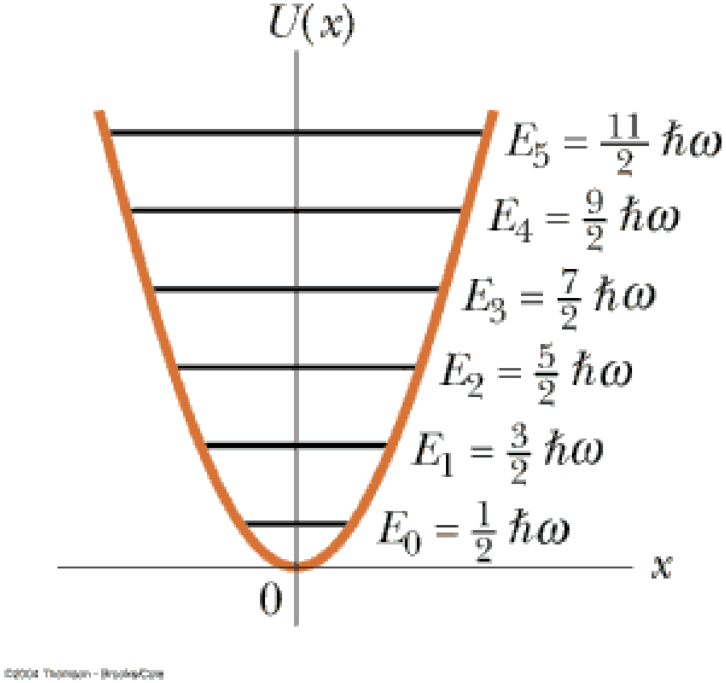


# Energy Levels and Transitions

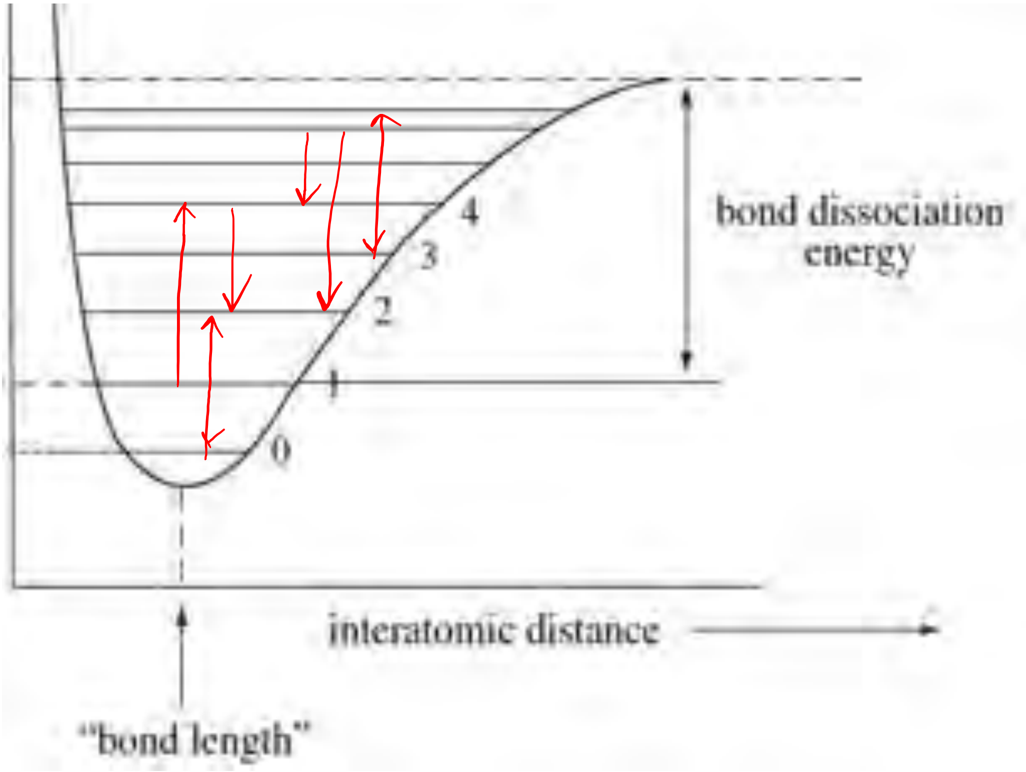
It’s all about the potential!

A quantum state describes a *system*, e.g. an electron in a potential

Harmonic Oscillator



Bond between atoms



# Spectrum of Hydrogen Lamp

**Spectrum spread out using a diffraction grating**

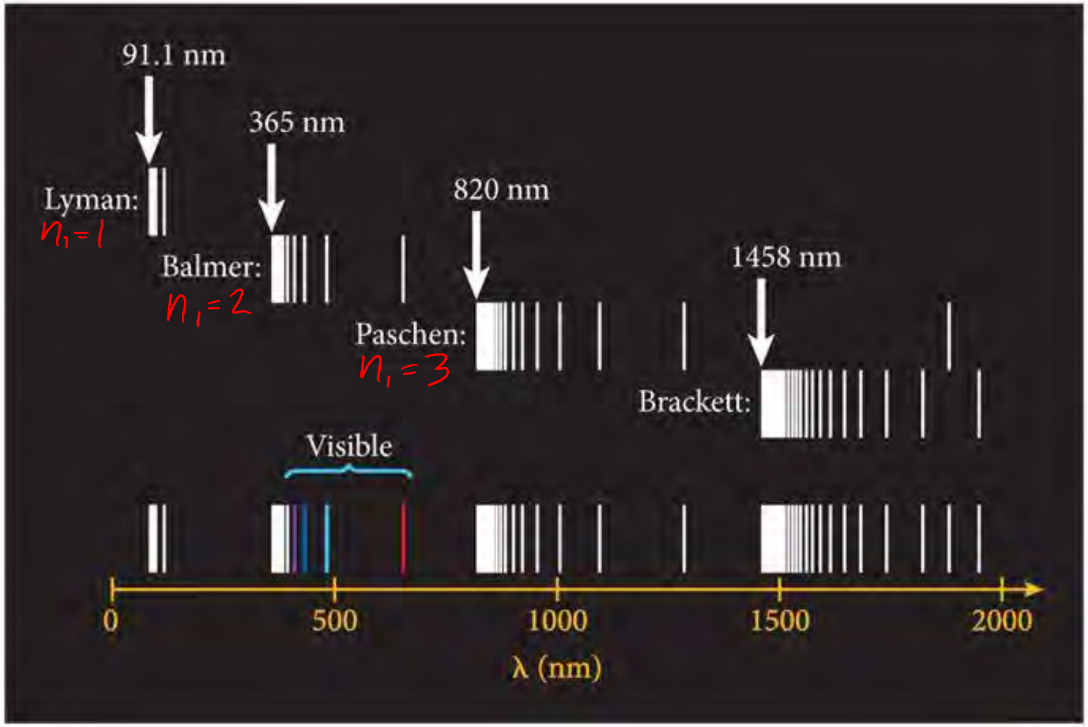
(Better than using dispersion in a glass prism)

**Empirical formula by Balmer:** $\lambda = (364.56\,nm)\,\dfrac{n^2}{(n^2-4)}$ $= \dfrac{(\ )}{4}\,\dfrac{1}{\left(\frac{1}{4}-\frac{1}{n^2}\right)}$

for integers /

**Full spectrum of hydrogen emission lines:**

- Includes UV and infrared
- Must be from transitions between energy levels



# Bohr Model for the Atom

**Picture electrons orbiting the nucleus**

Problems with that, from classical theory:

- Electron should be able to have any energy level
- Charged particle in orbit should radiate energy and collapse

**Bohr's model:**

Assume that electrons can only occupy discrete orbits with angular momentum equal to a multiple of $\hbar$

Solving the circular motion problem gives

orbit radii:

$r_n = a_0 n^2$ with $a_0 = \hbar^2/\mu k e^2 = 5.295\times10^{-11}\,m$

↖ (reduced) mass

$E_n = -E_0/n^2$ with $E_0 = ke^2/2a_0 = 13.6\ eV$

(Neglecting fine structure from electron spin-orbit coupling, and hyperfine structure from nuclear spin couplings)

# Hydrogen Atom Transitions

Alternatively,

$$E_n = \frac{-R_\infty hc}{n^2}$$

$R_\infty$ is the “Rydberg constant”, $1.09737 \times 10^7\ \mathrm{m}^{-1}$

$R_\infty hc$ is the “Rydberg energy”, $\sim 13.6$ eV

But for a hydrogen atom, we should use the reduced mass

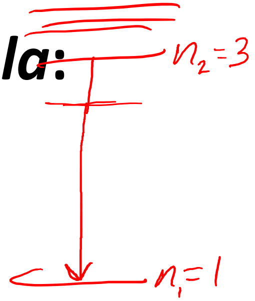
$$\mu = \frac{m_p m_e}{m_p + m_e}$$

➔ $R_H$ is Rydberg constant for hydrogen, $1.09678 \times 10^7\ \mathrm{m}^{-1}$

Starting from $E_n \propto -1/n^2$ …

A photon emitted or absorbed in a transition must have energy equal to the difference of two energy levels

**Photon wavelengths are given by the *Rydberg formula*:**



$$\frac{1}{\lambda} = R_H \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

Example: $\frac{1}{\lambda} = R_H \left( \frac{1}{1^2} - \frac{1}{3^2} \right)$

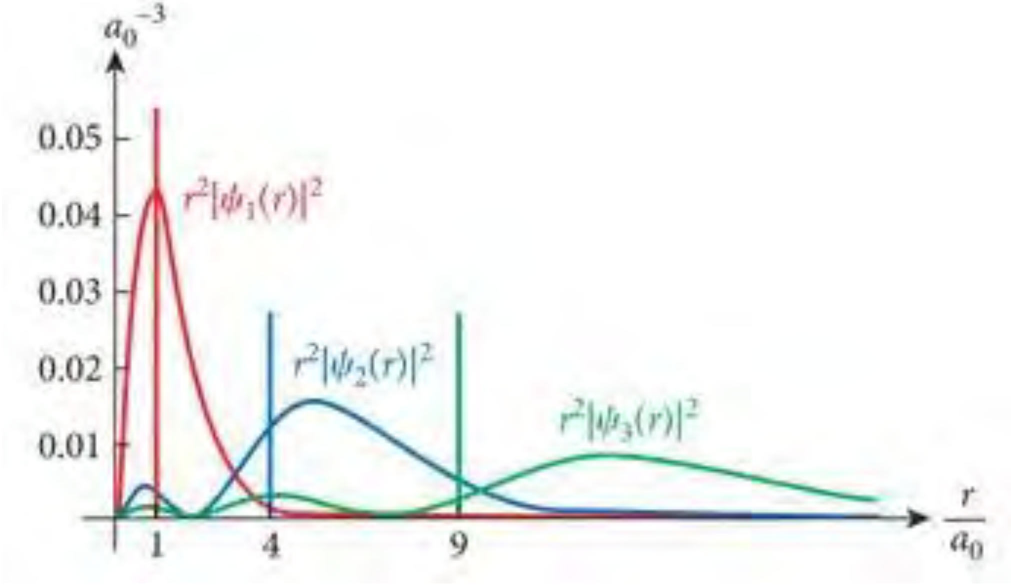
# Quantum Mechanics Solution

**Quantum mechanical system with one electron in Coulomb (electrostatic) potential**

3-D system

Exactly solvable, but the math is complicated

$$\frac{-\hbar^2}{2\mu}\left[\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right]+\left(\frac{-ke^2}{r}\right)\psi = E\,\psi$$



# Extending to Other Atoms

**Single-electron atoms**

Simple!

Change $e^2$ to $\underset{\uparrow \text{ charge of nucleus}}{Z}e^2$ and use appropriate reduced mass $\mu$

**Multi-electron atoms**

Complicated!

Multi-particle quantum state with interacting electrons

# Notes about Atomic Spectra Experiment

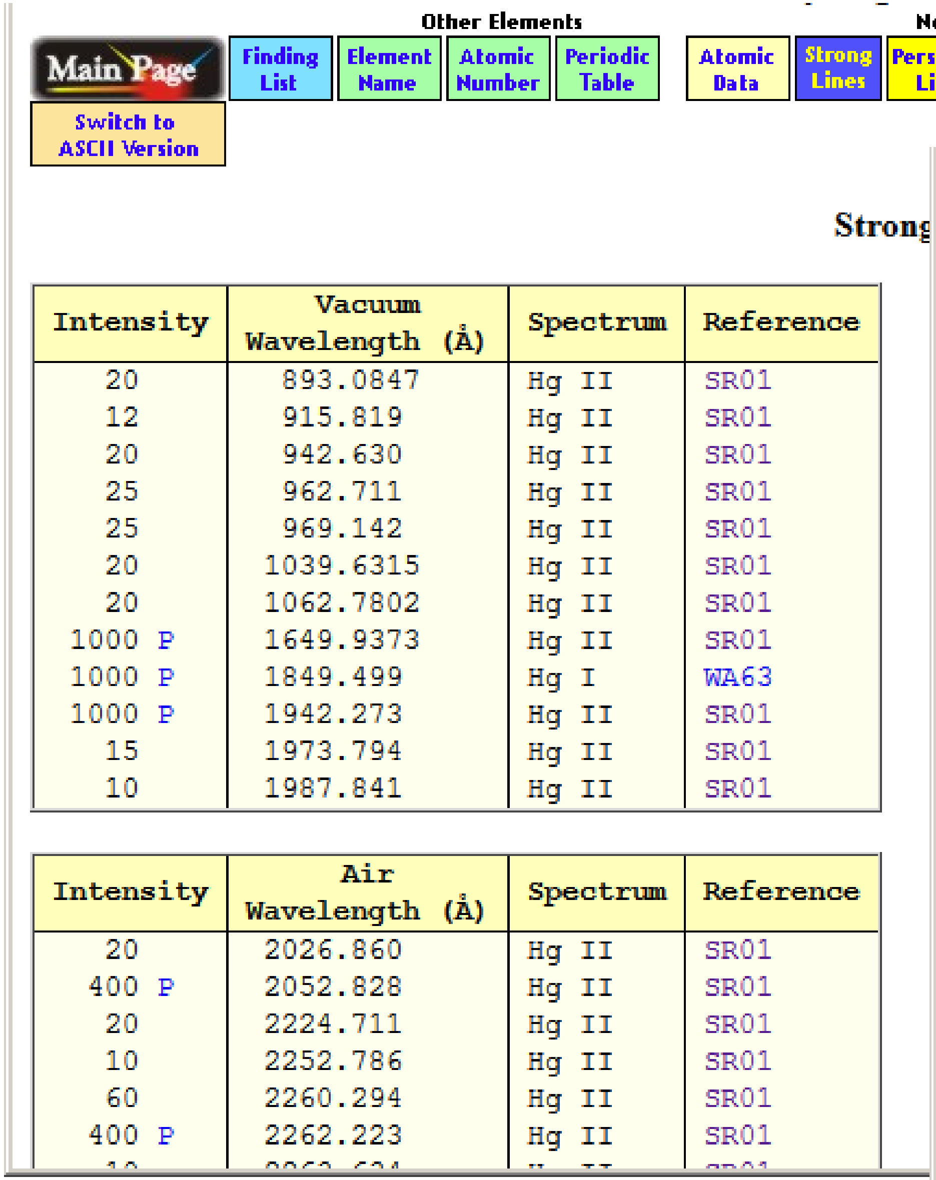
**Manual equipment and data recording**

- Uses a glass diffraction grating
- Figure out what the knobs do
- Vernier scale for angles – do you know how to read it?
- Grating needs to be aligned (might be OK already, or might not)

**Suggest using Matlab scripts for data analysis calculations**

**Evaluate measurement uncertainties**

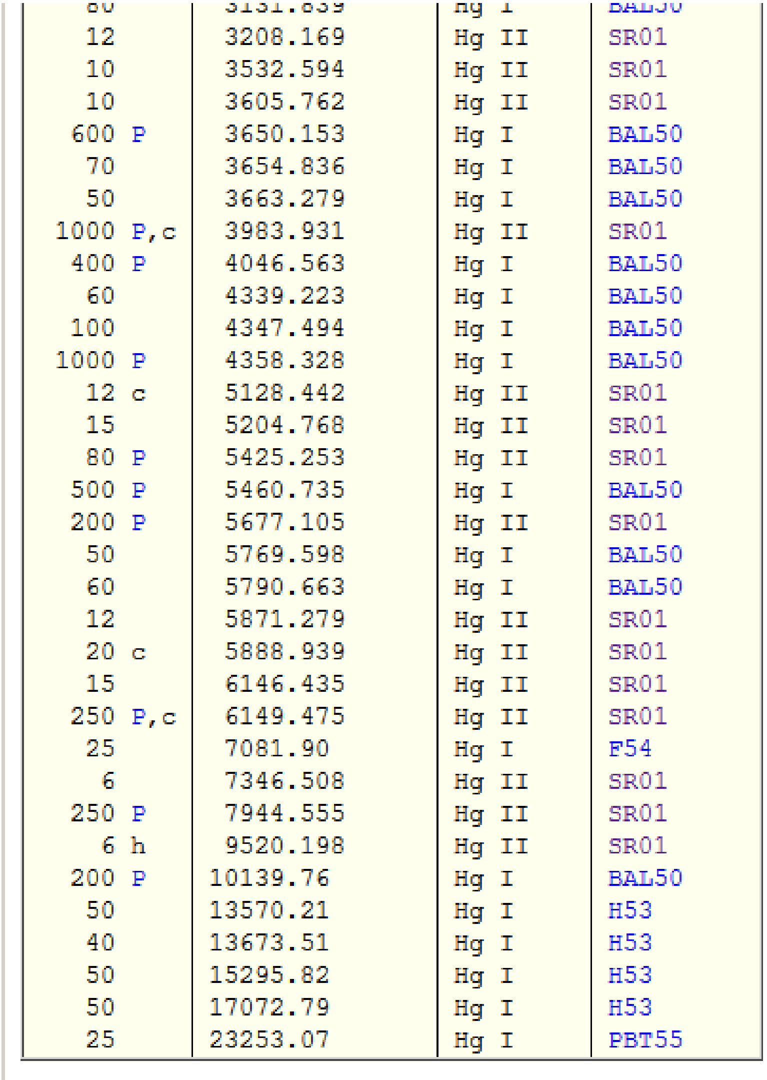
# http://physics.nist.gov/PhysRefData/Handbook/Tables/mercurytable2.htm



Strong

| Intensity | Vacuum Wavelength (Å) | Spectrum | Reference |
|---|---|---|---|
| 20 | 893.0847 | Hg II | SR01 |
| 12 | 915.819 | Hg II | SR01 |
| 20 | 942.630 | Hg II | SR01 |
| 25 | 962.711 | Hg II | SR01 |
| 25 | 969.142 | Hg II | SR01 |
| 20 | 1039.6315 | Hg II | SR01 |
| 20 | 1062.7802 | Hg II | SR01 |
| 1000 P | 1649.9373 | Hg II | SR01 |
| 1000 P | 1849.499 | Hg I | WA63 |
| 1000 P | 1942.273 | Hg II | SR01 |
| 15 | 1973.794 | Hg II | SR01 |
| 10 | 1987.841 | Hg II | SR01 |

| Intensity | Air Wavelength (Å) | Spectrum | Reference |
|---|---|---|---|
| 20 | 2026.860 | Hg II | SR01 |
| 400 P | 2052.828 | Hg II | SR01 |
| 20 | 2224.711 | Hg II | SR01 |
| 10 | 2252.786 | Hg II | SR01 |
| 60 | 2260.294 | Hg II | SR01 |
| 400 P | 2262.223 | Hg II | SR01 |



| | | | |
|---|---|---|---|
| 80 | 3131.839 | Hg I | BAL50 |
| 12 | 3208.169 | Hg II | SR01 |
| 10 | 3532.594 | Hg II | SR01 |
| 10 | 3605.762 | Hg II | SR01 |
| 600 P | 3650.153 | Hg I | BAL50 |
| 70 | 3654.836 | Hg I | BAL50 |
| 50 | 3663.279 | Hg I | BAL50 |
| 1000 P,c | 3983.931 | Hg II | SR01 |
| 400 P | 4046.563 | Hg I | BAL50 |
| 60 | 4339.223 | Hg I | BAL50 |
| 100 | 4347.494 | Hg I | BAL50 |
| 1000 P | 4358.328 | Hg I | BAL50 |
| 12 c | 5128.442 | Hg II | SR01 |
| 15 | 5204.768 | Hg II | SR01 |
| 80 P | 5425.253 | Hg II | SR01 |
| 500 P | 5460.735 | Hg I | BAL50 |
| 200 P | 5677.105 | Hg II | SR01 |
| 50 | 5769.598 | Hg I | BAL50 |
| 60 | 5790.663 | Hg I | BAL50 |
| 12 | 5871.279 | Hg II | SR01 |
| 20 c | 5888.939 | Hg II | SR01 |
| 15 | 6146.435 | Hg II | SR01 |
| 250 P,c | 6149.475 | Hg II | SR01 |
| 25 | 7081.90 | Hg I | F54 |
| 6 | 7346.508 | Hg II | SR01 |
| 250 P | 7944.555 | Hg II | SR01 |
| 6 h | 9520.198 | Hg II | SR01 |
| 200 P | 10139.76 | Hg I | BAL50 |
| 50 | 13570.21 | Hg I | H53 |
| 40 | 13673.51 | Hg I | H53 |
| 50 | 15295.82 | Hg I | H53 |
| 50 | 17072.79 | Hg I | H53 |
| 25 | 23253.07 | Hg I | PBT55 |