

Lecture 12

Waves, Particles, and Uncertainty

Outline of Lecture 12

- Matter and radiation have both attributes of *particles* and *waves*.
- The wave-particle duality endows all entities with a complementary *uncertainty* in position-momentum and energy-time, yielding new insight into the nature of why telescopes have an intrinsic limitation to their angular resolution.
- Electrons are *fermions* and satisfy *Pauli's exclusion principle*. The resulting *shell structure of electrons in atoms* explains the *periodic table of the elements* and the chemical properties of matter (and thereby of living organisms).

Code: uncertainty

The Quantum Revolution

- First Phase (Lectures 10 & 11):
 - **Max Planck** (1858-1947) introduces a new constant of nature to explain blackbody radiation: $h = 6.63 \times 10^{-34}$ joule s, $\hbar \equiv h / 2\pi$.
 - **Albert Einstein** (1879-1955) postulates in 1905 a *quantum of light* \equiv *photon* with energy $E = hc / \lambda$, where λ is the wavelength, to explain the photoelectric effect. Light is both a particle and a wave.
 - **Niels Bohr** (1885-1962) applies ideas of Einstein and de Broglie to explain the radiation spectrum of H atom.
- Second Phase (Lecture 12):
 - **Louis de Broglie** (1892-1987) hypothesizes *wave-particle duality* to hold also for matter. If p is the momentum of any kind of particle, then it has an associated wave whose wavelength is given by $\lambda = h / p$.
 - **Werner Heisenberg** (1901-1976) and **Erwin Schroedinger** (1887-1961) provides mathematical theories of new quantum theory:
 - Schroedinger's theory makes direct use of de Broglie's hypothesis.
 - Both descriptions imply the *uncertainty principle* $\Delta x \Delta p_x \geq \hbar$ and are different mathematical representations of the same physical theory -- *quantum mechanics*.
 - **Wolfgang Pauli** (1900-1958) proposes that electrons (and all other particles of half-integer spin -- *fermions*) satisfy an *exclusion principle*: no more than one fermion can occupy a given quantum microstate.

In 1924 De Broglie Writes Shortest PhD Thesis in History of Physics

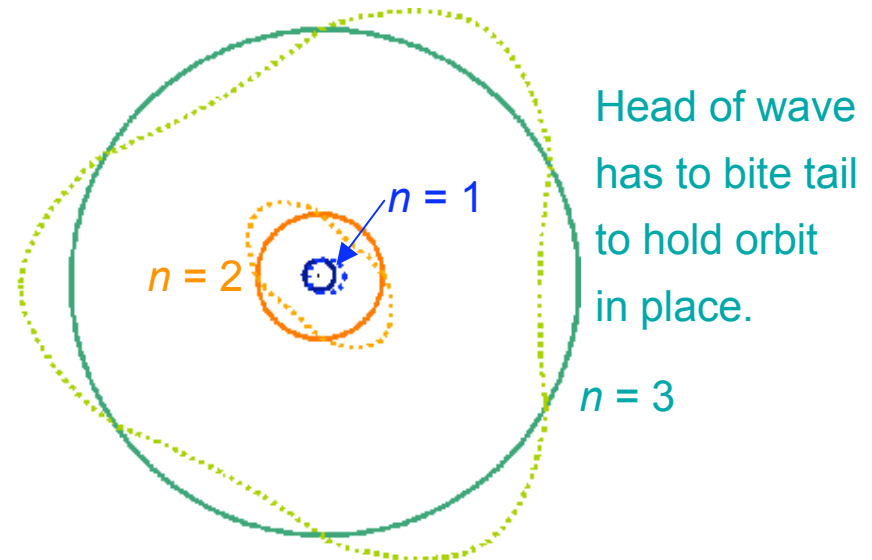
- Light of wavelength λ comes in indivisible packets (photons), each of momentum p with

$$p = \frac{E}{c} = \frac{h}{\lambda}.$$

- Matter particles of momentum $p = mv$ must have associated wavelength

$$\lambda = \frac{h}{p}.$$

- Einstein asked by Sorbonne examiners to comment on thesis.



$$2\pi r = n\lambda = n \frac{h}{m_e v}, \text{ with } n = 1, 2, 3, \dots,$$

which together with $e^2/r^2 = F = ma = m_e \frac{v^2}{r}$

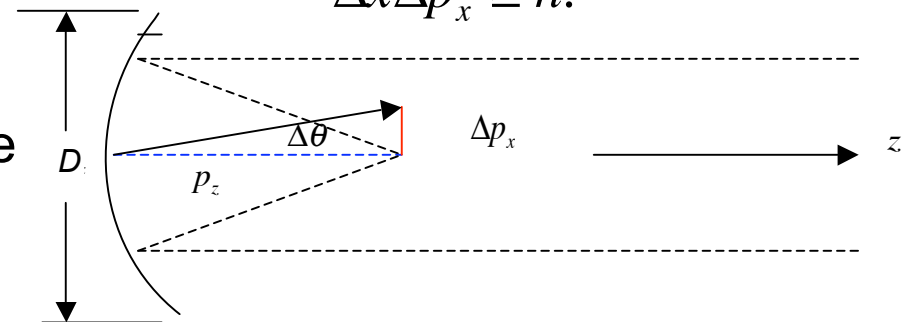
gives the same result as Bohr's hydrogen atom obtained from the quantization of angular momentum!

Quantum Mechanics

- In 1925 Heisenberg invents matrix mechanics, which is a correct version of quantum mechanics, but difficult to use to get practical answers.
- In 1926 Schroedinger invents wave mechanics, which is much easier to use and understand.
- What is waving? Max Born: function whose square gives probability distribution in space.
- In attempt to prove Schroedinger wrong, Heisenberg discovers uncertainty relations instead. These relations provide the key to understanding the equivalence of the matrix and wave approaches.

Product of uncertainties in simultaneous measurement of position and momentum:

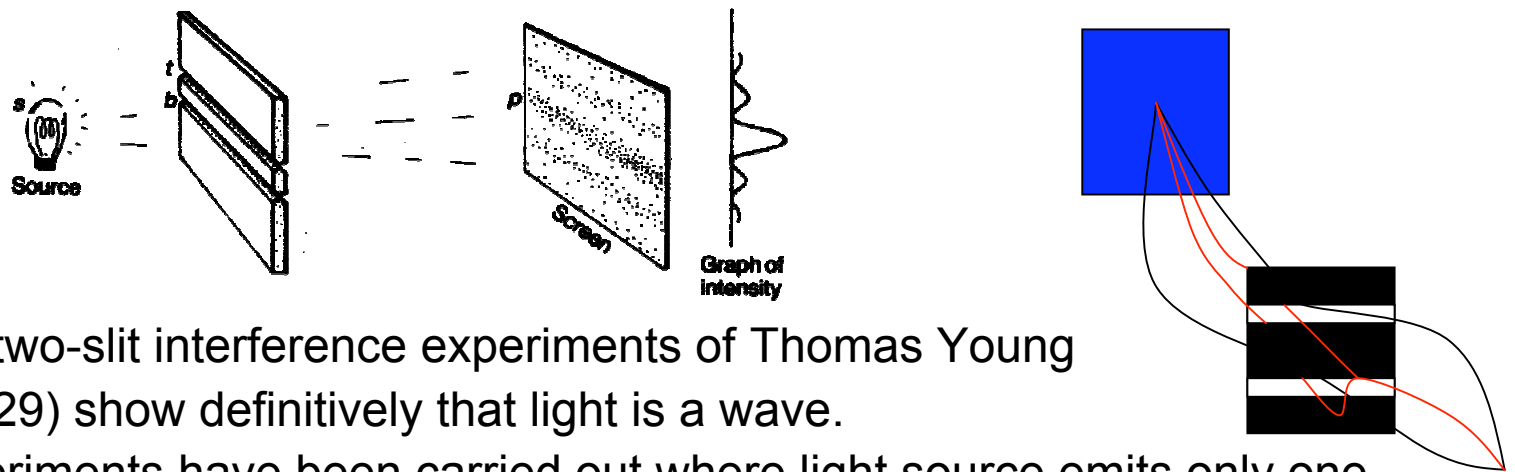
$$\Delta x \Delta p_x \geq \hbar.$$



$$\Delta \theta = \frac{\Delta p_x}{p_z} \geq \frac{\hbar / \Delta x}{h / \lambda} = \frac{\lambda}{D}$$

(with $\Delta x \sim D/2\pi$ somewhat arbitrarily), which is the statement of the diffraction limit of telescopes derived from treating light (photons) as a wave with $\lambda \ll D$.

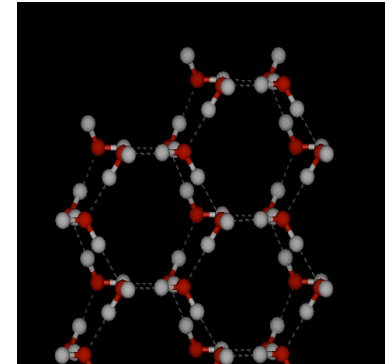
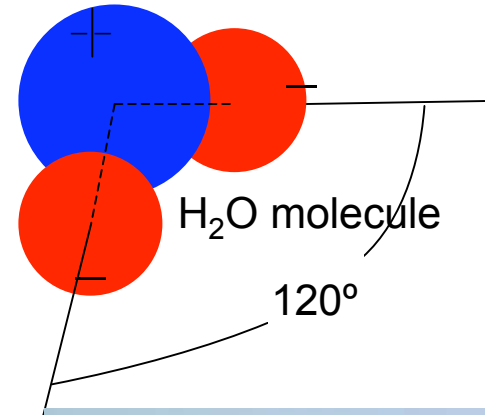
Two-Slit Experiment and Wave-Particle Duality



- Famous two-slit interference experiments of Thomas Young (1773-1829) show definitively that light is a wave.
- Yet, experiments have been carried out where light source emits only one photon at a time, and the same interference pattern still occurs. Photons (and everything else) always behave as both a particle and a wave.
- One might have thought that each photon must go through one slit or another. But in that case, how can it know how to go ahead of time so as to form statistically a brightness pattern appropriate for the two-slit experiment?
- Richard Feynman's interpretation is that each photon goes through both slits, by many paths (!), and interferes with itself (!). How can this be? (A person cannot go through two open doors at the same time. But you are physically much larger than your de Broglie wavelength.) Nevertheless, no one truly understands quantum mechanics, although many people can calculate its consequences given its mathematical rules.

Relationship of Quantum Theory to Chemistry and Materials Science

- The laws of quantum mechanics explain the structure of electronic shells surrounding atoms, which determine an atom's position in the periodic table of elements.
- Energy differences determine the pattern of spectral lines formed when radiative transitions induces changes in the electronic structure.
- The affinity of atoms for each other to become molecules depends on the ability of their outer electronic shells to form chemical bonds.
- Closed shells are preferred in such bonds because they represent states of least energy. Example: two hydrogen atoms plus one oxygen atom = water molecule H_2O .



Difference Between Fermions & Bosons

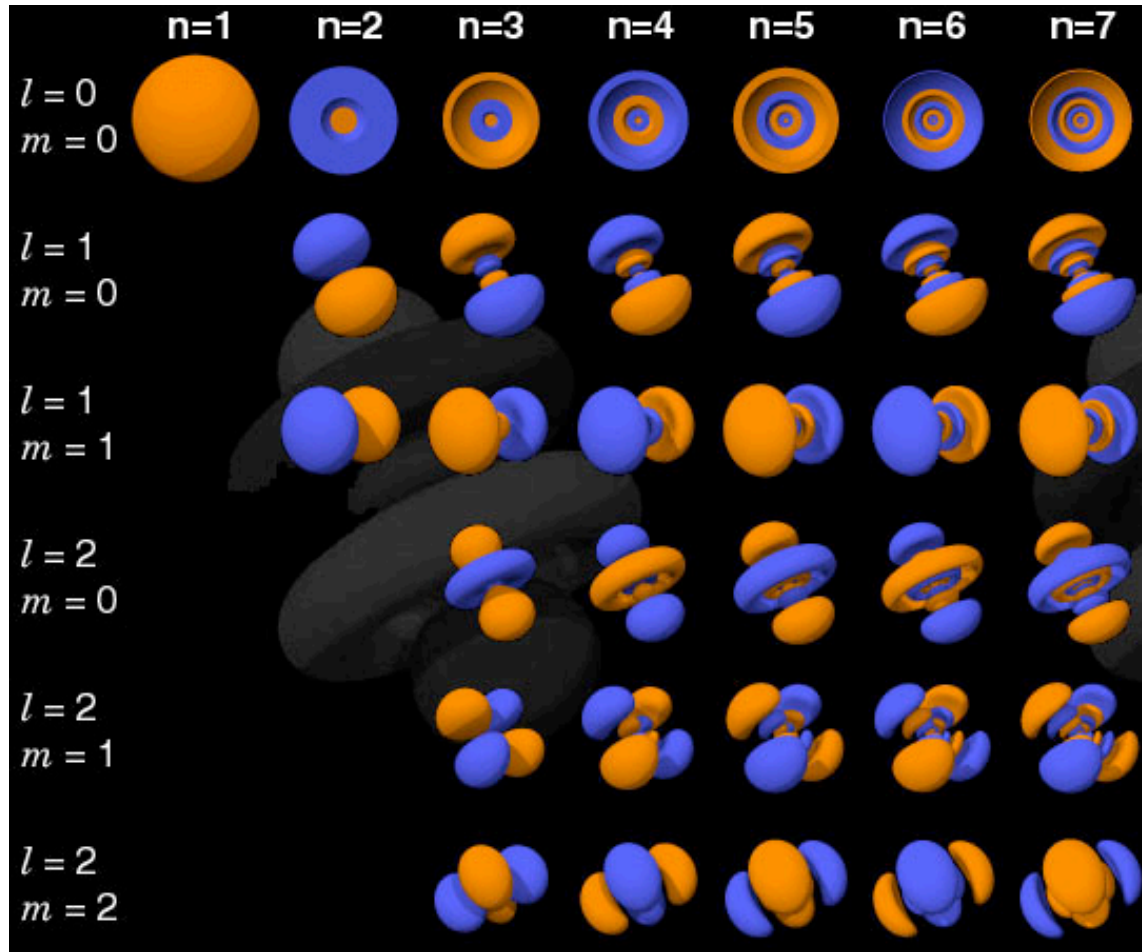
- Quantum Angular Momentum
 - Orbital angular momentum of an electron can only have integer multiples ℓ of \hbar with $\ell = 0, 1, 2, \dots, n-1$. For given ℓ , there are $2\ell+1$ possible orientations $m_\ell = -\ell, -\ell+1, \dots, 0, \dots, \ell-1, \ell$, of the vector angular momentum.
 - Spin angular momentum for an electron can take only one value $s = 1/2$ times \hbar , and have only $2s+1 = 2$ orientations $m_s = -1/2$ or $+1/2$. (“parallel” or “anti-parallel”).
- Pauli’s Exclusion Principle
 - All known particles have either integer spin (e.g., $s = 1$ for photons) and are called bosons (after Satyendranath Bose) or half-integer spin (e.g., $s = 1/2$ for electrons) and are called fermions (after Enrico Fermi).
 - A quantum state is defined by the collection of its quantum numbers, e.g., n, ℓ, m_ℓ, s, m_s .
 - Any number of bosons can occupy a given quantum state, but no more than one fermion of a given kind (e.g., electron, proton, or neutron) can occupy a given quantum state.

Periodic Table of the Elements

PERIODIC TABLE OF ELEMENTS

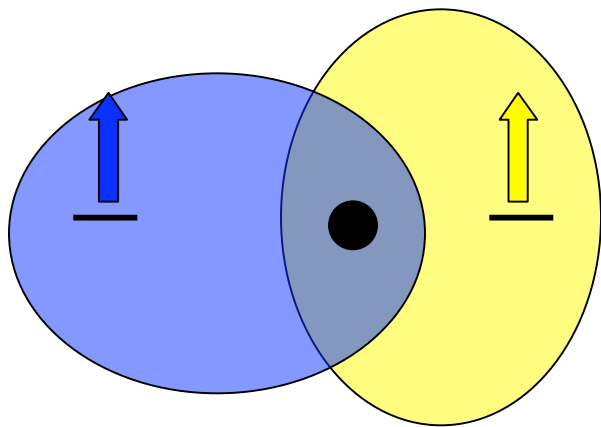
$n=1, l=0$	1 H																			$n=1, l=0$	2 He					
$n=2, l=0$	3 Li	4 Be																		$n=2, l=1$	5 B	6 C	7 N	8 O	9 F	10 Ne
$n=3, l=0$	11 Na	12 Mg																		$n=3, l=1$	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
$n=4, l=0$	19 K	20 Ca	$n=3, l=2$	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	4, 1	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr						
$n=5, l=0$	37 Rb	38 Sr	$n=4, l=2$	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	5, 1	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe						
$n=6, l=0$	55 Cs	56 Ba	$n=5, l=2$	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	6, 1	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn						
$n=7, l=0$	87 Fr	88 Ra	$n=6, l=2$	89 Ac	104 Rf	105 Ha								7, 1												
			$n=4, l=3$	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	Lanthanum series								
			$n=5, l=3$	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	Actinum series								

Shape of Electron Cloud in Different Atomic Orbitals

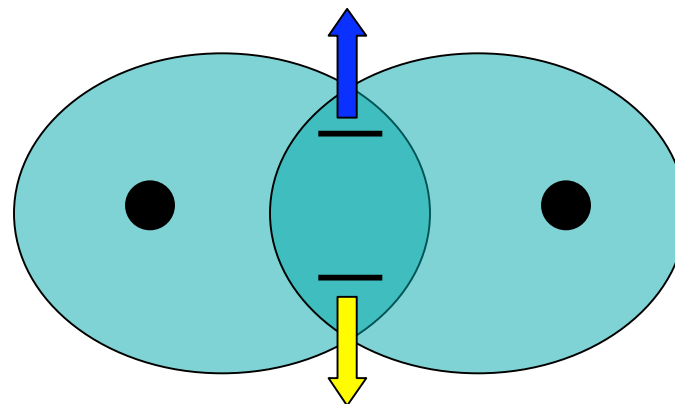


Role of Total Spin in Multi-Electron Atoms and Molecules

- Two electrons with the same spin orientation (arrows) orbiting a central nucleus (black dot) in an atom have different spatial orbitals (colored blobs) that tend to avoid one another, which is then less disruptive from an energetic viewpoint.

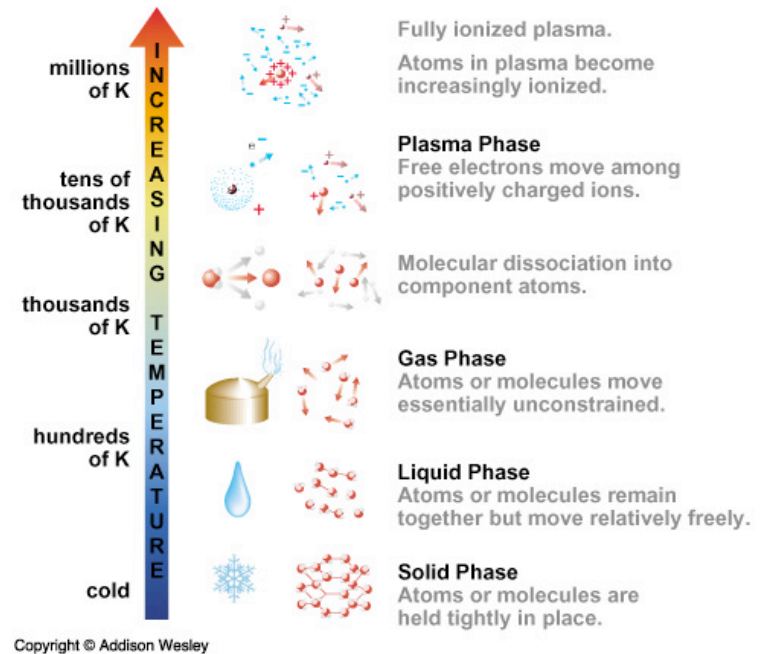


- Two electrons with opposite spin orientations in a diatomic molecule can have the same spatial orbital, allowing them to concentrate more their negative charge in the space between the two positively repulsing nuclei, thereby providing the chemical bond that holds the system together.



Reaction of Matter to Changing Temperature

- Raising temperature (at a given pressure) corresponds to greater random motions at microscopic levels.
- Bound states (gravitational, chemical, or nuclear) arise because of attractive forces. Repulsive forces are disruptive.
- At low temperatures, matter wants to settle into states with least energy (most bound).
- At high temperatures, matter wants to break free of its bonds (gravitational, chemical, or nuclear) and have more free particles (greater freedom).
- Maximizing entropy under given conditions of temperature and pressure represents then a tension between wanting to be more bound and having more freedom.
- As T increases: solid \rightarrow liquid \rightarrow molecular gas \rightarrow atomic gas \rightarrow lightly ionized gas \rightarrow fully ionized plasma \rightarrow gas of elementary particles \rightarrow sea of quarks & gluons \rightarrow ?



Summary

- Because **Planck's constant** $h = 6.64 \times 10^{-34}$ joule s is such a small quantity, its being nonzero escaped notice until scientists began to deal with microscopic bodies like **atoms** and **molecules**.
- Moreover, because **Pauli's exclusion principle** forbids **fermions** like electrons, protons, and neutrons, which are the constituents of ordinary matter, to occupy the same quantum state, the wavelike property of matter was late to attract notice relative to their particle-like attributes.
- In contrast, because light particles can act in unison – indeed, **photons like to be in the same state** (as in a laser beam), then the wavelike attributes of light are readily observable macroscopically. In turn, the particulate nature of photons is only apparent in the quantum interactions of light with individual particles of matter (such as electrons).