Modern Physics

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Lesson IX
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Seated (left to right): Erwin Schrödinger, Irène Joliot-Curie, Niels Bohr, Abram Ioffe, Marie Curie, Paul Langevin, Owen Willans Richardson, Lord Ernest Rutherford, Théophile de Donder, Maurice de Broglie, Louis de Broglie, Lise Meitner, James Chadwick.

Standing (left to right): Émile Henriot, Francis Perrin, Frédéric Joliot-Curie, Werner Heisenberg, Hendrik Kramers, Ernst Stahel, Enrico Fermi, Ernest Walton, Paul Dirac, Peter Debye, Francis Mott, Blas Cabrera y Felipe, George Gamow, Walther Bothe, Patrick Blackett, M. Rosenblum, Jacques Errera, Ed. Bauer, Wolfgang Pauli, Jules-Émile Verschaffelt, Max Cosyns, E. Herzen, John Douglas Cockcroft, Charles Ellis, Rudolf Peierls, Auguste Piccard, Ernest Lawrence, Léon Rosenfeld. (October 1933)

Balmer-Rydberg-Ritz formula

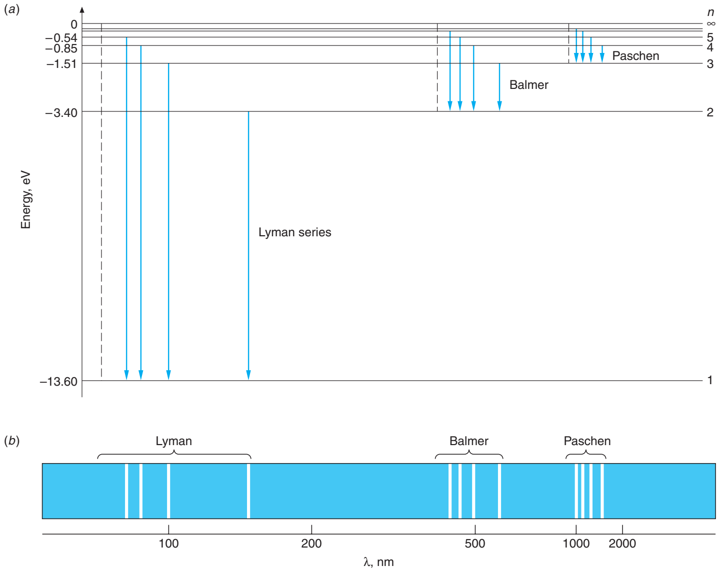
- When hydrogen in glass tube is excited by $5,000$ V discharge 4 lines are observed in visible part of emission spectrum
  - red @ 656.3 nm
  - blue-green @ 486.1 nm
  - blue violet @ 434.1 nm
  - violet @ 410.2 nm
- Explanation ☞ Balmer's empirical formula

$$\lambda = 364.56\, n^2/(n^2 - 4)\ \text{nm} \qquad n = 3, 4, 5, \cdots \tag{1}$$

- Generalized by Rydberg and Ritz to accommodate newly discovered spectral lines in UV and IR

$$\frac{1}{\lambda} = \mathcal{R}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) \qquad \text{for} \quad n_2 > n_1 \tag{2}$$

Atomic spectra



Rydberg constant

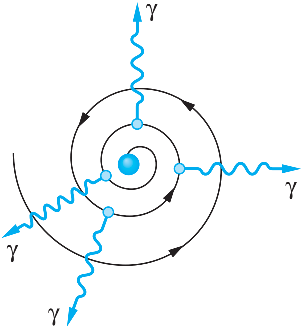
- For hydrogen ☞ $\mathcal{R}_{\rm H} = 1.096776 \times 10^7 \ {\rm m}^{-1}$
- Balmer series of spectral lines in visible region correspond to $n_1 = 2$ and $n_2 = 3, 4, 5, 6$
- Lines with $n_1 = 1$ in ultraviolet make up Lyman series
- Line with $n_2 = 2$ ☞ designated Lyman alpha has longest wavelength in this series: $\lambda = 121.57 \ {\rm nm}$
- For very heavy elements ☞ $\mathcal{R}_\infty = 1.097373 \times 10^7 \ {\rm m}^{-1}$

Thomson's atom

- Many attempts were made to construct atom model that yielded Balmer-Rydberg-Ritz formula
- It was known that:
  - atom was about 10^{-10} m in diameter
  - it contained electrons much lighter than the atom
  - it was electrically neutral
- Thomson hypothesis ☞ electrons embedded in fluid that contained most of atom mass and had enough positive charge to make atom electrically neutral
- He then searched for configurations that were stable and had normal modes of vibration corresponding to known frequencies of spectral lines
- One difficulty with all such models is that electrostatic forces alone cannot produce stable equilibrium

Rutherford's atom

- Atom ☞ positively-charged nucleus
  around which much lighter negatively-charged electrons circulate
  (much like planets in the Solar system)
- Contradiction with classical electromagnetic theory
  accelerating electron should radiate away its energy
- Hydrogen atom should exist for no longer than 5×10^{-11} s



Bohr's atom

- Attraction between two opposite charges ☞ Coulomb's law

$$\vec{F} = \frac{e^2}{r^2}\,\hat{\imath}_r\,, \tag{3}$$

- Since Coulomb attraction is central force (dependent only on r)

$$|\vec{F}| = -\frac{dV(r)}{dr} \tag{4}$$

- For mutual potential energy of proton and electron

$$V(r) = -\frac{e^2}{r} \tag{5}$$

- Bohr considered electron in circular orbit of radius r around proton
- To remain in this orbit ☞ electron needs centripetal acceleration

$$a = v^2/r \tag{6}$$

Bohr's atom (cont'd)

- Using (4) and (6) in Newton's second law

$$\frac{e^2}{r} = \frac{m_e v^2}{r} \tag{7}$$

- Assume m_p is infinite so that proton's position remains fixed (actually $m_p \approx 1836 m_e$)
- Energy of hydrogen atom is sum of kinetic and potential energies

$$E = K + V = \frac{1}{2} m_e v^2 - \frac{e^2}{r} \tag{8}$$

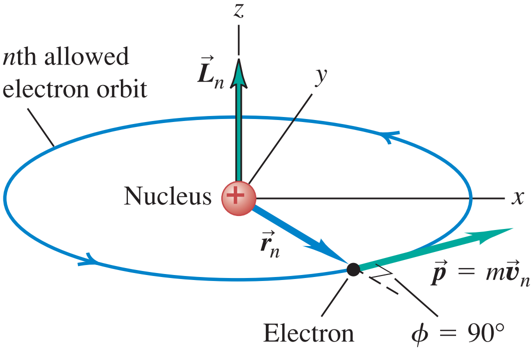
- Using (7)

$$K = -\frac{1}{2} V \quad \text{and} \quad E = \frac{1}{2} V = -K \tag{9}$$

- Energy of bound atom is negative since it is lower than energy of separated electron and proton which is taken to be zero

Bohr's atom (cont'd)

- For further progress ☞ restriction on values of r or v
- Angular momentum ☞ $\vec{L} = \vec{r} \times \vec{p}$
- Since $\vec{p}$ is perpendicular to $\vec{r}$ ☞ $L = rp = mvr$
- Using (9) ☞ $r = \frac{L^2}{me^2}$



Bohr's quantization

- Introduce angular momentum quantization

$$L = n\hbar \quad \text{with} \quad n = 1, 2, \cdots \tag{10}$$

excluding $n = 0$ ☞ electron would then not be in circular orbit

- Allowed orbital radii ☞ $r_n = n^2 a_0$

(Bohr radius ☞ $a_0 \equiv \frac{\hbar^2}{m_e e^2} = 5.29 \times 10^{-11}$ m $\simeq 0.529$ $\mathring{A}$)

- Corresponding energy $E_n = -\frac{e^2}{2a_0 n^2} = -\frac{m_e e^4}{2\hbar^2 n^2}, \quad n = 1, 2 \cdots$
- Balmer-Rydberg-Ritz formula

$$\frac{hc}{\lambda} = E_{n_2} - E_{n_1} = \frac{2\pi^2 m_e e^4}{h^2} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \tag{11}$$

$$\mathcal{R} = \frac{2\pi m_e e^4}{h^3 c} \approx 1.09737 \times 10^7 \text{ m}^{-1}$$

- Slight discrepency with experimental value for hydrogen

due to finite proton mass

Hydrogen-like ions systems

- Generalization for single electron orbiting nucleus

  ($Z = 1$ for hydrogen, $Z = 2$ for He$^+$, $Z = 3$ for Li^{++})

- Coulomb potential generalizes to

$$V(r) = -\frac{Ze^2}{r} \tag{12}$$

- Radius of orbit becomes

$$r_n = \frac{n^2 a_0}{Z} \tag{13}$$

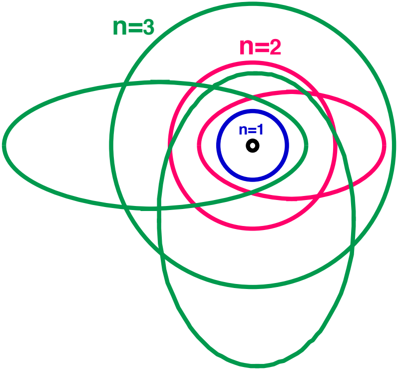
- Energy becomes

$$E_n = -\frac{Z^2 e^2}{2a_0 n^2} \tag{14}$$

Sommerfeld-Wilson quantization

Generalized Bohr's formula for allowed elliptical orbits

$$\oint p\, dr = nh \quad \text{with} \quad n = 1, 2, \cdots . \tag{15}$$



de Broglie wavelength

- In view of particle properties for light waves – photons – de Broglie ventured to consider reverse phenomenon
- Assign wave properties to matter:
  To every particle with mass m and momentum $\vec{p}$ ☞ associate

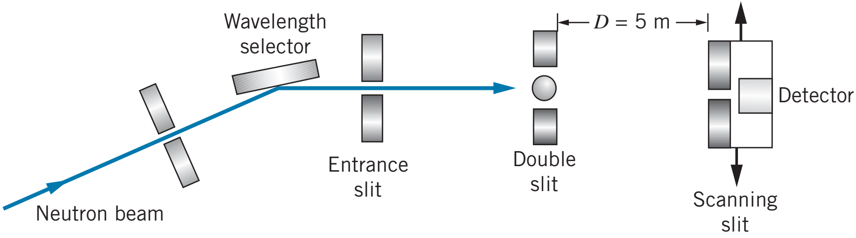
$$\lambda = h/|\vec{p}| \tag{16}$$

- Assignment of energy and momentum to matter
  in (reversed) analogy to photons

$$E = \hbar\omega \quad \text{and} \quad |\vec{p}| = \hbar|\vec{k}| = h/\lambda \tag{17}$$

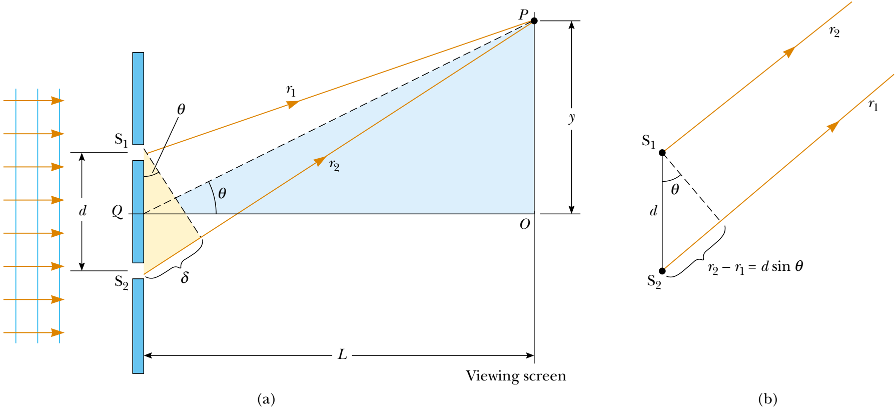
Neutron double-slit experiment

- Parallel beam of neutrons falls on double-slit
- Neutron detector capable of detecting individual neutrons
- Detector registers discrete particles localized in space and time
- This can be achieved if the neutron source is weak enough



- neutron kinetic energy ☞ 2.4×10^{-4} eV
- de Broglie wavelength ☞ 1.85 nm
- center-to-center distance between two slits ☞ $d = 126\ \mu\text{m}$

Recall Young's double-slit experiment



$$d \ll L \wedge \lambda \ll d \Rightarrow \theta \approx \sin\theta \approx \tan\theta \Rightarrow \delta(y)/d \approx y/L$$

Using approximations

- Bright fringes measured from O are @

$$y_{\rm bright} = \frac{\lambda L}{d} m \qquad m = 0, \pm 1, \pm 2, \cdots \tag{18}$$

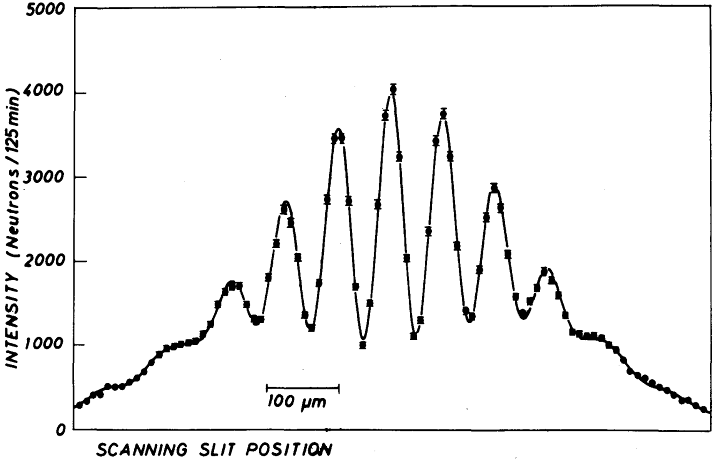
  m ☞ order number
  when $\delta = m\lambda$ ☞ constructive interference

- Dark fringes measured from O are @

$$y_{\rm dark} = \frac{\lambda L}{d} (m + \tfrac{1}{2}) \qquad m = 0, \pm 1, \pm 2, \cdots \tag{19}$$

  when δ is odd multiple of $\lambda/2$ ☞ two waves arriving at point P are out of phase by π and give rise to destructive interference

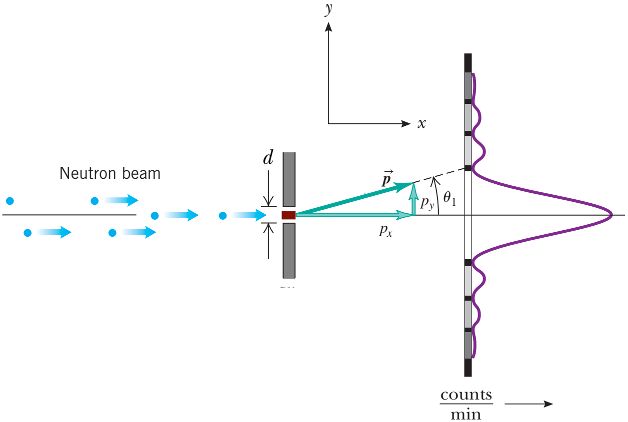
- In neutron double-slit experiment ☞ $L \to D$



Estimating spacing $(y_{n+1} - y_n) \approx 75\ \mu\mathrm{m}$

$$\lambda = \frac{d\ (y_{n+1} - y_n)}{D} = 1.89\ \mathrm{nm} \tag{20}$$

Result agrees with de Broglie wavelength predicted for neutron beam!



- θ_1 ☞ angle between central maximum and first minimum
- for $m = 1$ ☞ $\sin\theta_1 = \lambda/d$
- neutron striking screen at outer edge of central maximum must have component of momentum p_y as well as a component p_x
- from the geometry ☞ components are related by $p_y/p_x = \tan\theta_1$
- use approximation $\tan\theta_1 = \theta_1$ and $p_y = p_x\,\theta_1$

Heisenberg's uncertainty principle

- All in all ☞ $$p_y = p_x \, \lambda/d \tag{21}$$
- Neutrons striking detector within central maximum
  i.e. angles between $(-\lambda/d, +\lambda/d)$
  have y-momentum-component spread over $(-p_x\lambda/d, +p_x\lambda/d)$
- Symmetry of interference pattern shows $\langle p_y \rangle = 0$
- There will be an *uncertainty* Δp_y at least as great as $p_x\lambda/d$

$$\Delta p_y \geq p_x \, \lambda/d \tag{22}$$

- The narrower the separation between slits d
  the broader is the interference pattern
  and the greater is the uncertainty in p_y
- Using de Broglie relation $\lambda = h/p_x$ and simplifying

$$\Delta p_y \geq p_x \frac{h}{p_x d} = \frac{h}{d} \tag{23}$$

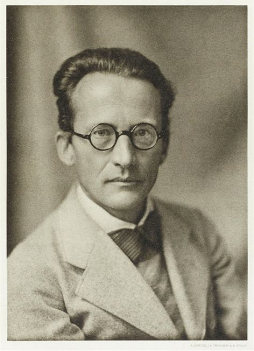
Heisenberg's uncertainty principle (cont'd)

What does this all mean?

- $d \equiv \Delta y$ represents uncertainty in y-component of neutron position as it passes through the double-slit gap
  (We don't know where in gap each neutron passes through)
- Both y-position and y-momentum-component have uncertainties related by ☞
  $$\Delta p_y \, \Delta y \geq h \qquad (24)$$
- We reduce Δp_y only by reducing width of interference pattern
  To do this ☞ increase d which increases position uncertainty Δy
- Conversely
  we decrease position uncertainty by narrowing doubl-slit gap
  interference pattern broadens
  and corresponding momentum uncertainty increases


$\Delta x \, \Delta p_x \geq \frac{\hbar}{2}$
Werner Heisenberg, 1927

- Schrödinger equation plays role of Newton's laws and conservation of energy in classical mechanics
  ☞ it predicts future behavior of dynamic system
- It is a wave equation in terms of wavefunction which predicts analytically and precisely the probability of events or outcome
- Actually ☞ detailed outcome is not strictly determined but given a large number of events Schrödinger equation will predict the distribution of results



Time dependent Schrödinger equation

- It is not possible to derive the Schrödinger equation in any rigorous fashion from classical physics
- However ☞ it had to come from somewhere and it is indeed possible to “derive” the Schrödinger equation using somewhat less rigorous means
- Consider particle with mass m and momentum p_x moving in 1-dimension in potential $V(x)$ ☞ total energy is

$$E = \frac{p_x^2}{2m} + V(x) \tag{25}$$

- Multiplying both sides of (25) by wave function $\psi(x,t)$ should not change equality

$$E\psi(x,t) = \left[\frac{p_x^2}{2m} + V(x)\right]\psi(x,t) \tag{26}$$

Time dependent Schrödinger equation (cont'd)

- Recall de Broglie relations

$$p_x = \hbar k_x \quad \text{and} \quad E = \hbar \omega \tag{27}$$

- Suppose wave function is plane wave traveling in x direction with a well defined energy and momentum

$$\psi(x,t) = A_0 e^{i(k_x x - \omega t)} \tag{28}$$

- Energy relation in terms of de Broglie variables becomes

$$\hbar \omega A_0 e^{i(k_x x - \omega t)} = E A_0 e^{i(k_x x - \omega t)} \tag{29}$$

$$\left[\frac{\hbar^2 k_x^2}{2m} + V(x)\right] A_0 e^{i(k_x x - \omega t)} = \left[\frac{p_x^2}{2m} + V(x)\right] A_0 e^{i(k_x x - \omega t)} \tag{30}$$

Time dependent Schrödinger equation (cont'd)

- For equality in (29) to hold

$$E\psi(x,t) = i\hbar \frac{\partial}{\partial t}\psi(x,t) \tag{31}$$

- For equality in (30) to hold

$$p_x\psi(x,t) = -\hbar \frac{\partial}{\partial x}\psi(x,t) \tag{32}$$

Puttin'all this together ☞ time-dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = \left[-\frac{h^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x,t) \tag{33}$$

Time dependent Schrödinger equation (cont'd)

2nd-order linear differential equation with 3 important properties

- it is consistent with energy conservation
- it is linear and singular value ☞ solutions can be constructed by superposition of two or more independent solutions
- free-particle solution ☞ $V(x) = 0$
  consistent with a single de Broglie wave

Time independent Schrödinger equation

- If potential energy is independent of time
  use mathematical technique known as separation of variables
- Assume

$$\psi(x,t) = \psi(x)\,\chi(t) \tag{34}$$

- Substitution into time dependent Schrödinger equation yields

$$i\hbar \frac{\partial}{\partial t}\chi(t) = E\chi(t) = \hbar\omega\chi(t) \tag{35}$$

$$\left[-\frac{h^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = E\psi(x) \tag{36}$$

- Solution to (35) ☞ oscillating complex exponential

$$\chi(t) = e^{-iEt/\hbar} = e^{-i\omega t} \tag{37}$$

- Solution to (36) ☞ an eigenvalue problem

Time independent Schrödinger equation

2nd-order linear differential equation with 3 important properties

- *Continuity:* Solutions $\psi(x)$ to (36) and its first derivative $\psi'(x)$ must be continuous $\forall x$ (the latter holds for finite potential $V(x)$)
- *Normalizable:* Solutions $\psi(x)$ to (36) must be square integrable integral of modulus squared of wave function over all space must be finite constant so that wave function can be normalized
$$\int |\psi(x)|^2 \, dx = 1$$
- *Linearity:* Given two independent solutions $\psi_1(x)$ and $\psi_2(x)$ can construct other solutions by taking superposition of these
$$\psi(x) = \alpha_1 \, \psi_1(x) + \alpha_2 \, \psi_2(x)$$
$\alpha_i \in \mathbb{C}$ satisfying $|\alpha_1|^2 + |\alpha_2|^2 = 1$ to ensure normalization.