Quantum Mechanics

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Lesson III
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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-mile Verschaffelt, Max Cosyns, E. Herzen, John Douglas Cockcroft, Charles Ellis, Rudolf Peierls, Auguste Piccard, Ernest Lawrence, Léon Rosenfeld. (October 1933)

So far in this class, we've learned these constants, in some sense parameters of the universe:

- e, the electron charge;
- m_e, the electron mass;
- h, Planck's constant.

Can we derive a length scale from these units? Let's say

$$l_{natural} = m_e^{\alpha}(e^2)^{\beta}h^{\gamma}.$$

Remember that e^2 has units

$$F \cdot l^2 = \frac{ml^3}{t^2}$$

and h has units

$$h = E \cdot t = \frac{ml^2}{t}.$$

We can plug these in:

$$l_{natural} = m^{\alpha} \cdot \left(ml^3t^{-2}\right)^{\beta} \cdot \left(ml^2t^{-1}\right)^{\gamma}.$$

We want the units on the right to multiply out to l, so:

$$\begin{aligned} \alpha + \beta + \gamma &= 0 && (4.1)\\ 3\beta + 2\gamma &= 1 && (4.2)\\ -2\beta - \gamma &= 0 && (4.3)\\ & && (4.4) \end{aligned}$$

Solving this (details omitted) gives us $(\alpha, \beta, \gamma) = (-1, -1, 2)$. Thus, the "natural" unit length derived from these constants is

$$l_{natural} = m_e^{-1}(e^2)^{-1}h^2 = \frac{h^2}{m_e e^2} = (2\pi)^2 \cdot 0.528\text{Å}.$$

It turns out that 0.528Å is the radius of a hydrogen atom. This isn't a coincidence! We'll see the constant

Balmer-Rydberg-Ritz formula

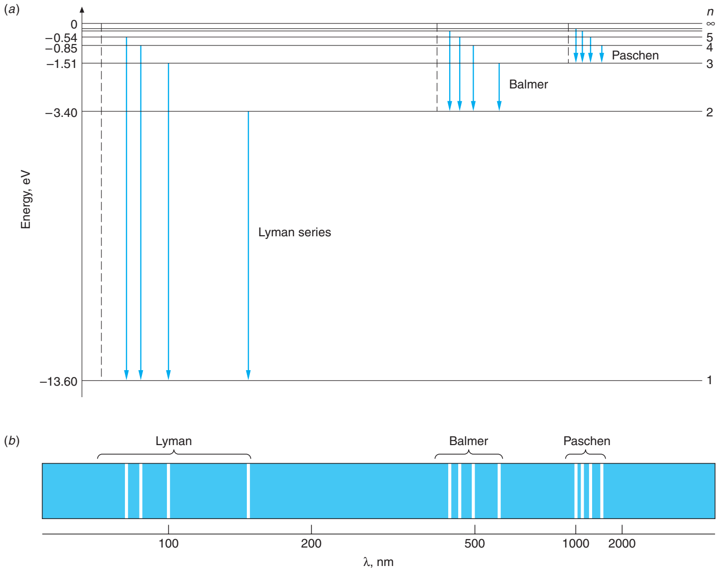
- When hydrogen in glass tube is excited by $5,000$ V discharge 4 lines are observed in visible part of emission spectrum
  - red @ 656.3 nm
  - blue-green @ 486.1 nm
  - blue violet @ 434.1 nm
  - violet @ 410.2 nm
- Explanation ☞ Balmer's empirical formula

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

- 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

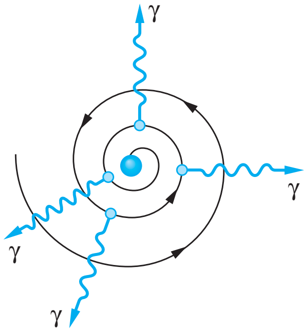
- For hydrogen ☞ $\mathcal{R}_{\rm H} = 1.096776 \times 10^7~{\rm m}^{-1}$
- Balmer series of spectral lines in visible region correspond to $n_1 = 2$ and $n_2 = 3, 4, 5, 6$
- Lines with $n_1 = 1$ in ultraviolet make up Lyman series
- Line with $n_2 = 2$ ☞ designated Lyman alpha has longest wavelength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

$$\vec{F} = \frac{e^2}{r^2}\,\hat{\imath}_r \qquad (\text{Gaussian} - \text{cgs units}) \tag{3}$$

- 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

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

- 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

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

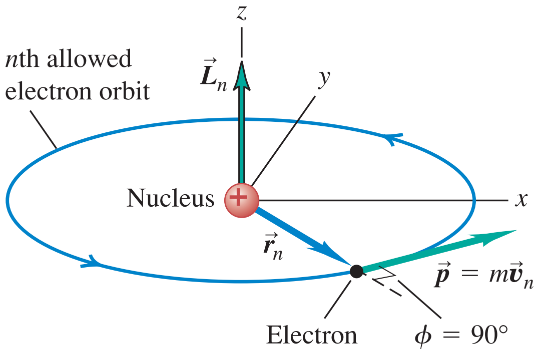
- Using (7)

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

- 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 $\vec{r}$ ☞ $L = rp = m_e v r$
- Using (9) ☞ $r = \frac{L^2}{m_e e^2}$



Bohr's quantization

- Introduce angular momentum quantization

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

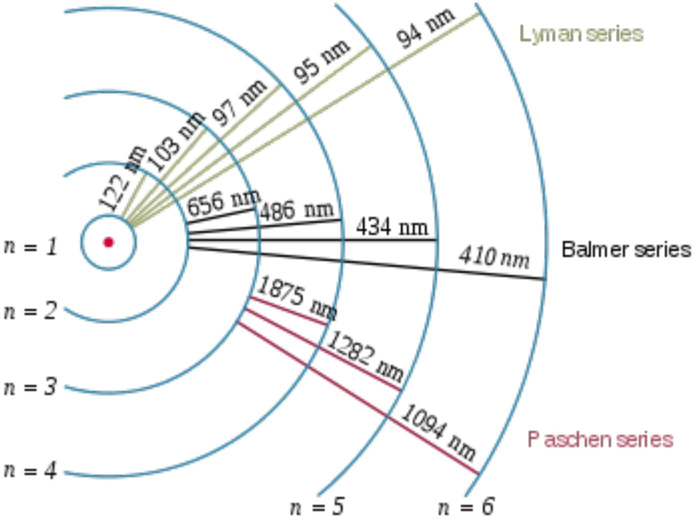
excluding $n = 0$ ☞ electron would then not be in circular orbit

- 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


Lyman series
Balmer series
Paschen series
94 nm
95 nm
97 nm
103 nm
122 nm
656 nm
486 nm
434 nm
410 nm
1875 nm
1282 nm
1094 nm
n = 1
n = 2
n = 3
n = 4
n = 5
n = 6

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

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

Quantize all the things!

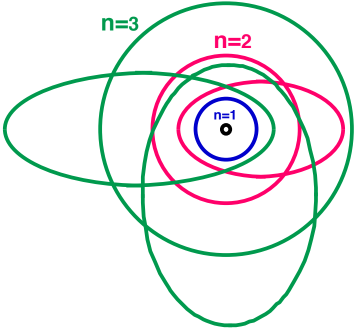
- So far we've discussed two kinds of quantization:
  - Quantization of EM energy for a harmonic oscillator into lumps h led to understanding of blackbody radiation
  - Quantization of angular momentum L led to the Bohr atom
- The natural question arising from this is: what else can we quantize?
- Wilson and Sommerfeld proposed general rule:
  If we integrate variables with respect to their conjugate variables in a closed action ☞ we get a multiple of h

$$\oint p \, dq = nh$$

if p, q are conjugate and the integral is over one cycle

Generalized Bohr's formula for allowed elliptical orbits

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



Applying rule to conjugate variables L, θ gives us:

$$\oint L \cdot d\theta = 2\pi L = nh = \frac{nh}{2\pi} = n\hbar$$

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

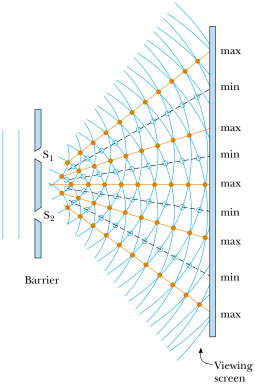
$$\lambda = h/|\vec{p}| \tag{16}$$

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

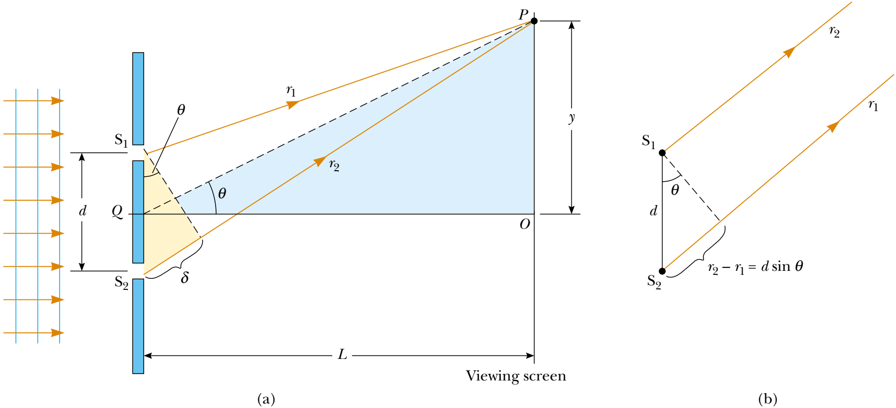
$$E = \hbar\omega \quad \text{and} \quad |\vec{p}| = \hbar|\vec{k}| = h/\lambda \tag{17}$$

Light waves ☞ Young's double slit experiment

- Monochromatic light from a single concentrated source illuminates a barrier containing two small openings
- Light emerging from two slits is projected onto distant screen
- Distinctly ☞ we observe light deviates from straight-line path and enters region that would otherwise be shadowed



Aproximations



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

Interference

- Bright fringes measured from O are @

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

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

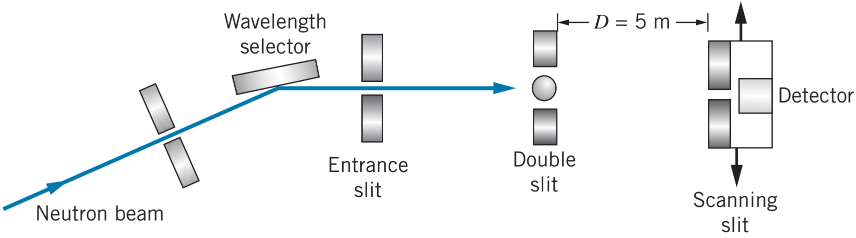
- Dark fringes measured from O are @

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

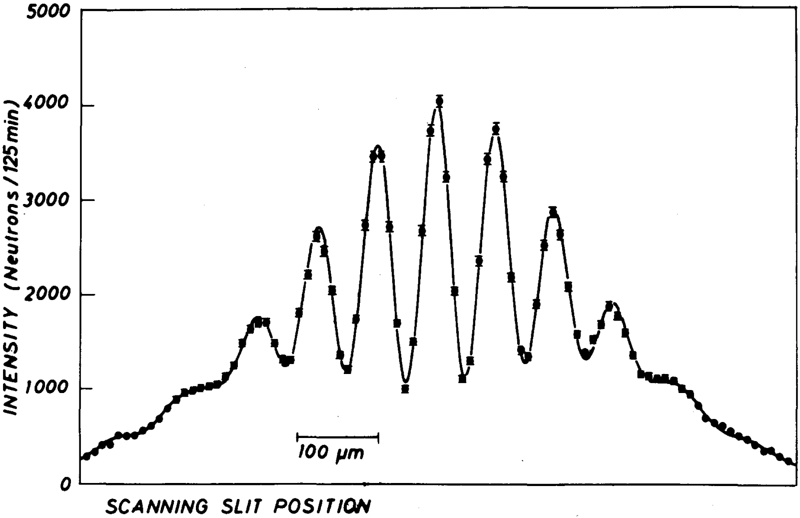
when δ is odd multiple of $\lambda/2$ ☞ two waves arriving at point P are out of phase by π and give rise to destructive interference

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 ☞ $d = 126\ \mu\text{m}$



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

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

Heisenberg's Uncertainty Principle

uncertainty in momentum

$$\Delta x \Delta p \geq \frac{h}{4\pi} = \frac{\hbar}{2}$$

uncertainty in position

The more accurately you know the position (i.e., the smaller Δx is), the less accurately you know the momentum (i.e., the larger Δp is); and vice versa

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Heisenberg realised that ...

- In the world of very small particles, one cannot measure any property of a particle without interacting with it in some way

- This introduces an unavoidable uncertainty into the result

- One can never measure all the properties exactly

Werner Heisenberg (1901-1976)
Image in the Public Domain

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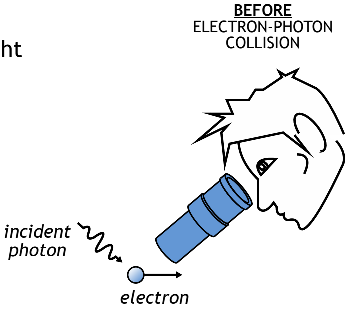
Measuring Position and Momentum of an Electron

- Shine light on electron and detect reflected light using a microscope
- Minimum uncertainty in position is given by the wavelength of the light
- So to determine the position accurately, it is necessary to use light with a short wavelength



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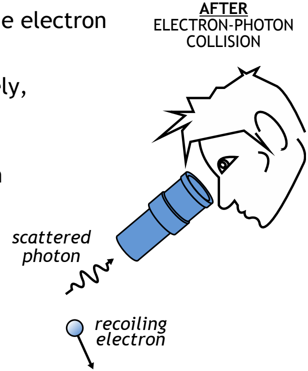
Measuring Position and Momentum of an Electron

- By Planck's law $E = hc/\lambda$, a photon with a short wavelength has a large energy
- Thus, it would impart a large 'kick' to the electron
- But to determine its momentum accurately, electron must only be given a small kick
- This means using light of long wavelength



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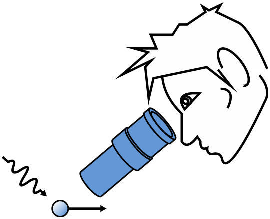
Light Microscopes



- Suppose the positions and speeds of all particles in the universe are measured to sufficient accuracy at a particular instant in time
- It is possible to predict the motions of every particle at any time in the future (or in the past for that matter)

"An intelligent being knowing, at a given instant of time, all forces acting in nature, as well as the momentary positions of all things of which the universe consists, would be able to comprehend the motions of the largest bodies of the world and those of the smallest atoms in one single formula, provided it were sufficiently powerful to subject all the data to analysis; to it, nothing would be uncertain, both future and past would be present before its eyes."

Pierre Simon Laplace

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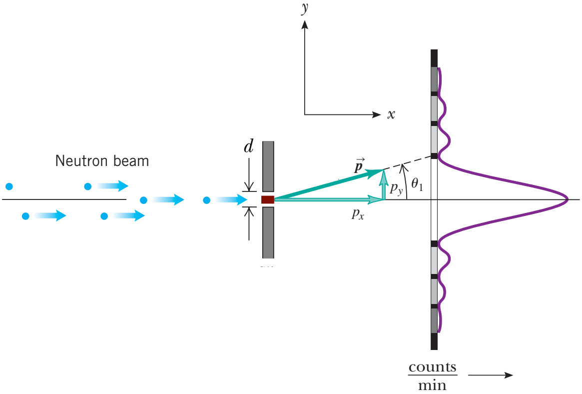
Feynman reasoning



- 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)

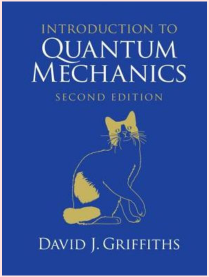
What does this all mean?

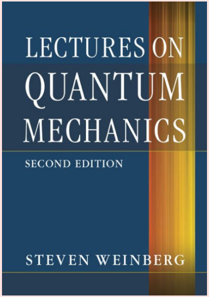
- $d \equiv \Delta y$ represents uncertainty in y-component of neutron position as it passes through the double-slit gap
  (We don't know where in gap each neutron passes through)
- Both y-position and y-momentum-component have uncertainties related by ☞

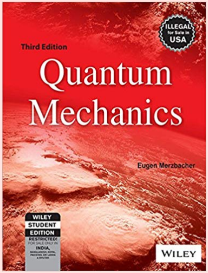
$$\Delta p_y \, \Delta y \geq h \tag{24}$$

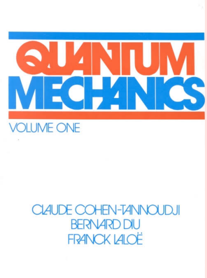
- We reduce Δp_y only by reducing width of interference pattern
  To do this ☞ increase d which increases position uncertainty Δy
- Conversely
  we decrease position uncertainty by narrowing doubl-slit gap
  interference pattern broadens
  and corresponding momentum uncertainty increases

Bibliography









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