Quantum Mechanics/Wave Theory

- Rapid progress made in development of QM thanks to many
  - Heisenberg, Born, Dirac…/DeBroglie, Schrödinger,…
- Historically
  - de Broglie (PhD student!) in1924 saw light was being described both by classic wave theory (e.g., Maxwell) and by particles (Planck-Einstein, with supporting evidence by Millikan (1916) and Compton (1923) showing $p_{photon}=h/\lambda$)
  - if photon could be described as particle and wave, why not matter particles too

    $\lambda=h/p=h/m\text{v}$ (h=6.626×10^{-34}Jsec)
    - so 1 g pebble moving at 1 cm/s ⇒ $\lambda\sim10^{-19}$ nm (λ/D<<1)

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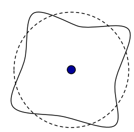
Electron Wavelength

- For electron in orbit, if electron is a wave, then an integral number of wavelengths must fit orbit perimeter



$$2\pi r = n\lambda = n\frac{h}{p} = n\frac{h}{m_e \text{v}_e}$$

$$\Rightarrow m_e \text{v}_e r = L = n\hbar$$ **same as Bohr model**

- If matter can be described as waves, need new dynamic equations (similar to EM/optical wave theory) to treat waves
  - will lead to **Schrödinger Equation**

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A Modern Interpretation of QM

- Understanding wave/matter duality has most commonly been approached based on the concepts of probability
- Postulate based on importance of observables
  - for “large” (macroscopic) systems, we can make measurements/observations without significantly disturbing our system
  - for “small” systems, the disturbance associated with making the observation is not negligible, it impacts the system

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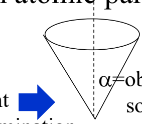
Example of Measurement Impact

- Consider optical microscope used to observe an atomic particle
  - optical theory says resolving power of a microscope given by $\Delta x \sim \lambda / \sin\alpha$ (λ = light wavelength)



- To characterize a particle’s dynamic state need to measure, for example: x (position) **and** p (momentum)
  - to improve Δx would need to reduce λ (e.g., from visible→uv→xrays)
  - BUT light (photon) involved in measurement would interact with particle, transfer some momentum to/from atom
- Uncertainty in momentum transferred due to photon being scattered into our observation solid angle

$$|\Delta p_x| = p\sin\alpha = \frac{h}{\lambda}\sin\alpha$$

Heisenberg Uncertainty Principle

- Multiplying both uncertainties to get our "least" uncertainty (best resolution) of this product $\Delta x\,|\Delta p_x| \cong \dfrac{\lambda}{\sin\alpha}\dfrac{h}{\lambda}\sin\alpha = h$
- Correct expression is $\boxed{\Delta x\,|\Delta p_x| \geq h/2\pi}$ **Heisenberg Uncertainty Principle**
  - can't know position **and** momentum of particle to arbitrarily high accuracy
- Causality only applies to undisturbed systems
  - observation causes non-negligible disturbance
- With causality "broken", we can only examine probabilities for subsequent measurements
  - wave aspect of matter connected to probability of finding a particle at some specific location

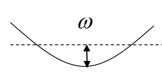
Review of Wave Equation Solutions

- Consider 1-d wave equation in space (x) and time (t)

$$\frac{\partial^2\omega}{\partial x^2} = \frac{1}{u^2}\frac{\partial^2\omega}{\partial t^2}$$

wave displacement

propagation speed



- x and t dependence independent, so can use separation of variables (SOV)
  - assume solution of form $\omega = \mathrm{f}(x)\,\mathrm{g}(t) = \mathrm{f}(x)\,e^{i2\pi\nu t}$
  - insert into wave equation

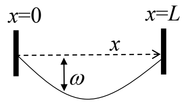
wavenumber

$$\frac{\partial^2 \mathrm{f}}{\partial x^2} = \frac{1}{u^2}(i2\pi\nu)^2\,\mathrm{f} \quad \rightarrow \boxed{\mathrm{f}''(x) + K^2\mathrm{f}(x) = 0} \qquad K \equiv \frac{2\pi\nu}{u} = \frac{2\pi}{\lambda}$$

  - standing wave eqn. (Helmholtz eqn)

Boundary Conditions: Vibrating String

$$f''(x) + K^2 f(x) = 0$$



- Problem not well-posed yet, need boundary conditions (BC)
  - consider string fixed at ends
  - BC are $\omega(t,0) = \omega(t,L) = 0$
  - which means $f(0) = f(L) = 0$

so BC are periodic

- By inspection, general solution should be of form

$$f = B\sin(Kx) + C\cos(Kx)$$

- Applying BC: $f(0) = 0 = C\cos(0) \Rightarrow C=0$

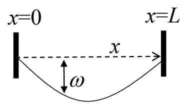
  $f(L) = 0 = B\sin(KL)$
  - either B=0 (boring) or $\sin(KL) = 0 \Rightarrow KL = n\pi$

    $n=0, 1, 2, \ldots$

Eigenvalues and Eigenfunctions

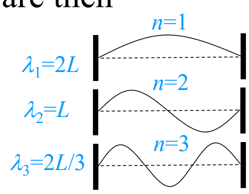
- So BC produce requirement that $KL=n\pi$ or we can write $\boldsymbol{K_n = n\pi/L}$

  n related to quantum numbers



  - **quantized wavenumbers**
  - can also define quantized wavelengths
    - $\lambda_n = 2\pi/K_n = \mathbf{2L/n}$
  - K_n (or λ_n) are the **eigenvalues** of the system
- Solutions for this 1-d wave problem are then

$$f(x) = \sum_{n=0}^{\infty} \underbrace{B_n}_{\text{amplitudes}} \underbrace{\sin(K_n x)}_{\text{eigenfunctions}} = \sum_{n=0}^{\infty} B_n \underbrace{\sin(2\pi x/\lambda_n)}_{\text{eigenfunctions}}$$



all possible solutions are superpositions of the eigenfunctions, scaled by their amplitudes

Superposition Example

- Any possible f(x) must be superposition of eigenmodes
- Example: non-symmetric (spatially) decaying oscillation

$$f(x) = \overset{B_1}{0.02}\sin\left(\frac{2\pi x}{\underset{\lambda_1}{2L}}\right) + \overset{B_2}{0.05}\sin\left(\frac{2\pi x}{\underset{\lambda_2}{L}}\right)$$
$$+\overset{B_3}{0.02}\sin\left(\frac{2\pi x}{\underset{\lambda_3}{2L/3}}\right) - \overset{B_4}{0.01}\sin\left(\frac{2\pi x}{\underset{\lambda_4}{L/2}}\right)$$