Lecture 13 - Waves and Particles

Classical mechanics is great for many, many situations. However, if particles are small enough, their quantum nature needs to be accounted for. We will quantify what "small enough" means in a few minutes.

A. Mathematics of waves

It really helps in Q.M. to be familiar with waves. Let's quickly review. Classical wave equation in 1D:

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

u: thing propagating
t: time
c: wave propagation speed
x: space

Solution for a traveling wave:

$$u = A e^{-i(kx-\omega t)} + B e^{i(kx-\omega t)}$$

k: wave number $\left(\frac{rad}{cm}\right)$

$$\omega = 2\pi f \qquad k = 2\pi/\lambda \qquad \omega = kc$$

f: frequency
λ: wavelength (continuous wavenumber)

ω: angular frequency $\left(\frac{rad}{s}\right)$

A, B: constants determined by ICs, BCs

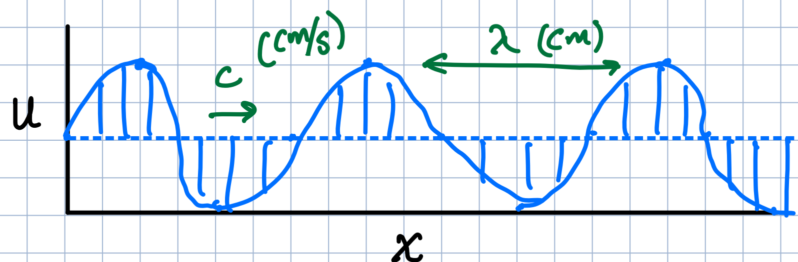
Solution for a standing wave (single mode):

$$u = \left(a e^{-i\omega_n t} + b e^{i\omega_n t}\right)\left(c e^{-ik_n x} + d e^{ik_n x}\right)$$

discrete wavenumber and angular frequency

Recall (Euler's formula):

$$e^{i\theta} = \cos\theta + i\sin\theta \Rightarrow \sin\theta = \frac{(e^{i\theta} - e^{-i\theta})}{2i}, \quad \cos\theta = \frac{(e^{i\theta} + e^{-i\theta})}{2}$$



$$f = c/\lambda = \frac{\#\text{ waves}}{\text{time}} \left(\frac{\text{cycles}}{s}\right)$$

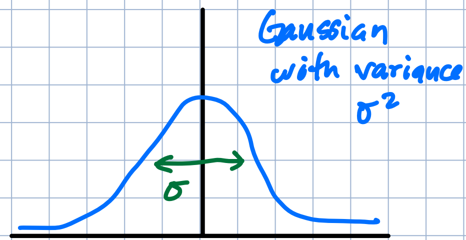
Note: Solutions are derived in the appendix.

B. Uncertainty principle of waves

There is a general uncertainty principle of Fourier transform conjugate variables that we can use to understand waves and localization.

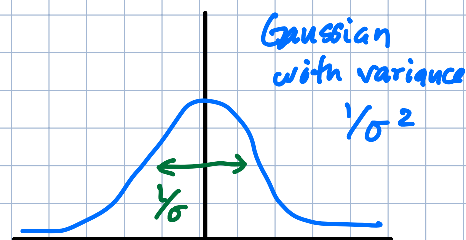
Suppose I have a Gaussian function

$$f(x) = \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left(-\frac{x^2}{2\sigma^2}\right)$$



The Fourier Transform of f is

$$\hat{f}(k) = \exp\left(-\tfrac{1}{2}k^2\sigma^2\right)$$



This is also a Gaussian, but the variance is $1/\sigma^2$.

lets define $\sigma_x^2 = \sigma^2$ and σ_k^2 as follows:

$$\hat{f}(k) = \exp\left(-\frac{k^2}{2\sigma_k^2}\right) \Rightarrow \sigma_k^2 = 1/\sigma^2$$

Therefore: $\boxed{\sigma_x^2 \cdot \sigma_k^2 = 1}$

single point in space

Also: $F[\delta(x-x_0)] = e^{-ikx_0}$

single wavelength

If the variance in the position goes up (down), then the variance in the wavenumber, k, goes down (up).

3Blue1Brown has a good example for giving us intuition here. If I am sitting at a stop light in the turn lane, and the blinkers seem to be in sync (frequency), the longer I wait, the more sure I am that they do have the same frequency. In other words, longer times tell me more information about frequencies. It would take infinite time to tell they were the exact same frequency (and not just off by a little bit). Conversely, suppose there were very many frequencies of blinkers. It would only take a very short time to tell they were all different.

"When did I know" that the blinkers were the same?

- Frequencies very close → spread out over time
- Frequencies spread out → located more precisely in time.

C. Wave-Particle Duality

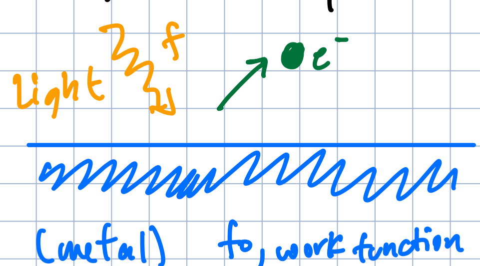
There is this sort of fundamental split at the heart of physics, and really, in mathematics. We have discrete things (e.g., number of apples) and continuous things (e.g., time). In physics prior to c.1900 — and it should be noted in everyday experience — the world was neatly divided into these two things. Two pertinent examples are light and electrons.

Light was seen as continuous. It obeyed Maxwell's equations. It propagates as a wave (see above).

$$\frac{\partial^2 \underline{E}}{\partial t^2} = c^2 \nabla^2 \underline{E} \qquad \frac{\partial^2 \underline{B}}{\partial t^2} = c^2 \nabla^2 \underline{B} \qquad c: \text{speed of light}$$

$\underline{E}$: electric field $\qquad$ $\underline{B}$: magnetic field.

Particles, as we have been talking about, were seen as discrete. Electrons were known to be a type of particle. There were a series of surprising experimental discoveries. The photoelectric effect demonstrated that light had a particle nature.



- minimum frequency of light needed to excite an electron
- higher intensity didn't matter if frequency too low.

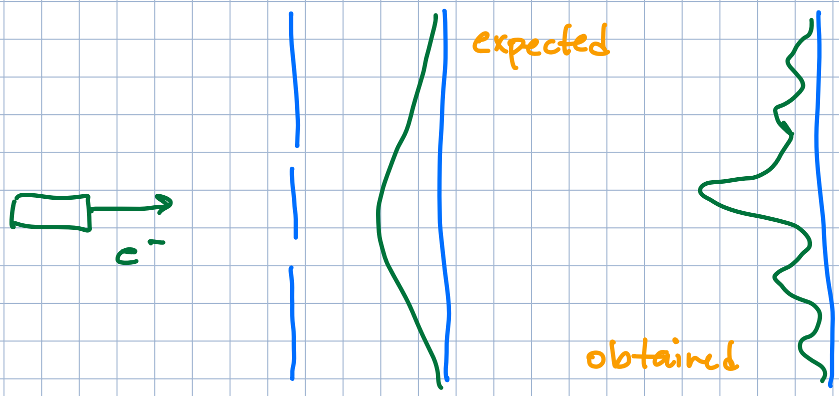
The conclusion is that light has a particle nature (photon) and the energy of the light was hypothesized to be given by

$E = hf$ or $\boxed{E = \hbar\omega}$ $\hbar = \frac{h}{2\pi}$

(Planck's Formula) $h = 6.626 \times 10^{-34}$ Js

(Aside) Planck developed formula while trying to solve the blackbody radiation UV catastrophe. Einstein connected it to the photoelectric effect. Einstein given the nobel prize for this.

Subsequently, electrons (particles) were discovered to have a wave-like character in the double-slit experiment.



Matter diffracted (interfered) like light. Show video from wikipedia.

Notes:

- Even one particle acts as if interfering with itself.
- Pattern is built up statistically. Particles appear in a "random" fashion.
- If you try to detect the particle before it hits, it changes its state.
- Measurements always result in interactions that cannot be neglected. This is a result of scale. E.g., even a single photon messes with the state of an electron.

Resulting conclusion: matter particles are wavelike in some way.

$$\boxed{\underline{p} = \hbar \underline{k}}.$$ Particle momentum $\propto$ wave number.

Equations for E & $\underline{p}$ are Planck-Einstein equations. They are fundamental to Q.M. They are like "laws." They are postulates based on experimental observations.

(Aside) The second P-E equation is equivalent to the de Broglie wavelength : $\lambda = \frac{h}{p} = \frac{h}{mv}$ ← very small number λ is big when p is small.

<u>Main takeaways:</u>

- Light and matter are not particles or waves, they are "particle-waves." They are both things. This is what is meant by "wave-particle duality."
- These effects only happen for matter if momentum is small.

<u>Example</u>: Colloidal particle in water (e.g. polyethylene)

size: $R = 1\,\mu m$ speed: $v = 1\,{}^{\mu m}/_{s}$ density: $\rho \approx 1\,{}^{g}/_{cm^3}$

$$m = \rho \cdot V = \rho \cdot \frac{4}{3}\pi R^3 = \frac{1g}{cm^3} \cdot \frac{4}{\cancel{3}}\cancel{\pi}(1\,\mu m)^3 \approx \frac{1000\,kg}{m^3} \cdot 4 \cdot 10^{-18}\,m^3$$

$$m \approx 4 \times 10^{-15}\,kg$$

$$p = mv = 4 \times 10^{-15}\,kg \cdot 10^{-6}\,\frac{m}{s} = 4 \times 10^{-21}\,kg\,{}^{m}/_{s}$$

$$\lambda = \frac{h}{p} = \frac{6.626 \times 10^{-34}\,Js}{4 \times 10^{-21}\,\frac{kg\,m}{s}} \approx 1.5 \times 10^{-13}\,\frac{\cancel{kg}\,m^{\cancel{2}}}{\cancel{s}} \cdot \frac{\cancel{s}}{\cancel{kg\,m}} = 1.5 \times 10^{-13}\,m$$

$$Js = \frac{kg\,m^2}{s}$$

$$\frac{\lambda}{R} = \frac{1.5 \times 10^{-13}\,m}{10^{-6}\,m} = \boxed{1.5 \times 10^{-7}}$$ negligible!

Example 2: Electron accelerated at 100 V.

$E = qV \qquad q_e = 1.602 \times 10^{-19}\,C \qquad E = 1.6 \times 10^{-19}\,C \cdot 100\,V = 1.6 \times 10^{-17}\,J$

$E = \dfrac{p^2}{2m_e} \Rightarrow p = \sqrt{2m_e E} \qquad m_e = 9.109 \times 10^{-31}\,kg$

$p = \left[2 \cdot 9.1 \times 10^{-31}\,kg \cdot 1.6 \times 10^{-17}\,\dfrac{kg\,m^2}{s^2}\right]^{1/2} = 5. \times 10^{-24}\,kg\,m/s$

$\lambda = \dfrac{h}{p} = \dfrac{6 \times 10^{-34}\,kg\,m^2/s}{5 \times 10^{-24}\,kg\,m/s} \approx 1.2 \times 10^{-10}\,m \approx 1.2\,Å$

atomic radius of hydrogen, $r_{H_2} \approx 0.25\,Å$

$\boxed{\dfrac{\lambda}{r_{H_2}} \approx 5}$ definitely not negligible!

D. Appendix: Solving the wave equation – traveling wave

$$\frac{\partial^2 \hat{u}}{\partial t^2} = c^2(-k^2 \hat{u}) = -k^2 c^2 \hat{u}$$

$$\frac{\partial^2 \hat{u}}{\partial t^2} + k^2 c^2 \hat{u} = 0 \qquad kc = \omega$$

Fourier transform

$$\hat{u} = \int e^{-ikx} u(x,t)\,dx$$

$$u = \frac{1}{2\pi}\int e^{ikx} \hat{u}(k,t)\,dx$$

2nd order, linear, homogeneous.
constant coefficient

$\omega^2 > 0 \rightarrow$ sines & cosines

$$\hat{u} = A(k)e^{ikct} + B(k)e^{-ikct} = A(k)\,e^{i\omega t} + B(k)e^{-i\omega t}$$

Boundary conditions for a traveling wave with a single wavelength, λ_0: $k_0 = 2\pi/\lambda_0$, $\omega_0 = ck_0$

$$\lim_{x \to -\infty} u(x,t) = \lim_{x \to \infty} u(x,t) = a\,e^{i(k_0 x - \omega_0 t)}$$

Definition of the B.C.

$$\hat{u}(-\infty,t) = \hat{u}(\infty,t) = 2\pi a e^{-i\omega_0 t}\delta(k-k_0)$$ ← Take F.T. of B.C.

Matching with our solution gives:

$$\hat{u}(k,t) = 2\pi a e^{-i\omega t}\delta(k-k_0) = A(k)e^{i\omega t} + B(k)e^{-i\omega t}$$

$$A(k)=0 \qquad B(k) = 2\pi a\,\delta(k-k_0)$$

Now take the inverse Fourier transform

$$\boxed{u(x,t) = a e^{i(k_0 x - \omega_0 t)}}$$ ← the single mode traveling wave we proscribed at the boundaries.

E. Appendix: Solving the wave equation – standing wave

Solve by separation of variables

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \qquad \text{let } u = f(t)\,g(x)$$

$$\frac{\partial^2 (fg)}{\partial t^2} = c^2 \frac{\partial^2 (fg)}{\partial x^2} \Rightarrow g\frac{\partial^2 f}{\partial t^2} = c^2 f \frac{\partial^2 g}{\partial x^2}$$

$$\frac{1}{c^2}\frac{1}{f}\frac{\partial^2 f}{\partial t^2} = \frac{1}{g}\frac{\partial^2 g}{\partial x^2} = -\gamma^2$$ ← must equal a constant because LHS = fn of t and RHS = fn of x.

must be negative because exponential growth won't satisfy physical B.C.s

Solve time ODE for f(t):

$$\frac{d^2 f}{dt^2} = -\gamma^2 c^2 f \Rightarrow \frac{d^2 f}{dt^2} + \gamma^2 c^2 f = 0$$ ← 2nd order, linear, constant coefficient gives sines & cosines.

$$f(t) = a e^{-i\gamma c t} + b e^{i\gamma c t}$$ ← a or b depends on ICs.

Solve space ODE for $g(x)$:

$$\frac{d^2g}{dx^2} = -g\gamma^2 \Rightarrow \frac{d^2g}{dx^2} + g\gamma^2 = 0$$

← Again; 2nd order, linear constant coefficient. Gives sines & cosines.

$$g(x) = c\,e^{-i\gamma x} + d\,e^{i\gamma x}$$

When stationary, only fixed values of γ are allowed.

Example: $g(0) = 0$, $g(2\pi) = 0$ (string w/ fixed ends)

$$g(0) = c\,e^0 + d\,e^0 = c + d = 0 \quad \Rightarrow c = -d$$

$$g(2\pi) = c\,e^{-i\gamma(2\pi)} + d\,e^{i\gamma(2\pi)}$$

$$= d\left(e^{2\pi i\gamma} - e^{-2\pi i\gamma}\right)$$

we can identify γ as $1/\lambda$ now.

$$= 2id\,\sin(2\pi\gamma) = 0$$

either $d = 0$ or $\gamma_n = 0, 1/2, 1, 3/2, \ldots$ for $n = 0, 1, 2, \ldots$

$$g(x) = c\,e^{-ik_nx} + d\,e^{ik_nx} \qquad k_n = \pi n, \quad n = 0, 1, \ldots$$

Putting it all together gives:

$$u(x,t) = g(t)f(x)$$

$$= \left(a\,e^{-i\gamma_nct} + b\,e^{i\gamma_nct}\right)\left(c\,e^{-ik_nx} + d\,e^{ik_nx}\right)$$

shift be $e^{2\pi}$ $\quad 2\pi\gamma_nc = \omega_n$

$$\boxed{u(x,t) = \left(a\,e^{-i\omega_nt} + b\,e^{i\omega_nt}\right)\left(c\,e^{-ik_nx} + d\,e^{ik_nx}\right)}$$

This is for a single mode only. For all modes the solution is

$$u(x,t) = \sum_{n=0}^{\infty}\left(a\,e^{-i\omega_nt} + b\,e^{i\omega_nt}\right)\left(c\,e^{-ik_nx} + d\,e^{ik_nx}\right)$$