States, amplitudes, interference

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Quantum Mechanics 1
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1. Classical mechanics of a point particle

2. Classical waves

3. The double-slit experiment

Outline

Newton's laws of motion

- In classical mechanics a point particle (of mass m) has a well-defined position ($\mathbf{q}$), which changes according to Newton's laws:

$$m\frac{d^2\mathbf{q}}{dt^2} = \mathbf{F},$$

  where **F** is the instantaneous force acting on the particle.
- This second order differential equation can be solved if the initial position and velocity of the particle are known. This requires the knowledge of 6 quantities (3 components of the position vector and 3 components of the velocity vector).
- We will consider a conservative system, *i.e.*, one in which the force depends only on the position and not explicitly on time. In this case, one can write

$$\mathbf{F} = -\frac{dV}{d\mathbf{q}}.$$

Reference: Classical Mechanics, Goldstein

Hamilton's formulation

- Any second order differential equation can be written as a set of coupled first order equations

$$m\frac{d\mathbf{q}}{dt} = \mathbf{p} \qquad \frac{d\mathbf{p}}{dt} = -\frac{dV}{d\mathbf{q}}.$$

  These equations can be solved if the initial position and momenta are known. This requires the knowledge of 6 quantities (which?).
- Hamilton's equations specify that the particle has a well-defined position ($\mathbf{q}$) and a well-defined momentum ($\mathbf{p}$). Nothing new: this just replaces velocity by momentum.
- The 6 component vector

$$\gamma = (\mathbf{q}, \mathbf{p}) = (q_1, q_2, q_3, p_1, p_2, p_3)$$

  can be thought of as a single point in phase space. Give γ at one time (and the forces), and the value of γ at any other time can be obtained by solving Hamilton's equations.

Reference: Classical Mechanics, Goldstein

Some problems

1. The equation for a simple harmonic oscillator in one dimension of space can be written as

$$\frac{d^2q}{dt^2} = -\omega^2 q.$$

   Write down the potential $V(q)$ for the harmonic oscillator. Write down Hamilton's equations for the harmonic oscillator.

2. Two coupled second order differential equations are

$$\frac{d^2q_1}{dt^2} = -q_2, \qquad \frac{d^2q_2}{dt^2} = -q_1.$$

   Rewrite these as a system of four coupled first order equations. Can these equations be written as Newton's or Hamilton's equations with some potential $V(q_1, q_2)$?

Hamilton's equations

- A Hamiltonian is the function on phase space—

$$H(\mathbf{p},\mathbf{q}) = \frac{1}{2m}\mathbf{p}^2 + V(\mathbf{q}).$$

  A Hamiltonian is just the energy: kinetic and potential.

- Hamilton's equations are

$$\frac{d\mathbf{q}}{dt} = \frac{dH}{d\mathbf{p}}, \qquad \frac{d\mathbf{p}}{dt} = -\frac{dH}{d\mathbf{q}}$$

  These equations are exactly equivalent to Newton's equations.

- Problems: For the previous two problems write down the Hamiltonians.
- The state of a system is the vector $\gamma = (\mathbf{q},\mathbf{p})$, because, given the state of a system at any time, one can obtain the state of a system at any other time by solving Hamilton's equations.

Outline

Wave trains and localization

- An infinite wave train $Exp[-ix]$ is not localized. If you say that the wave is at $x = x_0$, then it can equally well be at $x = x_0 + 1$.
- A "shaped" wave can be roughly localized. The Gaussian wave train

$$\mathrm{e}^{-x^2/(2a^2)}\ \mathrm{e}^{-ix}$$

is roughly localized between $-a \leq x \leq a$.
- The box wave train

$$\mathrm{e}^{-ix} \quad (\text{for } -a \leq x \leq a), \qquad\qquad 0 \quad (\text{otherwise})$$

is certainly localized between $-a \leq x \leq a$.

Power spectra

A wave $f(x)$ has a Fourier transform

$$\widetilde{f}(k) = \int_{-\infty}^{\infty} dx \mathrm{e}^{ikx} f(x).$$

The power spectrum of the wave is

$$P(k) = \left|\widetilde{f}(k)\right|^2.$$

Here k is the wavenumber.
The power spectra of various waves are—

	Shape	Spectrum
Infinite	constant	$\delta(1-k)$
Gaussian	$\exp[-x^2/(2a^2)]$	$a^2 \exp[-(1-k)^2 a^2]$
Box	$\Theta(a+x)\Theta(a-x)$	$\sin^2[a(1-k)]/(1-k)^2$

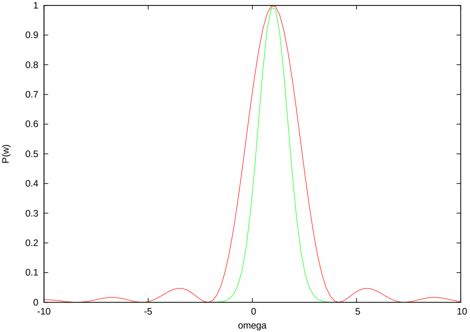
Note that for the Gaussian and Box wave trains, the width of the power spectrum is the inverse of the width of the wave train.

Duality of position and wavenumber

This is true of wave trains of all shapes—

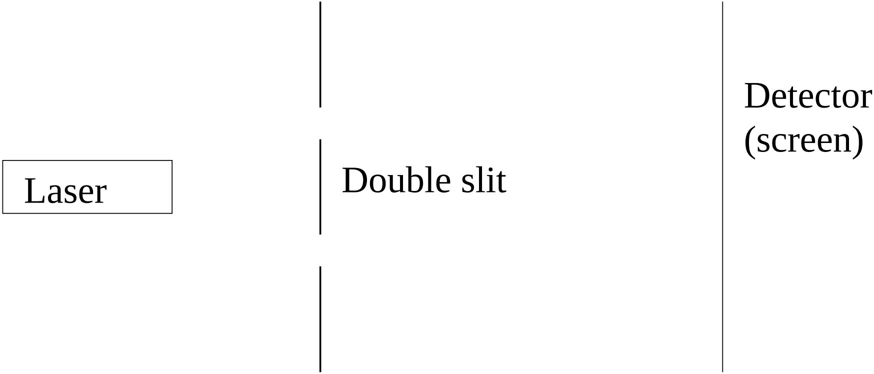
$$(\Delta x)\,(\Delta k) \geq 1,$$

where Δx is a measure of the width of the wave train and Δk is a measure of the width of the Fourier transform of the wave train (*i.e.*, of the power spectrum).



Outline

Wave-particle unity



Use a laser which emits one photon at a time. Use the screen as a detector.

Wave-particle unity

Since the laser emits one photon at a time, each photon appears as a single pointlike flash when it arrives at the screen. This is exactly what you expect of a particle.

When you plot the positions of many such flashes, then the density of points is governed by the interference fringes. The variation of the intensity through interference is exactly what you expect of a wave.

A quantum particle is both a wave and a particle: a wave when it travels through the slit, a particle when seen by the detector.

The state of a quantum particle must have a wave description. This is one complex number at each point of space. The square of the modulus of the wave is proportional to the probability of finding the particle at a point (**Born**).

Heisenberg's uncertainty principle

Planck hypothesized that a wave of frequency ω carries energy $E = \hbar\omega$. **de Broglie** extended this hypothesis to state that the momentum, p, carried by a wave of wavenumber k is $p = \hbar k$.
Note that the two statements are compatible with each other under dimensional analysis.
The uncertainty relation for waves then allows us to write

$$(\Delta x)\,(\Delta p) \geq \hbar.$$

This is **Heisenberg**'s uncertainty relation. It is therefore a direct consequence of the wave nature of particles.
Note that this can be made compatible with the phase space description if one realizes that there is an unit volume element in phase space— $\hbar^D$. Phase space volumes smaller than this are unphysical.

Some problems

1. For the classical one-dimensional harmonic oscillator, the phase space is two dimensional (q and p). The loci of constant energy, *i.e.*, constant value of the Hamiltonian, must be curves. Find these curves. Find the values of the energy which bound areas of magnitude $n\hbar$ (where $n \geq 1$ is any integer). What is the physics of these shapes?
2. For any classical particle moving in one dimension the phase space is two dimensional. Assume that the particle is confined within a "box", *i.e.*, a region with $-a \leq q \leq a$. Find the phase space trajectories of constant energy. Find the energy values which bound phase space areas of magnitude $n\hbar$. What is the physics of these shapes?
3. What happens when the box size goes to infinity? How do the shapes of phase space cells of area $n\hbar$ change? What is the physics behind this?