States, amplitudes, interference

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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:

$$m\ddot{\mathbf{q}} = \mathbf{F},$$

  where $\mathbf{F}$ 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

$$\mathbf{F} = -\nabla V.$$

Reference: Classical Mechanics, Goldstein

Hamilton's formulation

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

$$m\dot{\mathbf{q}} = \mathbf{p}, \qquad \dot{\mathbf{p}} = -\nabla V.$$

  So the particle has a well-defined position ($\mathbf{q}$) and a well-defined momentum ($\mathbf{p}$). These equations can be solved if $\mathbf{q}(0)$ and $\mathbf{p}(0)$ are known.
- 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. Given γ at one time, and the potential, the value of γ at any other time can be obtained by solving Hamilton's equations.

Reference: Classical Mechanics, Goldstein

Hamilton's equations

- A Hamiltonian is the function on phase space—
$$H(\mathbf{p},\mathbf{q}) = \frac{1}{2m}\mathbf{p}^2 + V(\mathbf{q}).$$
We will study time-independent Hamiltonians in this course. Then the Hamiltonian is just the total energy: the sum of kinetic and potential.
- Hamilton's equations are
$$\dot{\mathbf{q}} = \frac{dH}{d\mathbf{p}}, \qquad \dot{\mathbf{p}} = -\frac{dH}{d\mathbf{q}}.$$
These equations are exactly equivalent to Newton's equations. This is the decomposition shown earlier.
- The state of the system is completely specified by $\gamma = (\mathbf{q},\mathbf{p})$, because any mechanical quantity can be computed from $\mathbf{q}$ and $\mathbf{p}$. The state may also be specified by $\gamma(0)$, since all successive γ can be found from it.

Some problems

Problem 1.1: A classical harmonic oscillator

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

$$\ddot{q} = -\omega^2 q.$$

Write down the potential $V(q)$ for the harmonic oscillator. Write down Hamilton's equations for the harmonic oscillator. What are the trajectories of the particle in phase space?

Problem 1.2: A classical square well problem

A particle moves in one dimension (along a line) subject to a square well potential: $V(q) = 0$ except when $|q| < a$. In the range $|q| < a$ we have $V(q) = -V_0$. What are the forces on the particle? What are the trajectories of the particle in phase space?

Outline

Wave trains and localization

Waves can be described either in space ($\mathbf{x}$) or in wave-number ($\mathbf{k}$). Descriptions are related by a Fourier transform.

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Wave trains and localization

Waves can be described either in space ($\mathbf{x}$) or in wave-number ($\mathbf{k}$). Descriptions are related by a Fourier transform.

- The infinite wave train $\exp[-i\mathbf{k}\cdot\mathbf{x}]$ is not localized. Why?
- A "shaped" wave may be roughly localized. The Gaussian wave train

  $$\mathrm{e}^{-x^2/(2a^2)}\,\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{x}}$$

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

  $$\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{x}} \quad (\text{for } -a \le x \le a), \qquad\qquad 0 \quad (\text{otherwise})$$

  is definitely localized between $-a \le x \le a$.

Duality in wave-number

A wave $f(\mathbf{x})$ has a Fourier transform

$$\widetilde{f}(\mathbf{k}) = \int_{-\infty}^{\infty} d\mathbf{x} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x}).$$

So knowing $f(\mathbf{x})$ is equivalent to knowing $\widetilde{f}(\mathbf{k})$. The squared amplitude of a wave is $|f(\mathbf{x})|^2$. The power spectrum of the wave is

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

Examine a change of length scale $\mathbf{x} \to \mathbf{x}' = \xi\mathbf{x}$. Then the amplitude becomes narrower (if $\xi > 1$) without changing shape. Then

$$\widetilde{f}\left(\frac{\mathbf{k}}{\xi}\right) = \int_{-\infty}^{\infty} d\mathbf{x} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}/\xi} f(\mathbf{x}) = \xi^D \int_{-\infty}^{\infty} d\mathbf{x}' \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}'} f\left(\frac{\mathbf{x}'}{\xi}\right) = \xi^D \widetilde{f}(\mathbf{k}).$$

So the scale of wave-number changes to $\mathbf{k} \to \mathbf{k}' = \mathbf{k}/\xi$.

Gaussian wave trains

For a Gaussian wave train in one dimension

$$\widetilde{f}(k) = \int_{-\infty}^{\infty} dx \mathrm{e}^{ikx} \, \mathrm{e}^{-x^2/(2a^2)}.$$

Combine the exponentials, and complete the square to get

$$\widetilde{f}(k) = \mathrm{e}^{-a^2k^2/2} \int_{-\infty}^{\infty} dx \mathrm{e}^{-(x+ia^2k)^2/(2a^2)}.$$

The integrand vanishes everywhere in the upper-half of the complex plane of $z = x + ia^2k$. So one can close the contour of integration in the upper-half plane, and evaluate the constant (k-independent) value of the integral.

Since the width of the squared amplitude, $\Delta x = a$, the width of the squared amplitude $\Delta k = 1/a$. So, for a one dimensional Gaussian wave train one has

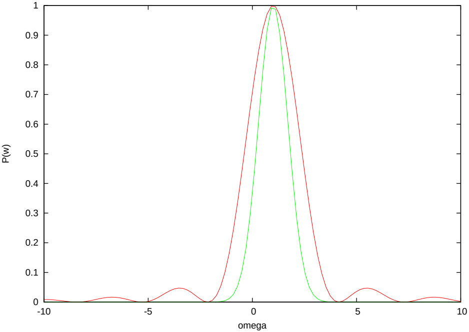
$$\Delta x \, \Delta k = 1.$$

Duality of position and wavenumber

This is true of wave trains of all shapes—

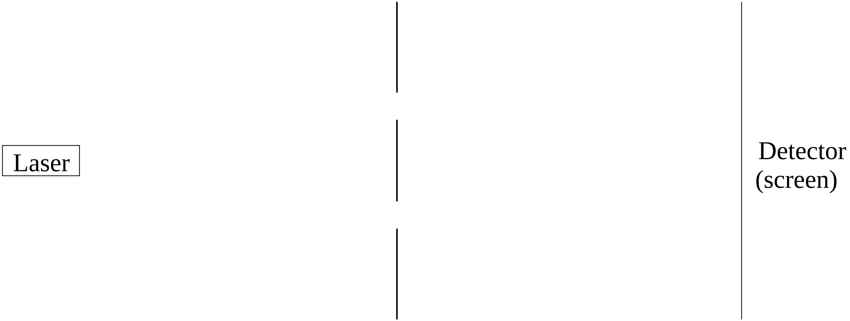
$$(\Delta x)\,(\Delta k) \geq 1,$$

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.

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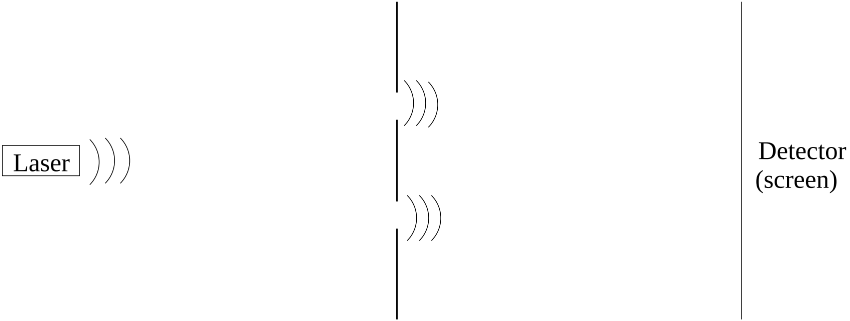

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A quantum particle is both a wave and a particle: a wave when it travels through the slit, a particle when seen by the detector.

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**).

Interference

- x is the position of a point on the screen.
- Wave function of photon at x if lower slit closed: $\Psi_1(x)$.
- Wave function of photon at x if upper slit closed: $\Psi_2(x)$.
- Wave function if both slits open: $\Psi(x) = \Psi_1(x) + \Psi_2(x)$.
- Fixed phase relationship between the two needed for interference, *i.e.*, if $\Psi_2(x) = \Psi_1(x) A(x) \mathrm{e}^{i\phi(x)}$, then

  $$|\Psi(x)|^2 = |\Psi_1(x)|^2 \times \left\{1 + A(x)^2 + 2A(x)\cos\phi(x)\right\}.$$

  Usual case of interference: $\phi(x) = k \times \mathrm{path\ difference}(x)$.
- If phase relationship randomized, then interference disappears. If one slit closed then interference disappears. If the two slits have light of different polarization, then interference disappears.
- Interference only if at least two possible paths available.

Quantum unification

Quantum reality

A particle and a wave are not different things: there is something wave-like about quantum particles.

Measurable consequences

Every unification has measurable consequences.

- The first law of thermodynamics includes the law of intercovertibility of mechanical energy and heat. This implies that the units of measurment of these two should be the same. Thus the Joule's constant is just a constant factor relating two different systems of units for the same thing.
- The principle of relativity says that time and space are equivalent and interconvertible. This implies that the units of measurement of the two are the same. Thus the speed of light in vacuum is just a constant relating two different units for the same thing.
- A precise statement of the principle of quantum mechanics must also relate two physical quantities which until now were considered to be different.

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 dimensionally compatible.) 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.

The old quantum theory

Problem 1.3: One-dimensional harmonic oscillator

For the classical one-dimensional harmonic oscillator, the phase space is two dimensional. Find the loci of constant energy. 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?

Problem 1.4: One-dimensional free particle

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? 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?

Outline

1. Classical mechanics of a point particle
2. Classical waves
3. The double-slit experiment
4. Keywords and References

Keywords and References

Keywords

Classical mechanics, Hamiltonian formulation, phase space, state, classical waves, wave train, amplitude, wave-number, Fourier transforms, power spectrum, position-wavenumber duality, double slit experiment, Born waves, Planck hypothesis, de Broglie hypothesis, Planck's constant, Heisenberg uncertainty relations, the old quantum theory.

References

The Feynman Lectures in Physics (Vol 3), by R. P. Feynman *et al*
Quantum Mechanics (Non-relativistic theory), by L. D. Landau and E. M. Lifschitz.