The wave function

Exercise 1: Dirac delta function

The Dirac delta function is a distribution defined by

$$\int_{-\infty}^{\infty} \mathrm{d}x\, \delta(x-x_0)\, f(x) = \int_{x_0-\epsilon}^{x_0+\epsilon} \mathrm{d}x\, \delta(x-x_0)\, f(x) = f(x_0)$$

for any smooth function in $x = x_0$. It also satisfies

$$\int_{-\infty}^{\infty} \mathrm{d}x\, \delta(x-x_0) = 1 \quad \text{and} \quad \delta(x) = 0,\ \forall\, x \neq 0.$$

i) Show that the Dirac delta function can be written as the limit when $L \to \infty$ or $\epsilon \to 0^+$ of the following functions:

(a) $\delta_L(x) = \dfrac{1}{2\pi} \displaystyle\int_{-L}^{L} \mathrm{d}k\, \mathrm{e}^{ikx} = \dfrac{\sin Lx}{\pi x}$

(b) $\delta_\epsilon(x) = \dfrac{1}{(2\pi\epsilon^2)^{1/2}}\, \mathrm{e}^{-x^2/2\epsilon^2}$

(c) $\delta_\epsilon(x) = \dfrac{\epsilon/\pi}{x^2+\epsilon^2}$

(d) $\delta_\epsilon(x) = \dfrac{\theta(x+\frac{\epsilon}{2}) - \theta(x-\frac{\epsilon}{2})}{\epsilon}$ where $\theta(x)$ is the Heaviside step function.

ii) Check the following properties of the Dirac delta function where the prime means derivative *in the sense of distributions*:

(a) $\delta(x) = \delta(-x)$

(b) $\delta'(x) = -\delta'(-x)$

(c) $x\delta(x) = 0$

(d) $x\delta'(x) = -\delta(x)$

(e) $x^2\delta'(x) = 0$

(f) $\delta(ax) = \dfrac{1}{|a|}\delta(x), \quad a \neq 0$

(g) $\delta(f(x)) = \displaystyle\sum_{f(x_i)=0} \dfrac{1}{|f'(x_i)|}\delta(x-x_i)$

(h) $f(x)\delta(x-a) = f(a)\delta(x-a)$

(i) $\displaystyle\int_{-\infty}^{\infty} \mathrm{d}x\, \delta(x-a)\, \delta(x-b) = \delta(a-b)$

(j) $\displaystyle\int_{-\infty}^{\infty} \mathrm{d}x\, \delta'(x-a)\, \delta(x-b) = \delta'(b-a)$

(k) $\delta'(x) = \dfrac{i}{2\pi} \displaystyle\int_{-\infty}^{\infty} \mathrm{d}k\, k\mathrm{e}^{ikx}$

(l) $\delta(x) = \theta'(x)$ (compare with *i)* (d) of this exercise)

Exercise 2: Fourier transform

Let us consider the function $f(x)$ defined in the interval $-\infty < x < \infty$. When we can write $f(x)$ as

$$f(x) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} \mathrm{d}k\, \mathrm{e}^{ikx} g(k)$$

then $g(k)$ is the *Fourier transform* of $f(x)$.

i) Using a representation of the Dirac delta function provided in the previous exercise, show that we can invert the relation:

$$g(k) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-ikx} f(x),$$

where now $f(x)$ is the *inverse Fourier transform* of $g(k)$.

ii) Compute the Fourier transform of the following functions: [*solutions*]

i) $f(x) = \delta(x - x_0)$ — $g(k) = (2\pi)^{-1/2} \mathrm{e}^{-ikx_0}$

ii) $f(x) = c_0 \mathrm{e}^{ik_0 x}$ — $g(k) = (2\pi)^{1/2} c_0 \delta(k - k_0)$

iii) $f(x) = c_0 \cos k_0 x$ — $g(k) = (2\pi)^{1/2} c_0 \dfrac{\delta(k - k_0) + \delta(k + k_0)}{2}$

iv) $f(x) = c_0 \sin k_0 x$ — $g(k) = (2\pi)^{1/2} c_0 \dfrac{\delta(k - k_0) - \delta(k + k_0)}{2i}$

v) $f(x) = c_0 \mathrm{e}^{-x^2/2\sigma^2}\, \mathrm{e}^{ik_0 x}$ — $g(k) = c_0 \sigma \mathrm{e}^{-(k-k_0)^2 \sigma^2/2}$

vi) $f(x) = c_0 \mathrm{e}^{-a|x|}\, \mathrm{e}^{ik_0 x}$ — $g(k) = (2/\pi)^{1/2} c_0 \dfrac{a}{a^2 + (k - k_0)^2}$

vii) $f(x) = \begin{cases} c_0 \mathrm{e}^{ik_0 x}, & |x| < A \\ 0, & |x| > A \end{cases}, \quad A > 0$ — $g(k) = (2/\pi)^{1/2} c_0 \dfrac{\sin(k - k_0)A}{k - k_0}$

viii) $f(x) = c_0 \dfrac{\sin ax}{x}, \quad a > 0$ — $g(k) = \begin{cases} (\pi/2)^{1/2} c_0 & , \ |k| < a \\ 0 & , \ |k| > a \end{cases}$

Exercise 3: Wave functions and time evolution

The Fourier transform takes a wave function in the position representation into the momentum representation and *viceversa*:

$$\langle x|p\rangle = \frac{1}{(2\pi\hbar)^{1/2}} e^{ipx/\hbar} \Rightarrow \begin{cases} \langle x|\psi\rangle \equiv \psi(x) = \dfrac{1}{(2\pi\hbar)^{1/2}} \displaystyle\int_{-\infty}^{\infty} \mathrm{d}p\ e^{ipx/\hbar}\ \hat{\psi}(p) \\ \langle p|\psi\rangle \equiv \hat{\psi}(p) = \dfrac{1}{(2\pi\hbar)^{1/2}} \displaystyle\int_{-\infty}^{\infty} \mathrm{d}x\ e^{-ipx/\hbar}\ \psi(x). \end{cases}$$

If the wave function has a well defined momentum p_0, then its transform gives a plane wave:

$$\hat{\psi}(p) = \delta(p - p_0), \quad \psi(x) = \frac{1}{(2\pi\hbar)^{1/2}} e^{ip_0 x/\hbar}.$$

Suppose that at time $t = 0$ the state of a 1-dimensional free massive particle is given by the Gaussian wave function

$$\xi(x) = \frac{1}{\pi^{1/4}\sqrt{d}} e^{ik_0 x - \frac{x^2}{2d^2}},$$

where d and k_0 are positive real numbers.

i) Plot the wave function ξ.

ii) Normalize ξ to one.

iii) Write the wave function in the momentum representation.

iv) Find the expectation values and the uncertainties in $\hat{x}$ and $\hat{p}$, and show that the product of uncertainties is minimal.

v) Find the time evolution of the wave function.

vi) Comment on the limit $d \to \infty$.

Exercise 4: Wave function, probability and time evolution

A particle of mass m is inside a 1-dimensional box of length a (i.e., an infinite quantum well at $0 \le x \le a$). Let as suppose that at $t = 0$ its wave function is

$$\psi(x, t = 0) = \sqrt{\frac{8}{5a}} \left[1 + \cos\left(\frac{\pi x}{a}\right)\right] \sin\left(\frac{\pi x}{a}\right).$$

i) Solve Schrodinger equation and find the energy eigestates and eigenvalues.

ii) Find the wave function of the particle at an arbitrary time t.

iii) Determine the probability to find the particle in the left half of the box at time t.

Exercise 5: Probability density and density current

i) Prove that a stationary state in a non-degenerate energy level implies a vanishing density current $\vec{J}(x)$.

ii) Consider the following eigenstate in a 3-dimensional harmonic oscillator of frequency ω and mass M:

$$\psi(x) = \pi^{-3/4}\alpha^{5/2}(x + iy)\exp(-\alpha^2 r^2/2), \quad \alpha = (M\omega/\hbar)^{1/2}.$$

Show that its probability density current is not zero. Is its energy level degenerate? Is this state stationary?

Exercise 6: Retarded propagator

i) Calculate the retarded propagator for evolution of a free particle in one dimension.

ii) Calculate the evolution of a wave packet with minimum dispersion at $t = 0$, i.e. a plane wave modulated with a Gaussian function,

$$\psi(x, t = 0) = \frac{1}{(\pi a^2)^{1/4}} \mathrm{e}^{-x^2/2a^2} \mathrm{e}^{ip_0 x/\hbar},$$

where a and p_0 are positive real numbers. What is the dispersion of the wave packet at $t > 0$?

iii) A particle of mass M moves freely in a straight line, with wave function at $t = 0$ given by the expression above, and an initial uncertainty in position of 1 Å. At which time is the uncertainty in position equal to 1 mm? Calculate this time for an electron with mass $m_e = 9 \times 10^{-28}$ g and a particle with mass $M = 1$ g.

Exercise 7: Test exercise, September 2012 [2.5P]

A free particle of mass m evolving in one dimension is in a state described at $t = 0$ by the wave function $\Psi(x, 0) = A\sin(k_0 x)$.

i) Find the wave function at a time t.

ii) What are the possible values for its momentum and what is the probability they will be measured?

iii) We measure the momentum at $t = t_0$ to be $\hbar k_0$. What is the wave function at $t > t_0$?

Exercise 8: Ehrenfest theorem

Consider a 1-dimensional particle in a region with potential energy $V(x)$.

i) Find the time evolution of the expectation values of its position and its momentum [*Ehrenfest theorem*]. Integrate these equations and compare them with the classical equations of motion for a massive particle in a potential $V(x) = -Fx$, where F is a constant.

ii) Does the center of the wave function follow the classical laws of motion for a generic potential $V(x) = -\lambda x^n$?

Exercise 9: Virial theorem

The *virial theorem* establishes that $2\langle K\rangle_\psi = \langle \vec{x}\cdot\nabla V(\vec{x})\rangle_\psi$, where K is the kinetic energy of a stationary state ψ with potential energy V. Show that

i) The theorem applied to a potential $V(x) = kx^n$ implies $2\langle K\rangle = n\langle V\rangle$.

ii) If $V(\vec{x})$ decreases radially $\forall\, x \neq 0$, then H has no eigenvectors.

iii) If $\vec{x}\cdot\nabla V(\vec{x}) \leq -\gamma V(\vec{x})$, $\forall\,\vec{x}\neq 0$, $0<\gamma<2$, then H has no eigenvalues $E>0$.

iv) If $V(r) = -g\mathrm{e}^{-kr}/r$ (where g and k are positive real numbers), then $\vec{x}\cdot\nabla V(r) \leq -V(r)+gk$ and all the energy eigenvalues verify $E \leq gk$.

v) Use that the observable $\vec{X}\cdot\vec{P}$ is a constant of motion of an arbitrary stationary state (why?) to prove the virial theorem.

Exercise 4 must be turned in [deadline: 29 October 2020 at 15:00]