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Problem 1: Free propagator (Oral)

Learning objective

In this exercise, we study the concept of the propagator in order to solve the Schrödinger equation. As an example, we calculate the propagator of a single, free particle in one dimension.

The propagator $K(x, x', t)$ of a Hamiltonian operator H (some differential operator in x) is defined as the solution of the Schrödinger equation

$$i\hbar\partial_t K(x, x', t) = HK(x, x', t) \tag{1}$$

with the initial condition $K(x, x', 0) = \delta(x - x')$.

a) Show that for the initial condition $\psi(x, t = 0) = \psi_0(x)$ the solution of the Schrödinger equation is given by

$$\psi(x, t) = \int \; dx' \, K(x, x', t)\psi_0(x') \, . \tag{2}$$

b) Show using Fourier transformation (plane wave expansion) that the propagator of a free particle with Hamiltonian operator $H = -\hbar^2\partial_x^2/2m$ is given by

$$K(x, x', t) = \sqrt{\frac{m}{2\pi\hbar i t}} \exp\left(\frac{im(x - x')^2}{2\hbar t}\right) \, . \tag{3}$$

Problem 2: Wave packet (Written, 5 points)

Learning objective

Gaussian Wave functions are very useful in quantum mechanics, as they allow for the derivation of many exact results. In this exercise, we study the time evolution of such an initial wave function.

We consider a free particle of mass m. Its dispersion relation is $\omega(k) = \frac{\hbar}{2m}k^2$. As shown in the lecture, the functions $\psi_k(x, t) = e^{i(kx - \omega(k)t)}$ form a basis for the solution space of the Schrödinger equation for the free particle.

At time $t = 0$, the particle is prepared in the state

$$\psi(x, 0) = A \, e^{ik_0 x} e^{-\frac{(x - x_0)^2}{4\sigma}} \, . \tag{4}$$

a) Calculate the normalization constant A.

b) Show that the wave packet becomes

$$\psi(x,t) = \left(\frac{\sigma}{2\pi\sigma_t^2}\right)^{\frac{1}{4}} e^{ik_0x} e^{-i\frac{\hbar}{2m}k_0^2 t} e^{-\frac{(x-(x_0+\hbar k_0 t/m))^2}{4\sigma_t}} \quad \text{with} \quad \sigma_t = \sigma + i\frac{\hbar}{2m}t \tag{5}$$

for arbitrary time t.

c) Determine the velocity of the particle which is described by the wave packet. Use the equations

$$\langle v\rangle = \partial_t \langle x\rangle \ , \quad \langle x\rangle = \int_{-\infty}^{\infty} \mathrm{d}x\ \psi^*(x,t)x\psi(x,t) \ . \tag{6}$$

d) The uncertainty Δx is defined by $(\Delta x)^2 = \langle x^2\rangle - \langle x\rangle^2$. It is a measure of the width of a probability distribution. At $t=0$, the uncertainty of the particle's position is given by $(\Delta x)^2|_{t=0} = \sigma$. Show that

$$(\Delta x)^2 = \sigma(a_0 + a_1 t^2) \tag{7}$$

for arbitrary time t.

e) A linear dispersion relation $\omega(k) = c_0 + c_1 k$ would have changed the results for the free particle. Show that the wave packet would not have broadened in time.

Problem 3: Harmonic oscillator in path integral formulation (Written, 2 points + 1 bonus)

Learning objective

The harmonic oscillator is a very important problem in quantum mechanics. In this exercise, we derive the propagator for the harmonic oscillator using the path integral approach.

The propagator for a particle of mass m in a harmonic potential $V(x) = \frac{1}{2}m\omega^2x^2$ is given by

$$K(x_b, x_a, t_b) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega t_b)}}\ \exp\left(\frac{im\omega}{2\hbar\sin(\omega t_b)}\left((x_a^2 + x_b^2)\cos(\omega t_b) - 2x_a x_b\right)\right) \ , \tag{8}$$

where we set $t_a = 0$ without loss of generality. We make use of the path integral formulation to derive this result.

a) In the path integral formulation, the propagator is calculated from the action $S[x]$ as

$$K(x_b, x_a, t_b) = \int_{x_a}^{x_b} \mathcal{D}x\ e^{iS[x]/\hbar} \ . \tag{9}$$

Express the quantum path as $x(t) = \overline{x}(t) + y(t)$ as a sum of the classical path $\overline{x}(t)$ and fluctuations $y(t)$. Write the action as the sum of the classical action and the contribution of the fluctuations. What are the boundary conditions for the fluctuations? Show that

$$K(x_b, x_a, t_b) = F(t_b)\ e^{iS[\overline{x}]/\hbar} \ , \tag{10}$$

and demonstrate that $F(t_b)$ is independent of the initial and final positions x_a and x_b.

b) Show that the classical solution of the harmonic oscillator takes the form

$$\overline{x}(t) = \frac{x_b - x_a \cos(\omega t_b)}{\sin(\omega t_b)} \sin(\omega t) + x_a \cos(\omega t) \ . \tag{11}$$

Evaluate the classical action for this solution.

c) **Bonus task:** Next, we determine the prefactor $F(t_b)$. Make use of the expansion of the fluctuations

$$y(t) = \sum_{n=1}^{\infty} a_n y_n(t) \ , \tag{12}$$

with $y_n(t) = \sqrt{\frac{2}{t_b}} \sin(n\pi t/t_b)$.

Hints

- Use the eigenvalue equation $(-\partial_t^2 - \omega^2) y_n(t) = \lambda_n y_n(t)$ and the orthonormality of y_n to evaluate $S[y]$.
- Rewrite $\mathcal{D}y = J \prod_{n=1}^{\infty} \mathrm{d}a_n$, where J is a undetermined normalization constant. Calculate $F(t_b)$ as a function J and λ_n.
- To get rid of J, we study the limit $\omega \to 0$ of the propagator. In this limit, we must obtain the solution for a free particle and we can derive $F_0(t_b) = F(t_b)|_{\omega \to 0}$ from equation (3) of problem 1. We can use this finding to obtain the result for arbitrary ω as $F(t_b) = \frac{F(t_b)}{F_0(t_b)} F_0(t_b)$. The fraction $\frac{F(t_b)}{F_0(t_b)}$ can be simplified using $\sin(x) = x \prod_{k=1}^{\infty} \left(1 - \frac{x^2}{k^1 \pi^1}\right)$.