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Problem 2.1: Free propagator **[Oral] (2 pts.)**

↪ ID: ex_free_propagator:qm2122

> **Learning objective**
>
> In this exercise, you study the concept of the propagator in order to solve the Schrödinger equation. As an example, you 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 an arbitrary 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 2.2: Wave packet **[Written] (5 pts.)**

↪ ID: ex_wave_packet:qm2122

> **Learning objective**
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> Gaussian wave functions are very useful in quantum mechanics, as they allow for the derivation of many exact results. In this exercise, you 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.

Assume that at time $t = 0$ the particle is prepared in the state

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

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a) Calculate the normalization constant A.

b) Show that the wave packet evolves into

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

with $\sigma_t = \sigma + i\frac{\hbar}{2m}t$ for arbitrary time t.

c) Determine the velocity of the particle which is described by the wave packet. To this end, use the definitions

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

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 (where a_0 and a_1 should be determined).

e) A *linear* dispersion relation $\omega(k) = c_0 + c_1 k$ would have changed the results for the free particle.

Show that in this case, the wave packet would not have broadened over time.

Problem 2.3: Harmonic oscillator in path integral formulation **[Written] (2 pts.)**

↪ ID: ex_harmonic_oscillator_path_integral_formulation:qm2122

Learning objective

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

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

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

where we set $t_a = 0$ without loss of generality.

Here we make use of the path integral formulation of quantum mechanics to derive this result.

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

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

where $x : [t_a, t_b] \to \mathbb{R}$ denotes trajectories of the particle with $x(t_a) = x_a$ and $x(t_b) = x_b$.

Express these trajectories $x(t) = \overline{x}(t) + y(t)$ 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 of this solution to obtain the factor $e^{iS[\overline{x}]/\hbar}$.

*c) Finally, determine the prefactor $F(t_b)$ by using 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 $S[y]$.
- Use the parametrization $\mathcal{D}y = J \prod_{n=1}^{\infty} \mathrm{d}a_n$, where J is a (yet) undetermined normalization constant. Calculate $F(t_b)$ as a function of J and λ_n.
- To get rid of J, study the limit $\omega \to 0$ of the propagator. In this limit, one must obtain the solution for a free particle and can derive $F_0(t_b) = F(t_b)|_{\omega \to 0}$ from equation (3) of the first problem. 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 the identity $\sin(x) = x \prod_{k=1}^{\infty} \left(1 - \frac{x^2}{k^2 \pi^2}\right)$.