Quantum Mechanics

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WS 24/25

Sheet 4 Saturday November 2 at 24:00

1 Free time evolution of Gaussian wave-packets

In this exercise, we consider the time-evolution of 'free' particles, i.e., particles that evolve under the Hamiltonian $H = P^2/(2m)$, which leads to the Scrödinger equation

$$i\hbar\partial_t\psi(t,x) = -\frac{\hbar^2}{2m}\partial_x^2\psi(t,x). \tag{1}$$

Here, we focus on Gaussian wave-packets

$$\psi_{\sigma,x_0,k_0}(x) = \left(\frac{1}{2\pi\sigma^2}\right)^{1/4} e^{-\frac{(x-x_0)^2}{4\sigma^2}} e^{ik_0(x-x_0)}, \tag{2}$$

where $\sigma, x_0, k_0, \in \mathbb{R}$ and $\sigma > 0$, and where ψ_{σ,x_0,k_0} is normalized such that $\int_{-\infty}^{\infty} |\psi_{\sigma,x_0,k_0}(x)|^2 dx = 1$.

a) Before we turn to the Gaussian wave-packets (2), let us for a moment consider general solutions. The strategy is to solve the Scrödinger equation (1) via Fourier transforms. Recall that we use conventions for the Fourier transform such that

$$\tilde{\psi}(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-ikx}\psi(x)dx, \quad \psi(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}\tilde{\psi}(k)dk.$$

Show that the Fourier transformed Schrödinger equation (1) has the solution

$$\tilde{\psi}(t,k) = \tilde{\psi}(0,k)e^{-it\frac{\hbar}{2m}k^2}, \tag{3}$$

where $\tilde{\psi}(0,k)$ is the Fourier transform of the initial state $\psi(0,x)$. You can use as a fact that if $\phi(x) = \partial_x^2\psi(x)$, then $\tilde{\phi}(k) = (ik)^2\tilde{\psi}(k)$. *Use (3) to show that the solution to (1) is*

$$\psi(t,x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \tilde{\psi}(0,k)e^{-it\frac{\hbar}{2m}k^2}e^{ikx}dk. \tag{4}$$

(2 points)

b) We can conclude that it is useful to determine the Fourier transform of ψ_{σ,x_0,k_0}. *Show that the Fourier transform of ψ_{σ,x_0,k_0} is*

$$\tilde{\psi}_{\sigma,x_0,k_0}(k) = \left(\frac{2\sigma^2}{\pi}\right)^{1/4} e^{-\sigma^2(k-k_0)^2}e^{-ikx_0}. \tag{5}$$

Hint: Try to use the results from sheet 1 as much as you can, in order to avoid unnecessary work.

(3 points)

c) We let $\tilde{\psi}(0,k) = \tilde{\psi}_{\sigma,x_0,k_0}(k)$ in (3). *Determine the expectation value* $\langle P\rangle(t)$ *and variance* $\mathrm{Var}[P](t)$ *for the evolving state.* It is fine to look up the expectation value and variance of normal distributions.

Hint: Recall that $p = \hbar k$.

(2 points)

d) Finally, we evaluate (4) for $\tilde{\psi}(0,k) = \tilde{\psi}_{\sigma,x_0,k_0}(k)$. For this purpose one can use the following generalization of the Gaussian integral[1]

$$\int_{-\infty}^{\infty} e^{-\alpha(k-\beta)^2} dk = \sqrt{\frac{\pi}{\alpha}}, \quad \alpha,\beta \in \mathbb{C}, \quad \mathrm{Re}(\alpha) > 0. \tag{6}$$

In other words, we allow the parameters α and β to be complex. *Show that*

$$\psi_{\sigma,x_0,k_0}(t,x) = \left(\frac{\sigma^2}{2\pi}\right)^{1/4} \frac{1}{\sqrt{\sigma^2 + i\frac{t\hbar}{2m}}} \exp\left[\frac{-(x-x_0)^2/4 + i\sigma^2 k_0(x-x_0) - i\sigma^2 k_0^2 \frac{t\hbar}{2m}}{\sigma^2 + i\frac{t\hbar}{2m}}\right]. \tag{7}$$

Hint: Use completion of squares in order to rewrite the right hand side of (5) and determine α and β in (6). Note that the completion yields a 'leftover' that does not depend on k. This leftover yields the exponent in (7).

(4 points)

2 Commutators and the Heisenberg picture.

a) Let A, B and C be operators.

Show that

$$[AB, C] = A[B,C] + [A,C]B, \quad [A, BC] = B[A,C] + [A,B]C.$$

Remark: These simple relations are actually quite useful. They are worth remembering.

(2 points)

b) Suppose that two operators A and B are such that $[A,B] = z\hat{1}$, where z is a complex number. *Show that*

$$[A, B^n] = znB^{n-1}, \quad n = 1, 2, \ldots.$$

Hint: Use induction and a).

(2 points)

c) Let A and B be operators such that $[A,B] = z\hat{1}$. Let f be a polynomial, or a function with a (nice) Taylor expansion. *Show that*

$$[A, f(B)] = zf'(B), \quad [f(A), B] = zf'(A), \tag{8}$$

where f' *denotes the derivative of* f.

(1 point)

Remark: An important special case of this result is the position operator X and momentum operator P, which satisfy the canonical commutation relation $[X,P] = i\hbar\hat{1}$, where we thus have

$$[f(X), P] = i\hbar f'(X), \quad [X, f(P)] = i\hbar f'(P).$$

[1] The square root has two branches (the solution to the equation $x^2 = \alpha$ has the two solutions $\sqrt{\alpha}$ and $-\sqrt{\alpha}$). In (6) we chose the branch such that the real part of $\sqrt{\alpha}$ is positive.

Another important special case is if A and B commute, i.e. $[A, B] = 0$ (and thus $z = 0$), in which case (8) yields

$$[A, f(B)] = 0.$$

d) For a (time-independent) Hamilton operator H, the time evolution is given by the family of unitary operators $U(t) = e^{-itH/\hbar}$. *Show that*

$$[U(t), H] = 0.$$

Hint: If there ever were a function with a nice Taylor expansion, it is the exponential function.

(1 point)

e) Let $F(t) = U(t)^\dagger F U(t)$ be the Heisenberg picture of an operator F. *Show that*

$$[F(t), H] = U(t)^\dagger [F, H] U(t).$$

(1 point)

f) *Use the fact that the Hamilton operator is Hermitian, $H = H^\dagger$, in order to show that $U(t)^\dagger = U(-t)$.*

(2 points)