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Physics 610 by Dr. Johnson
Master Homework Problem

"For a free particle, compute the time evolution of a Gaussian packet and how its expectation values change in time."

The Hamiltonian for a free particle is just the kinetic energy,

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \tag{1}$$

We start with the Gaussian wavepacket centered at $x = x_0$, which we write as

$$\Psi(x, t=0) = \Psi_0(x) = (2\pi\sigma^2)^{-1/4} e^{-\frac{(x-x_0)^2}{4\sigma^2}} \tag{2}$$

1 Normalization

"For the general Gaussian wavefunction $\Psi(x) = Ae^{(-ax^2/2)}$, with complex valued a, find the normalization A."

For normalization we require that $1 =< \Psi|\Psi >$. In position space we have that:

$$\begin{aligned} 1 &= \int_{-\infty}^{+\infty} dx\ \Psi^*(x)\ \Psi(x) \\ &= \int_{-\infty}^{+\infty} dx\ A^* e^{-\frac{a^* x^2}{2}}\ Ae^{-\frac{ax^2}{2}} \\ &= |A|^2 \int_{-\infty}^{+\infty} dx\ e^{-(a^*+a)x^2/2} \\ &= |A|^2 \int_{-\infty}^{+\infty} dx\ e^{-Re(a)x^2} \end{aligned} \tag{3}$$

To continue we need to solve the Guassian integral $I = \int_{-\infty}^{+\infty} dx\ e^{-ax^2}$. To do this we consider the quanity I^2, make a change of variables to polar coordinates, and solve by a simple substitution.

$$
\begin{aligned}
I^2 &= \Big(\int_{-\infty}^{+\infty} dx\ e^{-ax^2} \Big) \Big(\int_{-\infty}^{+\infty} dy\ e^{-ay^2} \Big) \\
&= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} dx\ dy\ e^{-a(x^2+y^2)} \\
&= \int_{0}^{2\pi} \int_{0}^{+\infty} r\ d\theta\ dr\ e^{-ar^2} \\
&= 2\pi \int_{0}^{+\infty} \frac{1}{2}\ du\ e^{-au} \\
&= \pi \Big(-\frac{1}{a} e^{-au} \Big|_0^{+\infty} \Big) \\
&= \frac{\pi}{a}
\end{aligned} \tag{4}
$$

We now have all we need to complete the normalization. Resuming from the last line of (3),

$$
\begin{aligned}
1 &= |A|^2 \int_{-\infty}^{+\infty} dx\ e^{-Re(a)x^2} \\
&= |A|^2 \sqrt{\frac{\pi}{Re(a)}}
\end{aligned} \tag{5}
$$

Thus, as long as $Re(A) > 0$ (otherwise the magnitude of A is imaginary),

$$
\boxed{A = \pm \Big(\frac{Re(a)}{\pi} \Big)^{\frac{1}{4}}} \tag{6}
$$

2 Expectation value $< x^2 >$

"For the normalized Gaussian wavefunction in problem 1, fine the expectation value $< x^2 >$."

For a general operator (observable) $\hat{\Omega}$ the expectation value in a state Ψ is calculated as $< \hat{\Omega} > = < \Psi | \hat{\Omega} | \Psi >$. Using the positive normalization found in problem 1, we arrive at the wavefunction

$$
\Psi(x) = \Big(\frac{Re(a)}{\pi} \Big)^{\frac{1}{4}}\ e^{-\frac{ax^2}{2}} \tag{7}
$$

Thus for the operator x^2,

$$
\begin{aligned}
< x^2 > &= < \Psi | x^2 | \Psi > \\
&= \int_{-\infty}^{+\infty} dx\ \Psi^*(x)\ x^2\ \Psi(x) \\
&= \Big(\frac{Re(a)}{\pi} \Big)^{\frac{1}{2}}\ \int_{-\infty}^{+\infty} dx\ x^2\ e^{-Re(a)x^2}
\end{aligned} \tag{8}
$$

The Guassian integral $I = \int_{-\infty}^{+\infty} dx\ x^2\ e^{-ax^2}$ can be solved by the method of differentiation under the integral which is demonstrated here. To begin, first notice that

$$x^2\ e^{-ax^2} = -\frac{\partial}{\partial a} e^{-ax^2} \tag{9}$$

Thus,

$$\begin{aligned} I &= \int_{-\infty}^{+\infty} dx\ x^2\ e^{-ax^2} \\ &= -\int_{-\infty}^{+\infty} dx\ \frac{\partial}{\partial a} e^{-ax^2} \\ &= -\frac{\partial}{\partial a} \int_{-\infty}^{+\infty} dx\ e^{-ax^2} \\ &= -\frac{\partial}{\partial a} \sqrt{\frac{\pi}{a}} \\ &= \frac{1}{2a} \sqrt{\frac{\pi}{a}} \end{aligned} \tag{10}$$

Where the third equality follows from a being a constant with respect to x, and where the fourth equality comes from the results of problem 1 (4). Picking up from the last line of (8),

$$\begin{aligned} < x^2 > &= \left(\frac{Re(a)}{\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{+\infty} dx\ x^2\ e^{-Re(a)x^2} \\ &= \left(\frac{Re(a)}{\pi}\right)^{\frac{1}{2}} \frac{1}{2Re(a)} \left(\frac{\pi}{Re(a)}\right)^{\frac{1}{2}} \end{aligned} \tag{11}$$

$$\boxed{< x^2 >= \frac{1}{2Re(a)}}$$

It's worth verifying the dimensions of this solution. Note that in order for the argument of the *exp* function in Ψ to be dimensionless, a must have dimensions of L^{-2}. So our solution has the correct dimensions, L^2.