PHYS-C0252 - Quantum Mechanics

Exercise set 4 - model solutions

Due date: May 22, 2024 by 23:59 on MyCourses
Return the exercises as a `.pdf`.
You can write by hand and take pictures, use digital note-taking or LaTeX etc.

1. (a) Using

$$\langle x|\psi\rangle = \psi(x), \tag{1}$$
$$\hat{x}\,|x\rangle = x\,|x\rangle\,, \tag{2}$$
$$\langle x'|\hat{p}|x\rangle = -\mathrm{i}\hbar\delta(x'-x)\frac{\partial}{\partial x}, \tag{3}$$

Derive the expressions

$$\langle\psi|\hat{x}|\psi\rangle = \int_{-\infty}^{\infty} x|\psi(x)|^2\mathrm{d}x,$$
$$\langle\psi|\hat{p}|\psi\rangle = -\mathrm{i}\hbar\int_{-\infty}^{\infty}\psi^*(x)\psi'(x)\mathrm{d}x$$

for the expectation values of position and momentum.
Hint: It maybe useful to insert the identity operator

$$\hat{I} = \int_{-\infty}^{\infty} |x\rangle\,\langle x|\,\mathrm{d}x$$

at some point(s) inside the expressions for the expectation values. For example, an inner product between two states $|\psi\rangle$ and $|\chi\rangle$ is given by

$$\langle\psi|\chi\rangle = \langle\psi|\underbrace{\left(\int_{-\infty}^{\infty}|x\rangle\,\langle x|\,\mathrm{d}x\right)}_{\hat{I}}|\chi\rangle$$
$$= \int_{-\infty}^{\infty}\langle\psi|x\rangle\,\langle x|\chi\rangle\,\mathrm{d}\alpha = \int_{-\infty}^{\infty}\psi^*(x)\chi(x)\mathrm{d}x.$$

(b) Consider a one-dimensional particle in a quantum state whose position-basis representation is

$$\langle x|\psi\rangle = \psi(x) = \begin{cases} A\sin(kx)\,\mathrm{e}^{\mathrm{i}kx}\mathrm{e}^{-\lambda x}, & \text{if } x\in[0,\infty),\\ 0, & \text{otherwise,}\end{cases}$$

where $\lambda > 0$ and $k \in \mathbb{R}\backslash\{0\}$. Find a suitable scalar A such that $\psi(x)$ is normalized. Hint: recall that $\sin x = \frac{\mathrm{e}^{\mathrm{i}x}-\mathrm{e}^{-\mathrm{i}x}}{2\mathrm{i}}$ to simplify the integral.

(c) For the wave function given in part (b), find the expectation values of position and momentum. Hint from (b) might prove to be useful here as well.

Solution:

(a)

$$\begin{aligned}
\langle\psi|\hat{x}|\psi\rangle &= \langle\psi|\,\hat{x}\int_{-\infty}^{\infty}|x\rangle\langle x|\,\mathrm{d}x\,|\psi\rangle \\
&= \langle\psi|\int_{-\infty}^{\infty}\hat{x}\,|x\rangle\langle x|\psi\rangle\,\mathrm{d}x \\
&= \langle\psi|\int_{-\infty}^{\infty}x\,|x\rangle\,\psi(x)\mathrm{d}x \\
&= \int_{-\infty}^{\infty}x\,\langle\psi|x\rangle\,\psi(x)\mathrm{d}x \\
&= \int_{-\infty}^{\infty}x\psi(x)^*\psi(x)dx = \int_{-\infty}^{\infty}x|\psi(x)|^2\mathrm{d}x
\end{aligned}$$

$$\begin{aligned}
\langle\psi|\hat{p}|\psi\rangle &= \langle\psi|\int_{-\infty}^{\infty}|x'\rangle\langle x'|\,dx'\hat{p}\int_{-\infty}^{\infty}|x\rangle\langle x|\,\mathrm{d}x\,|\psi\rangle \\
&= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\langle\psi|x'\rangle\langle x'|\,\hat{p}\,|x\rangle\langle x|\psi\rangle\,\mathrm{d}x\mathrm{d}x' \\
&= -\mathrm{i}\hbar\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi^*(x')\delta(x'-x)\frac{\partial}{\partial x}\psi(x)\mathrm{d}x\mathrm{d}x' \\
&= -\mathrm{i}\hbar\int_{-\infty}^{\infty}\psi^*(x)\psi'(x)\mathrm{d}x
\end{aligned}$$

(b) First let's massage the non-zero part of $\psi(x)$ into an expression that involves only exponential functions with the assistance of the identity $\sin x = \frac{\mathrm{e}^{\mathrm{i}x}-\mathrm{e}^{-\mathrm{i}x}}{2\mathrm{i}}$:

$$\begin{aligned}
\psi(x) &= \frac{A}{2\mathrm{i}}\left(\mathrm{e}^{\mathrm{i}kx}-\mathrm{e}^{-\mathrm{i}kx}\right)\mathrm{e}^{\mathrm{i}kx}\mathrm{e}^{-\lambda x} = \frac{A}{2\mathrm{i}}\left(\mathrm{e}^{\mathrm{i}kx}\mathrm{e}^{\mathrm{i}kx}\mathrm{e}^{-\lambda x}-\mathrm{e}^{-\mathrm{i}kx}\mathrm{e}^{\mathrm{i}kx}\mathrm{e}^{-\lambda x}\right) \\
&= \frac{A}{2\mathrm{i}}\left(\mathrm{e}^{2\mathrm{i}kx}\mathrm{e}^{-\lambda x}-\mathrm{e}^{-\lambda x}\right) = \frac{A}{2\mathrm{i}}\left(\mathrm{e}^{(-\lambda+2\mathrm{i}k)x}-\mathrm{e}^{-\lambda x}\right),
\end{aligned}$$

when $x \in [0,\infty)$. For future reference, let's also compute $\psi^*(x)$ on the same interval making use of the fact that $\left(\mathrm{e}^{\mathrm{i}x}\right)^* = \mathrm{e}^{-\mathrm{i}x}$:

$$\begin{aligned}
\psi^*(x) &= \left[\frac{A}{2\mathrm{i}}\left(\mathrm{e}^{(-\lambda+2\mathrm{i}k)x}-\mathrm{e}^{-\lambda x}\right)\right]^* = \left(\frac{A}{2\mathrm{i}}\right)^*\left(\mathrm{e}^{(-\lambda+2\mathrm{i}k)x}-\mathrm{e}^{-\lambda x}\right)^* \\
&= -\frac{A}{2\mathrm{i}}\left[\left(\mathrm{e}^{(-\lambda+2\mathrm{i}k)x}\right)^*-\left(\mathrm{e}^{-\lambda x}\right)^*\right] = -\frac{A}{2\mathrm{i}}\left(\mathrm{e}^{(-\lambda-2\mathrm{i}k)x}-\mathrm{e}^{-\lambda x}\right).
\end{aligned}$$

Finally, we proceed by determining the normalization scalar A after noting that $\int_a^b e^{cx}\mathrm{d}x = \frac{1}{c}e^{cx}\big|_{x=a}^b$ for any $c \in \mathbb{C}\setminus\{0\}$, as the exponential function is an analytic function (which you will learn/have learned about in an introductory complex analysis course), allowing us to extend some of the familiar results from calculus of real-valued functions into the complex plane:

$$\begin{aligned}
\langle\psi|\psi\rangle &= \int_{-\infty}^{\infty} \psi^*(x)\psi(x)\mathrm{d}x = \int_{0}^{\infty} \psi^*(x)\psi(x)\mathrm{d}x \\
&= \int_0^\infty -\frac{A}{2\mathrm{i}}\left(\mathrm{e}^{(-\lambda-2\mathrm{i}k)x} - \mathrm{e}^{-\lambda x}\right)\frac{A}{2\mathrm{i}}\left(\mathrm{e}^{(-\lambda+2\mathrm{i}k)x} - \mathrm{e}^{-\lambda x}\right)\mathrm{d}x \\
&= \frac{A^2}{4}\int_0^\infty \left(\mathrm{e}^{(-\lambda-2\mathrm{i}k)x} - \mathrm{e}^{-\lambda x}\right)\left(\mathrm{e}^{(-\lambda+2\mathrm{i}k)x} - \mathrm{e}^{-\lambda x}\right)\mathrm{d}x \\
&= \frac{A^2}{4}\int_0^\infty \left(\mathrm{e}^{-2\lambda x} - \mathrm{e}^{(-2\lambda-2\mathrm{i}k)x} - \mathrm{e}^{(-2\lambda+2\mathrm{i}k)x} + \mathrm{e}^{-2\lambda x}\right)\mathrm{d}x \\
&= \frac{A^2}{4}\int_0^\infty \left(2\mathrm{e}^{-2\lambda x} - \mathrm{e}^{-2(\lambda+\mathrm{i}k)x} - \mathrm{e}^{-2(\lambda-\mathrm{i}k)x}\right)\mathrm{d}x \\
&= \frac{A^2}{4}\left(-\frac{1}{\lambda}\mathrm{e}^{-2\lambda x} + \frac{1}{2(\lambda+\mathrm{i}k)}\mathrm{e}^{-2(\lambda+\mathrm{i}k)x} + \frac{1}{2(\lambda-\mathrm{i}k)}\mathrm{e}^{-2(\lambda-\mathrm{i}k)x}\right)\Bigg|_{x=0}^{\infty} \\
&= \frac{A^2}{4}\left(-\frac{1}{\lambda} + \frac{1}{2(\lambda+\mathrm{i}k)}\mathrm{e}^{-2\mathrm{i}kx} + \frac{1}{2(\lambda-\mathrm{i}k)}\mathrm{e}^{2\mathrm{i}kx}\right)\mathrm{e}^{-2\lambda x}\Bigg|_{x=0}^{\infty}
\end{aligned}$$

To evaluate the $x \to \infty$ limit of this expression, we remark that $\mathrm{e}^{-2\lambda x}$ is a term that corresponds to exponential decay for $\lambda > 0$ that approaches 0 as x tends to ∞, while the modulus of the phase factors $\mathrm{e}^{2\mathrm{i}kx}$ and $\mathrm{e}^{-2\mathrm{i}kx}$ is equal to 1. Thus the decay term dominates asymptotically. More generally, $\lim_{x\to\infty} x^n \mathrm{e}^{\mathrm{i}kx}\mathrm{e}^{-\lambda x} \to 0$ for any $n \in \mathbb{N}_0$, $k \in \mathbb{R}$, and $\lambda > 0$. Consequently, the norm of this wave function is

$$\begin{aligned}
\langle\psi|\psi\rangle &= \lim_{x\to\infty}\frac{A^2}{4}\left(-\frac{1}{\lambda} + \frac{1}{2(\lambda+\mathrm{i}k)}\mathrm{e}^{-2\mathrm{i}kx} + \frac{1}{2(\lambda-\mathrm{i}k)}\mathrm{e}^{2\mathrm{i}kx}\right)\mathrm{e}^{-2\lambda x} \\
&\quad - \lim_{x\to 0}\frac{A^2}{4}\left(-\frac{1}{\lambda} + \frac{1}{2(\lambda+\mathrm{i}k)}\mathrm{e}^{-2\mathrm{i}kx} + \frac{1}{2(\lambda-\mathrm{i}k)}\mathrm{e}^{2\mathrm{i}kx}\right)\mathrm{e}^{-2\lambda x} \\
&= 0 - \frac{A^2}{4}\left(-\frac{1}{\lambda} + \frac{1}{2(\lambda+\mathrm{i}k)}\mathrm{e}^{-2\mathrm{i}k\cdot 0} + \frac{1}{2(\lambda-\mathrm{i}k)}\mathrm{e}^{2\mathrm{i}k\cdot 0}\right)\mathrm{e}^{-2\lambda\cdot 0} \\
&= \frac{A^2}{4}\left(\frac{1}{\lambda} - \frac{1}{2(\lambda+\mathrm{i}k)} - \frac{1}{2(\lambda-\mathrm{i}k)}\right) = \frac{A^2}{4}\left(\frac{1}{\lambda} - \frac{\lambda-\mathrm{i}k}{2(\lambda^2+k^2)} - \frac{\lambda+\mathrm{i}k}{2(\lambda^2+k^2)}\right) \\
&= \frac{A^2}{4}\left(\frac{1}{\lambda} - \frac{\lambda}{\lambda^2+k^2}\right) = \frac{A^2}{4}\left(\frac{\lambda^2+k^2}{\lambda(\lambda^2+k^2)} - \frac{\lambda^2}{\lambda(\lambda^2+k^2)}\right) \\
&= \frac{A^2}{4}\left(\frac{k^2}{\lambda(\lambda^2+k^2)}\right) = 1 \Rightarrow A = 2\sqrt{\frac{\lambda(\lambda^2+k^2)}{k^2}}
\end{aligned}$$

In 1D, a wave function should have the dimensions of $\frac{1}{\sqrt{\text{length}}}$, and since both λ and k have the dimension of $\frac{1}{\text{length}}$, one can readily verify that the above expression for A gives the wave function the right dimensionality.

(c) We now proceed in a similar fashion to evaluate the other integrals, but before we do so, it might be worthwhile to recall the formula for integration by parts. Given two continuously differentiable functions $u(x)$ and $v(x)$, the following identity holds:

$$\int_a^b u(x)v'(x)\mathrm{d}x = u(x)v(x)\Big|_a^b - \int_a^b u'(x)v(x)\mathrm{d}x.$$

Now, skipping some of the intermediate algebraic simplification steps that are identical to what was done in part (b), the expectation value of $\hat{x}$ is given by

$$\begin{aligned}
\langle\psi|\hat{x}|\psi\rangle &= \int_{-\infty}^{\infty} x\psi^*(x)\psi(x)\mathrm{d}x \\
&= \int_0^{\infty} -\frac{A}{2\mathrm{i}}\left(\mathrm{e}^{(-\lambda-2\mathrm{i}k)x} - \mathrm{e}^{-\lambda x}\right) x\frac{A}{2\mathrm{i}}\left(\mathrm{e}^{(-\lambda+2\mathrm{i}k)x} - \mathrm{e}^{-\lambda x}\right)\mathrm{d}x \\
&= \frac{A^2}{4}\int_0^{\infty} x\left(2\mathrm{e}^{-2\lambda x} - \mathrm{e}^{-2(\lambda+\mathrm{i}k)x} - \mathrm{e}^{-2(\lambda-\mathrm{i}k)x}\right)\mathrm{d}x \\
&= \frac{A^2}{4}x\left(-\frac{1}{\lambda} + \frac{1}{2(\lambda+\mathrm{i}k)}\mathrm{e}^{-2\mathrm{i}kx} + \frac{1}{2(\lambda-\mathrm{i}k)}\mathrm{e}^{2\mathrm{i}kx}\right)\mathrm{e}^{-2\lambda x}\Big|_{x=0}^{\infty} \\
&\quad - \frac{A^2}{4}\int_a^b\left(-\frac{1}{\lambda}\mathrm{e}^{-2\lambda x} + \frac{1}{2(\lambda+\mathrm{i}k)}\mathrm{e}^{-2(\lambda+\mathrm{i}k)x} + \frac{1}{2(\lambda-\mathrm{i}k)}\mathrm{e}^{-2(\lambda-\mathrm{i}k)x}\right)\mathrm{d}x,
\end{aligned}$$

where we have used integration by parts with $u(x) = x$ and $v(x) = 2\mathrm{e}^{-2\lambda x} - \mathrm{e}^{-2(\lambda+\mathrm{i}k)x} - \mathrm{e}^{-2(\lambda-\mathrm{i}k)x}$. Now, since $\lim_{x\to\infty} x^n\mathrm{e}^{\mathrm{i}kx}\mathrm{e}^{-\lambda x} \to 0$ as mentioned in part (b), the first term in the last equality is in fact equal to zero. We are thus left with evaluating the second integral, which is quite straightforward as an integral of exponential functions:

$$\begin{aligned}
\langle\psi|\hat{x}|\psi\rangle &= -\frac{A^2}{4}\int_a^b\left(-\frac{1}{\lambda}\mathrm{e}^{-2\lambda x} + \frac{1}{2(\lambda+\mathrm{i}k)}\mathrm{e}^{-2(\lambda+\mathrm{i}k)x} + \frac{1}{2(\lambda-\mathrm{i}k)}\mathrm{e}^{-2(\lambda-\mathrm{i}k)x}\right)\mathrm{d}x \\
&= -\frac{A^2}{4}\left(\frac{1}{2\lambda^2}\mathrm{e}^{-2\lambda x} - \frac{1}{4(\lambda+\mathrm{i}k)^2}\mathrm{e}^{-2(\lambda+\mathrm{i}k)x} - \frac{1}{4(\lambda-\mathrm{i}k)^2}\mathrm{e}^{-2(\lambda-\mathrm{i}k)x}\right)\Big|_{x=0}^{\infty} \\
&= \lim_{x\to\infty} -\frac{A^2}{4}\left(\frac{1}{2\lambda^2}\mathrm{e}^{-2\lambda x} - \frac{1}{4(\lambda+\mathrm{i}k)^2}\mathrm{e}^{-2(\lambda+\mathrm{i}k)x} - \frac{1}{4(\lambda-\mathrm{i}k)^2}\mathrm{e}^{-2(\lambda-\mathrm{i}k)x}\right) \\
&\quad - \lim_{x\to 0} -\frac{A^2}{4}\left(\frac{1}{2\lambda^2}\mathrm{e}^{-2\lambda x} - \frac{1}{4(\lambda+\mathrm{i}k)^2}\mathrm{e}^{-2(\lambda+\mathrm{i}k)x} - \frac{1}{4(\lambda-\mathrm{i}k)^2}\mathrm{e}^{-2(\lambda-\mathrm{i}k)x}\right) \\
&= 0 - \left[-\frac{A^2}{4}\left(\frac{1}{2\lambda^2}\mathrm{e}^{-2\lambda\cdot 0} - \frac{1}{4(\lambda+\mathrm{i}k)^2}\mathrm{e}^{-2(\lambda+\mathrm{i}k)\cdot 0} - \frac{1}{4(\lambda-\mathrm{i}k)^2}\mathrm{e}^{-2(\lambda-\mathrm{i}k)\cdot 0}\right)\right] \\
&= \frac{A^2}{4}\left(\frac{1}{2\lambda^2} - \frac{1}{4(\lambda+\mathrm{i}k)^2} - \frac{1}{4(\lambda-\mathrm{i}k)^2}\right).
\end{aligned}$$

Let's further simplify this result with some algebra to get a slightly more elegant expression, first by multiplying numerators and the denominators of the second and the third terms of the expression by their respective complex conjugates to get rid of the imaginary units:

$$\begin{aligned}
\langle\psi|\hat{x}|\psi\rangle &= \frac{A^2}{4}\left(\frac{1}{2\lambda^2} - \frac{(\lambda-\mathrm{i}k)^2}{4(\lambda^2+k^2)^2} - \frac{(\lambda+\mathrm{i}k)^2}{4(\lambda^2+k^2)^2}\right) \\
&= \frac{A^2}{4}\left(\frac{1}{2\lambda^2} - \frac{\lambda^2-k^2-2\mathrm{i}\lambda k}{4(\lambda^2+k^2)^2} - \frac{\lambda^2-k^2+2\mathrm{i}\lambda k}{4(\lambda^2+k^2)^2}\right) \\
&= \frac{A^2}{4}\left(\frac{1}{2\lambda^2} - \frac{\lambda^2-k^2}{2(\lambda^2+k^2)^2}\right) = \frac{A^2}{4}\left(\frac{(\lambda^2+k^2)^2}{2\lambda^2(\lambda^2+k^2)^2} - \frac{\lambda^2(\lambda^2-k^2)}{2\lambda^2(\lambda^2+k^2)^2}\right) \\
&= \frac{A^2}{4}\left(\frac{\lambda^4+2\lambda^2k^2+k^4-\lambda^4+\lambda^2k^2}{2\lambda^2(\lambda^2+k^2)^2}\right) = \frac{A^2}{8}\left(\frac{3\lambda^2k^2+k^4}{\lambda^2(\lambda^2+k^2)^2}\right) \\
&= \frac{A^2}{8}\cdot\frac{k^2(3\lambda^2+k^2)}{\lambda^2(\lambda^2+k^2)^2}.
\end{aligned}$$

At last, let's substitute the expression for A we have obtained in part (a) to get the final result:

$$\begin{aligned}
\langle\psi|\hat{x}|\psi\rangle &= \frac{1}{8}\cdot\left(2\sqrt{\frac{\lambda(\lambda^2+k^2)}{k^2}}\right)^2\cdot\frac{k^2(3\lambda^2+k^2)}{\lambda^2(\lambda^2+k^2)^2} \\
&= \frac{4}{8}\cdot\frac{\lambda(\lambda^2+k^2)}{k^2}\cdot\frac{k^2(3\lambda^2+k^2)}{\lambda^2(\lambda^2+k^2)^2} = \frac{3\lambda^2+k^2}{2\lambda(\lambda^2+k^2)}.
\end{aligned}$$

We can see that the expectation value is real and strictly positive, which makes sense since our wave function is non-zero only on the interval $x \in (0,\infty)$, and furthermore it has the dimension of length, as is to be expected.

Now we proceed to compute the expectation value of $\hat{p}$ in a similar manner. First, let's calculate the derivative of $\psi(x)$:

$$\begin{aligned}
\psi'(x) &= \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{A}{2\mathrm{i}}\left(\mathrm{e}^{(-\lambda+2\mathrm{i}k)x} - \mathrm{e}^{-\lambda x}\right)\right) = \frac{A}{2\mathrm{i}}\left((-\lambda+2\mathrm{i}k)\mathrm{e}^{(-\lambda+2\mathrm{i}k)x} - (-\lambda)\mathrm{e}^{-\lambda x}\right) \\
&= \frac{A}{2\mathrm{i}}\left((-\lambda+2\mathrm{i}k)\mathrm{e}^{(-\lambda+2\mathrm{i}k)x} + \lambda\mathrm{e}^{-\lambda x}\right).
\end{aligned}$$

With this in mind, let's find $\langle\psi|\hat{p}|\psi\rangle$:

$$\begin{aligned}
\langle\psi|\hat{p}|\psi\rangle &= -\mathrm{i}\hbar\int_{-\infty}^{\infty}\psi^*(x)\psi'(x)\mathrm{d}x \\
&= -\mathrm{i}\hbar\int_0^{\infty} -\frac{A}{2\mathrm{i}}\left(\mathrm{e}^{(-\lambda-2\mathrm{i}k)x} - \mathrm{e}^{-\lambda x}\right)\frac{A}{2\mathrm{i}}\left((-\lambda+2\mathrm{i}k)\mathrm{e}^{(-\lambda+2\mathrm{i}k)x} + \lambda\mathrm{e}^{-\lambda x}\right)\mathrm{d}x \\
&= -\frac{\mathrm{i}\hbar A^2}{4}\int_0^{\infty}\left(\mathrm{e}^{(-\lambda-2\mathrm{i}k)x} - \mathrm{e}^{-\lambda x}\right)\left((-\lambda+2\mathrm{i}k)\mathrm{e}^{(-\lambda+2\mathrm{i}k)x} + \lambda\mathrm{e}^{-\lambda x}\right)\mathrm{d}x \\
&= -\frac{\mathrm{i}\hbar A^2}{4}\int_0^{\infty}\left((-\lambda+2\mathrm{i}k)\mathrm{e}^{-2\lambda x} + \lambda\mathrm{e}^{-2(\lambda+\mathrm{i}k)x} - (-\lambda+2\mathrm{i}k)\mathrm{e}^{-2(\lambda-\mathrm{i}k)x} - \lambda\mathrm{e}^{-2\lambda x}\right)\mathrm{d}x \\
&= -\frac{\mathrm{i}\hbar A^2}{4}\left(\frac{\lambda-2\mathrm{i}k}{2\lambda}\mathrm{e}^{-2\lambda x} - \frac{\lambda}{2(\lambda+\mathrm{i}k)}\mathrm{e}^{-2(\lambda+\mathrm{i}k)x} - \frac{\lambda-2\mathrm{i}k}{2(\lambda-\mathrm{i}k)}\mathrm{e}^{-2(\lambda-2\mathrm{i}k)x} + \frac{1}{2}\mathrm{e}^{-2\lambda x}\right)\Bigg|_{x=0}^{\infty} \\
&= -\frac{\mathrm{i}\hbar A^2}{4}\left(\frac{\lambda-2\mathrm{i}k}{2\lambda} - \frac{\lambda}{2(\lambda+\mathrm{i}k)}\mathrm{e}^{-2\mathrm{i}kx} - \frac{\lambda-2\mathrm{i}k}{2(\lambda-\mathrm{i}k)}\mathrm{e}^{2\mathrm{i}kx} + \frac{1}{2}\right)\mathrm{e}^{-2\lambda x}\Bigg|_{x=0}^{\infty}
\end{aligned}$$

Evaluating the limits similarly to before with the previously mentioned tricks, we arrive at the following:

$$
\begin{aligned}
\langle\psi|\hat{p}|\psi\rangle &= \lim_{x\to\infty} -\frac{\mathrm{i}\hbar A^2}{4}\left(\frac{\lambda-2\mathrm{i}k}{2\lambda} - \frac{\lambda}{2(\lambda+\mathrm{i}k)}\mathrm{e}^{-2\mathrm{i}kx} - \frac{\lambda-2\mathrm{i}k}{2(\lambda-\mathrm{i}k)}\mathrm{e}^{2\mathrm{i}kx} + \frac{1}{2}\right)\mathrm{e}^{-2\lambda x} \\
&\quad - \lim_{x\to 0} -\frac{\mathrm{i}\hbar A^2}{4}\left(\frac{\lambda-2\mathrm{i}k}{2\lambda} - \frac{\lambda}{2(\lambda+\mathrm{i}k)}\mathrm{e}^{-2\mathrm{i}kx} - \frac{\lambda-2\mathrm{i}k}{2(\lambda-\mathrm{i}k)}\mathrm{e}^{2\mathrm{i}kx} + \frac{1}{2}\right)\mathrm{e}^{-2\lambda x} \\
&= 0 - \left[-\frac{\mathrm{i}\hbar A^2}{4}\left(\frac{\lambda-2\mathrm{i}k}{2\lambda} - \frac{\lambda}{2(\lambda+\mathrm{i}k)}\mathrm{e}^{-2\mathrm{i}k\cdot 0} - \frac{\lambda-2\mathrm{i}k}{2(\lambda-\mathrm{i}k)}\mathrm{e}^{2\mathrm{i}k\cdot 0} + \frac{1}{2}\right)\mathrm{e}^{-2\lambda\cdot 0}\right] \\
&= \frac{\mathrm{i}\hbar A^2}{4}\left(\frac{\lambda-2\mathrm{i}k}{2\lambda} - \frac{\lambda}{2(\lambda+\mathrm{i}k)} - \frac{\lambda-2\mathrm{i}k}{2(\lambda-\mathrm{i}k)} + \frac{1}{2}\right) \\
&= \frac{\mathrm{i}\hbar A^2}{4}\left(1 - \frac{2\mathrm{i}k}{2\lambda} - \frac{\lambda}{2(\lambda+\mathrm{i}k)} - \frac{\lambda-2\mathrm{i}k}{2(\lambda-\mathrm{i}k)}\right)
\end{aligned}
$$

Now we simplify this expression by bringing all the terms under a common denominator:

$$
\begin{aligned}
\langle\psi|\hat{p}|\psi\rangle &= \frac{\mathrm{i}\hbar A^2}{4}\left(\frac{2\lambda(\lambda^2+k^2)}{2\lambda(\lambda^2+k^2)} - \frac{2\mathrm{i}k(\lambda^2+k^2)}{2\lambda(\lambda^2+k^2)} - \frac{\lambda^2(\lambda-\mathrm{i}k)}{2\lambda(\lambda^2+k^2)} - \frac{\lambda(\lambda-2\mathrm{i}k)(\lambda+\mathrm{i}k)}{2\lambda(\lambda^2+k^2)}\right) \\
&= \frac{\mathrm{i}\hbar A^2}{4}\cdot\frac{2\lambda^3+2\lambda k^2-2\mathrm{i}\lambda^2 k-2\mathrm{i}k^3-\lambda^3+\mathrm{i}\lambda^2 k-\lambda^3-\mathrm{i}\lambda^2 k+2\mathrm{i}\lambda^2 k-2\lambda k^2}{2\lambda(\lambda^2+k^2)} \\
&= \frac{\mathrm{i}\hbar A^2}{4}\cdot\frac{-2\mathrm{i}k^3}{2\lambda(\lambda^2+k^2)} = \frac{\hbar A^2}{4}\cdot\frac{k^3}{\lambda(\lambda^2+k^2)}.
\end{aligned}
$$

After a long battle, let's put the final nail in the coffin of this problem by substituting our expression for A:

$$
\begin{aligned}
\langle\psi|\hat{p}|\psi\rangle &= \frac{\hbar}{4}\cdot\left(2\sqrt{\frac{\lambda(\lambda^2+k^2)}{k^2}}\right)^2\cdot\frac{k^3}{\lambda(\lambda^2+k^2)} \\
&= \frac{\hbar}{4}\cdot\frac{4\lambda(\lambda^2+k^2)}{k^2}\cdot\frac{k^3}{\lambda(\lambda^2+k^2)} = \hbar k,
\end{aligned}
$$

a surprisingly simple answer! Once again, we see that the result is real-valued, as is to be expected from an expectation value of an observable. Let's also check the dimensionality as well to be certain. The dimension of momentum is $\frac{\text{mass}\cdot\text{length}}{\text{time}}$ (recall that it is classically defined as mass times velocity of a point particle), and since the dimension of the reduced Planck's constant $\hbar$ is $\frac{\text{mass}\cdot\text{length}^2}{\text{time}}$, while the dimension of k is $\frac{1}{\text{length}}$, the dimensions on both sides of the equation match. Phew!

2. Consider a particle of mass m in a one-dimensional potential

$$V(\hat{x}) = \frac{1}{2}m\omega^2\hat{x}^2 - \lambda\hat{x}$$

   (a) Given the corresponding Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$, find the ladder operators $\hat{b}$ and $\hat{b}^\dagger$ that allow an algebraic representation of the eigenstates.

Hint: Make a change of variables in $\hat{x}$ to simplify the Hamiltonian, and recall how $\hat{a}$ and $\hat{a}^\dagger$ are defined in terms of $\hat{x}$ and $\hat{p}$ for the harmonic oscillator. You should end up with a Hamiltonian of the form $\hat{A}^\dagger\hat{A} + C\hat{I}$, where $\hat{A} \in \mathcal{L}(\mathcal{H})$ and $C \in \mathbb{R}$.

(b) Find the eigenenergies of $\hat{H}$.

Solution:

(a) We can simplify $\hat{H}$ by completing the square for V:

$$\begin{aligned} V(\hat{x}) &= \frac{1}{2}m\omega^2\left(\hat{x}^2 - \frac{2\lambda\hat{x}}{m\omega^2}\right) \\ &= \frac{1}{2}m\omega^2\left(\hat{x}^2 - \frac{2\lambda\hat{x}}{m\omega^2} + \frac{\lambda^2}{m^2\omega^4}\right) - \frac{\lambda^2}{2m\omega^2} \\ &= \frac{1}{2}m\omega^2\left(\hat{x} - \frac{\lambda}{m\omega^2}\right)^2 - \frac{\lambda^2}{2m\omega^2}. \end{aligned}$$

Then, we define $\hat{x}' = \hat{x} - \frac{\lambda}{m\omega^2}$, so that

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}'^2 - \frac{\lambda^2}{2m\omega^2}\hat{I}$$

Defining the operators $\hat{b} = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x}' + \frac{i}{m\omega}\hat{p})$ and $\hat{b}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}(\hat{x}' - \frac{i}{m\omega}\hat{p})$, obtain

$$\hat{H} = \hbar\omega\left(\hat{b}^\dagger\hat{b} + \frac{1}{2}\right) - \frac{\lambda^2}{2m\omega^2}\hat{I}.$$

Annex

The algebraic trick for finding the eigenstates of the harmonic oscillator is based on the property $[\hat{a}, \hat{a}^\dagger] = 1$. Therefore, it is crucial to define your coordinates $\hat{x}$ and $\hat{p}$ so that they're canonical conjugates, that is $[\hat{x}, \hat{p}] = i\hbar$. For instance, defining $\hat{x}' = \hat{x}^2 - \frac{2\lambda}{m\omega^2}\hat{x}$ would give you the nice looking Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}'^2.$$

However, now $[\hat{x}', \hat{p}] = [\hat{x}^2 - \frac{2\lambda}{m\omega^2}\hat{x}, \hat{p}] = [\hat{x}^2, \hat{p}] - \frac{2\lambda}{m\omega^2}[\hat{x}, \hat{p}] = 2i\hbar\hat{x} - \frac{2\lambda}{m\omega^2}i\hbar$. Note that if we just add a constant to $\hat{x}$ like we've done in the solution, $\hat{x}' = \hat{x} + C$, the commutator doesn't change: $[\hat{x} + C, \hat{p}] = [\hat{x}, \hat{p}] + [C, \hat{p}] = i\hbar + 0$. There are other ways of defining the new variable, but in these cases you need to be more careful in defining the ladder operators and computing the eigenenergies. For instance, one could define $\hat{x}' = \alpha\hat{x} + \beta$, where α and β are constants. We'll then have $[\hat{x}', \hat{p}] = \alpha[\hat{x}, \hat{p}] = \alpha i\hbar$, which is not impossible to work with and still permits an expression in terms of ladder operators. However, one now needs to put some thought into defining $\hat{a}$ and $\hat{a}^\dagger$, and compute the commutator $[\hat{a}, \hat{a}^\dagger]$ which is no longer necessarily one, but some other constant, to make sure everything works out correctly.

(b) Using the above result,

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) - \frac{\lambda^2}{2m\omega^2}$$

where $n = 0, 1, 2, 3 \ldots$. The ground state energy is $E_0 = \frac{\hbar\omega}{2} - \frac{\lambda^2}{2m\omega^2}$.

3. Consider the time-independent Schrödinger's equation in position representation for a free particle ($V(x) = 0$):

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)$$

(a) Find a general solution for $\psi(x)$.

(b) Show that

$$\psi(x,t) = Ae^{ik(x-\frac{\hbar k}{2m}t)} + Be^{-ik(x+\frac{\hbar k}{2m}t)},$$

where A, B are constants and $k = \sqrt{2mE}/\hbar$.

(c) The first term in $\psi(x,t)$ represents a wave traveling to the right, and the second term represents a wave (of the same energy) going to the left. Since they only differ by the sign in front of k, we can write the wave function as

$$\psi_k(x,t) = Ae^{i(kx-\frac{\hbar k^2}{2m}t)},$$

where k can also be negative to cover the case of the wave travelling to the left. Find the velocity of this wave and compare it with the velocity of a classical free particle with energy E. Hint: compare $\psi_k(x,t)$ to the general plane wave solution $e^{ik(x-vt)}$.

Solution:

(a) The Schrödinger equation is

$$\frac{d^2\psi(x)}{dx^2} = -k^2\psi(x)$$

where $k = \sqrt{2mE}/\hbar$. The general solution to this differential equation is

$$\psi(x) = Ae^{\mathrm{i}kx} + Be^{-\mathrm{i}kx}.$$

(b) Note that the energy is $E = \hbar^2k^2/2m$. Recall that for an eigenstate, the time-dependent Schrödinger equation gives

$$-i\hbar\frac{d}{dt}\left|\psi(t)\right\rangle = \hat{H}\left|\psi(t)\right\rangle = E\left|\psi(t)\right\rangle.$$

With this, we have

$$\begin{aligned}
\left|\psi(t)\right\rangle &= e^{-iEt/\hbar}\left|\psi(0)\right\rangle \\
\Rightarrow \psi(x,t) = \langle x|\psi(t)\rangle &= e^{-iEt/\hbar}\langle x|\psi(0)\rangle = e^{-iEt/\hbar}\psi(x) \\
&= Ae^{\mathrm{i}k(x-\frac{\hbar k}{2m}t)} + Be^{-\mathrm{i}k(x+\frac{\hbar k}{2m}t)}.
\end{aligned}$$

(c) Comparing ψ_k to the general plane wave solution $Ae^{ik(x-vt)}$, we find

$$v_{\text{quantum}} = \frac{\hbar k}{2m} = \sqrt{\frac{E}{2m}}.$$

Classical energy of a free particle is $E = \frac{1}{2}mv^2$, so that

$$v_{\text{classical}} = \sqrt{\frac{2E}{m}} = 2v_{\text{quantum}}.$$

4. Consider a one-dimensional free particle in the following state at the time $t = 0$:

$$\psi(x, t = 0) = \frac{\sqrt{a}}{(2\pi)^{3/4}\hbar}\int_{-\infty}^{\infty} \mathrm{e}^{-a^2p^2/(2\hbar)^2}\mathrm{e}^{\mathrm{i}px/\hbar}\mathrm{d}p,$$

with $0 < a \in \mathbb{R}$. This is a Gaussian superposition of plane waves (also called a wave packet). Note that, unlike in the case of simple plane waves, this wave function is normalizable to unity, and hence can be interpreted as probability density for the particle.

(a) (4p) Show that the time evolution of the probability density is given by

$$|\psi(x,t)|^2 = \sqrt{\frac{2}{\pi a^2}}\frac{1}{\sqrt{1+4\hbar^2t^2/(m^2a^4)}} \cdot \exp\left(-\frac{2a^2x^2}{a^4+4\hbar^2t^2/m^2}\right).$$

Hint: the energy of a plane wave is given by $E = p^2/(2m)$. Also, for any complex numbers α and β such that $\mathrm{Re}(\alpha) > 0$,

$$\int_{-\infty}^{\infty} \mathrm{e}^{-\alpha(y+\beta)^2}\mathrm{d}y = \sqrt{\frac{\pi}{\alpha}},$$

and $(f(\beta))^* = f^*(\beta) = f(\beta^*)$ when $f : \mathbb{C} \to \mathbb{C}$ is an elementary function, such as $f(z) = 1/z$ or $f(z) = \exp(z)$.

(b) (2p) Sketch qualitatively the probability density $|\psi(x,t)|^2$ for some times $t = t_1$ and $t = t_2 > t_1$. What happens to the wave function over time?

Solution:

(a) As stated in the lecture notes, for a plane wave with momentum p,

$$\phi(x, t = 0) = \sqrt{\frac{1}{2\pi\hbar}}\mathrm{e}^{\mathrm{i}px/\hbar},$$

the time evolution is given by

$$\phi(x,t) = \phi(x, t=0)\cdot \mathrm{e}^{-\mathrm{i}Et/\hbar} = \sqrt{\frac{1}{2\pi\hbar}}\mathrm{e}^{-\mathrm{i}Et/\hbar}\mathrm{e}^{\mathrm{i}px/\hbar} = \sqrt{\frac{1}{2\pi\hbar}}\mathrm{e}^{-\mathrm{i}p^2t/(2m\hbar)}\mathrm{e}^{\mathrm{i}px/\hbar},$$

where we have used $E = p^2/2m$. The given wave function is a superposition of such plane waves, so it's time-evolution is given by

$$\begin{aligned}\psi(x,t) &= \frac{\sqrt{a}}{(2\pi)^{3/4}\hbar}\int_{-\infty}^{\infty} \mathrm{e}^{-a^2p^2/(2\hbar)^2}\mathrm{e}^{-\mathrm{i}p^2t/(2m\hbar)}\mathrm{e}^{\mathrm{i}px/\hbar}\mathrm{d}p \\ &= \frac{\sqrt{a}}{(2\pi)^{3/4}\hbar}\int_{-\infty}^{\infty} \exp\left(-\frac{a^2p^2}{(2\hbar)^2} - \frac{\mathrm{i}p^2t}{2m\hbar} + \frac{\mathrm{i}px}{\hbar}\right)\mathrm{d}p.\end{aligned}$$

Let us rearrange the terms in the exponential:

$$-\frac{a^2p^2}{(2\hbar)^2}-\frac{\mathrm{i}p^2t}{2m\hbar}+\frac{\mathrm{i}px}{\hbar}=-\left(\frac{\mathrm{i}t}{2m\hbar}+\frac{a^2}{2\hbar^2}\right)p^2+\frac{\mathrm{i}x}{\hbar}p.$$

Completing the square, this is

$$-\underbrace{\left(\frac{\mathrm{i}t}{2m\hbar}+\frac{a^2}{(2\hbar)^2}\right)}_{=\alpha}\left(p-\underbrace{\frac{\mathrm{i}x}{2\hbar\left(\frac{\mathrm{i}t}{2m\hbar}+\frac{a^2}{(2\hbar)^2}\right)}}_{=\beta}\right)^2+\underbrace{\frac{\left(\frac{\mathrm{i}x}{\hbar}\right)^2}{4\left(\frac{\mathrm{i}t}{2m\hbar}+\frac{a^2}{(2\hbar)^2}\right)}}_{\text{doesn't depend on } p}.$$

Using the given Gaussian integral identity, we find

$$\begin{aligned}\psi(x,t)&=\frac{\sqrt{a}}{(2\pi)^{3/4}\hbar}\sqrt{\frac{\pi}{\frac{\mathrm{i}t}{2m\hbar}+\frac{a^2}{(2\hbar)^2}}}\cdot\exp\left(\frac{\left(\frac{\mathrm{i}x}{\hbar}\right)^2}{4\left(\frac{\mathrm{i}t}{2m\hbar}+\frac{a^2}{(2\hbar)^2}\right)}\right)\\&=\frac{\sqrt{a}}{(2\pi)^{3/4}\hbar}\sqrt{\frac{\pi}{\frac{a^2}{(2\hbar)^2}+\frac{\mathrm{i}t}{2m\hbar}}}\cdot\exp\left(\frac{-x^2}{a^2+\frac{2\mathrm{i}\hbar t}{m}}\right)\end{aligned}$$

We obtain the complex conjugate of this by changing all i's to −i:

$$\psi^*(x,t)=\frac{\sqrt{a}}{(2\pi)^{3/4}\hbar}\sqrt{\frac{\pi}{\frac{a^2}{(2\hbar)^2}-\frac{\mathrm{i}t}{2m\hbar}}}\cdot\exp\left(\frac{-x^2}{a^2-\frac{2\mathrm{i}\hbar t}{m}}\right),$$

so that

$$\begin{aligned}|\psi(x,t)|^2=\psi^*(x,t)\psi(x,t)&=\frac{a}{(2\pi)^{3/2}\hbar^2}\frac{\pi}{\sqrt{\left(\frac{a^2}{(2\hbar)^2}-\frac{\mathrm{i}t}{2m\hbar}\right)\left(\frac{a^2}{(2\hbar)^2}+\frac{\mathrm{i}t}{2m\hbar}\right)}}\\&\qquad\times\exp\left(-x^2\left(\frac{1}{a^2-\frac{2\mathrm{i}\hbar t}{m}}+\frac{1}{a^2+\frac{2\mathrm{i}\hbar t}{m}}\right)\right)\\&=\frac{a\pi}{(2\pi)^{3/2}\hbar^2\sqrt{\frac{a^4}{(2\hbar)^4}+\frac{t^2}{(2\hbar)^2m^2}}}\exp\left(-x^2\left(\frac{a^2+\frac{2\mathrm{i}\hbar t}{m}+a^2-\frac{2\mathrm{i}\hbar t}{m}}{a^4+\frac{(2\hbar)^2t^2}{m^2}}\right)\right)\\&=\frac{a\pi}{(2\pi)^{3/2}\hbar^2\frac{a^2}{(2\hbar)^2}\sqrt{1+\frac{(2\hbar)^2t^2}{m^2a^4}}}\exp\left(\frac{-2x^2a^2}{a^4+4\hbar^2t^2/m^2}\right)\\&=\frac{4\pi}{(2\pi)^{3/2}a\sqrt{1+\frac{(2\hbar)^2t^2}{m^2a^4}}}\exp\left(\frac{-2x^2a^2}{a^4+4\hbar^2t^2/m^2}\right)\\&=\sqrt{\frac{2^4\pi^2}{(2\pi)^3a^2}}\frac{1}{\sqrt{1+\frac{(2\hbar)^2t^2}{m^2a^4}}}\exp\left(\frac{-2x^2a^2}{a^4+4\hbar^2t^2/m^2}\right)\\&=\sqrt{\frac{2}{\pi a^2}}\frac{1}{\sqrt{1+\frac{4\hbar^2t^2}{m^2a^4}}}\exp\left(\frac{-2x^2a^2}{a^4+4\hbar^2t^2/m^2}\right).\end{aligned}$$

(b) With a fixed value of t, the probability density $|\psi(x,t)|^2$ is a Gaussian function, i.e., of the form $A\mathrm{e}^{-x^2/(2\sigma^2)}$. When t increases, the prefactor A becomes smaller and the standard deviation $\sigma = \sqrt{(a^2 + 4\hbar^2 t^2/(a^2 m^2))/2}$ becomes larger. In other words, the wave packet spreads, or widens, and simultaneously the amplitude decreases to keep the total area under it equal to 1. This is illustrated below for $t_1 = ma^2/2\hbar$ and $t_2 = 2ma^2/2\hbar$, with $a = 1$: