With problems from "Modern Quantum Mechanics Third Edition" (J.J. Sakurai & Jim Napolitano)

One-Dimensional Free Particle

Consider a 1D free particle in a wavefunction of

$$\psi(x) \propto e^{-\frac{(x-x_0)^2}{d^2}}$$

where x_0 and d are both certain constants with the unit of length. Verify the uncertainty principle by evaluating $\sigma_x\sigma_y$ for this wavefunction. Firstly, you need to explicitly show how to do the integration of

$$\int_{-\infty}^{\infty} dx x^2 e^{-ax^2} = \frac{\sqrt{\pi}}{2a^{3/2}}$$

and then you can use this result to do the remaining calculations.

The given integral can be integrated by parts by writing it as

$$\int_{-\infty}^{\infty} dx x \cdot x e^{-ax^2} = I$$

Using the tabular method for integration by parts yields:

$$I = x \cdot \frac{-1}{2a} e^{-ax^2}\bigg|_{-\infty}^{\infty} - 1 \cdot \frac{-1}{2a} \int_{-\infty}^{\infty} dx e^{-ax^2}$$

The Gaussian integral evaluates to $\sqrt{\pi/a}$:

$$I = \frac{\sqrt{\pi}}{2\sqrt{a^3}}$$

To normalize the wavefunction, we perform the usual calculation:

$$A^2 \int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = 1$$

$$A^2 \int_{-\infty}^{\infty} e^{-\frac{2(x-x_0)^2}{d^2}} dx = 1$$

This is a Gaussian integral with the solution $d\sqrt{\pi/2}$ for $a = 2/d^2$. So A is then:

$$A^2 = \frac{1}{d}\sqrt{\frac{2}{\pi}}$$

And the normalized wavefunction is:

$$\psi(x) = \left(\frac{2}{d^2\pi}\right)^{1/4} e^{-\frac{(x-x_0)^2}{d^2}}$$

The variance σ_x is given by:

$$\sigma_x = \langle x^2 \rangle - \langle x \rangle^2$$

$$\langle x \rangle = \sqrt{\frac{2}{d^2\pi}} \int_{-\infty}^{\infty} e^{-\frac{(x-x_0)^2}{d^2}} x e^{-\frac{(x-x_0)^2}{d^2}} dx$$

$$\langle x\rangle = \sqrt{\frac{2}{d^2\pi}}\int_{-\infty}^{\infty} x e^{-\frac{2(x-x_0)^2}{d^2}}dx$$

This modified Gaussian integral evaluates to $x_0 d\sqrt{\pi/2}$:

$$\langle x\rangle = \sqrt{\frac{2}{d^2\pi}}\left(\frac{x_0 d\sqrt{\pi}}{\sqrt{2}}\right)$$

$$\langle x\rangle = \sqrt{\frac{2}{d^2\pi}}\left(\frac{x_0 d\sqrt{\pi}}{\sqrt{2}}\right) = x_0$$

$$\langle x^2\rangle = \sqrt{\frac{2}{d^2\pi}}\int_{-\infty}^{\infty} e^{-\frac{(x-x_0)^2}{d^2}} x^2 e^{-\frac{(x-x_0)^2}{d^2}}dx$$

$$\langle x^2\rangle = \sqrt{\frac{2}{d^2\pi}}\int_{-\infty}^{\infty} x^2 e^{-2\frac{(x-x_0)^2}{d^2}}dx$$

$$\langle x^2\rangle = \sqrt{\frac{2}{d^2\pi}}\left(\frac{\sqrt{\pi}(2/d^2)x_0^2+\sqrt{\pi}}{2\sqrt{8/d^6}}\right)$$

$$\langle x^2\rangle = \sqrt{\frac{2}{d^2}}\left(\frac{x_0^2 d}{\sqrt{8}}\right)$$

$$\langle x^2\rangle = \frac{x_0^2}{2}$$

The variance σ_p is given by:

$$\sigma_p = \langle p^2\rangle - \langle p\rangle^2$$

$$\langle p\rangle = (-i\hbar)\sqrt{\frac{2}{d^2\pi}}\int_{-\infty}^{\infty} e^{-\frac{(x-x_0)^2}{d^2}}\frac{d}{dx}e^{-\frac{(x-x_0)^2}{d^2}}dx$$

$$\langle p\rangle = (-i\hbar)\sqrt{\frac{2}{d^2\pi}}\int_{-\infty}^{\infty} e^{-\frac{(x-x_0)^2}{d^2}}\left(-\frac{2}{d^2}(x-x_0)\right)e^{-\frac{(x-x_0)^2}{d^2}}dx$$

$$\langle p\rangle = i\hbar\frac{2}{d^2}\sqrt{\frac{2}{d^2\pi}}\int_{-\infty}^{\infty}(x-x_0)e^{-2\frac{(x-x_0)^2}{d^2}}dx = 0$$

This is an integral of an odd function over a symmetric interval, so it evaluates to zero.

$$\langle p^2\rangle = -\hbar^2\sqrt{\frac{2}{d^2\pi}}\int_{-\infty}^{\infty} e^{-\frac{(x-x_0)^2}{d^2}}\frac{d^2}{dx^2}e^{-\frac{(x-x_0)^2}{d^2}}dx$$

$$\langle p^2\rangle = \frac{2\hbar^2}{d^2}\sqrt{\frac{2}{d^2\pi}}\int_{-\infty}^{\infty} e^{-\frac{(x-x_0)^2}{d^2}}\frac{d}{dx}\left((x-x_0)e^{-\frac{(x-x_0)^2}{d^2}}\right)dx$$

The product rule introduces a second term:

$$\langle p^2\rangle = \frac{2\hbar^2}{d^2}\sqrt{\frac{2}{d^2\pi}}\left[\int_{-\infty}^{\infty} e^{-2\frac{(x-x_0)^2}{d^2}}dx - \frac{2}{d^2}\int_{-\infty}^{\infty}(x-x_0)^2 e^{-\frac{2(x-x_0)^2}{d^2}}dx\right]$$

The first integral evaluates to $d\sqrt{\pi/2}$, and we can use the integral we first evaluated I for the second one:

$$\langle p^2\rangle = \frac{2\hbar^2}{d^2}\sqrt{\frac{2}{d^2\pi}}\left[\frac{d\sqrt{\pi}}{\sqrt{2}} - \frac{2}{d^2}\frac{d^3\sqrt{\pi}}{2\sqrt{8}}\right]$$

$$\langle p^2 \rangle = \frac{2\hbar^2}{d^2}\sqrt{\frac{2}{d^2\pi}}\left[\frac{d\sqrt{\pi}}{\sqrt{2}} - \frac{d\sqrt{\pi}}{\sqrt{8}}\right]$$

$$\langle p^2 \rangle = \frac{2\hbar^2}{d^2}\sqrt{\frac{2}{\pi}}\left[1 - \frac{1}{2}\right]$$

$$\langle p^2 \rangle = \frac{\hbar^2}{d^2}\sqrt{\frac{2}{\pi}}$$

The uncertainty principle is given by:

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}$$

$$\left(\frac{x_0^2}{2} - x_0\right)\left(\sqrt{\frac{2}{\pi}}\frac{\hbar^2}{d^2} - 0\right) \geq \frac{\hbar}{2}$$

$$\sqrt{\frac{2}{\pi}}\frac{\hbar^2 x_0^2}{2d^2} - \sqrt{\frac{2}{\pi}}\frac{\hbar^2 x_0}{d^2} \geq \frac{\hbar}{2}$$

Problem 2.1

Consider the spin-precession problem discussed in the text. It can also be solved in the Heisenberg picture. Using the Hamiltonian

$$H = -\left(\frac{eB}{mc}\right) S_z = \omega S_z$$

write the Heisenberg equations of motion for the time-dependent operators $S_x(t)$, $S_y(t)$ and $S_z(t)$. Solve them to obtain $S_{x,y,z}$ as functions of time.

Equation 2.93 gives the Heisenberg equation of motion for an observable O as:

$$\frac{dO}{dt} = \frac{1}{i\hbar}[O, H]$$

For S_x:

$$\frac{dS_x}{dt} = \frac{\omega}{i\hbar}[S_x, S_z] = -\frac{\omega}{i\hbar}(i\hbar S_y)$$

$$\boxed{\frac{dS_x}{dt} = -\omega S_y}$$

For S_y:

$$\frac{dS_y}{dt} = \frac{\omega}{i\hbar}[S_y, S_z] = \frac{\omega}{i\hbar}(i\hbar S_x)$$

$$\boxed{\frac{dS_y}{dt} = \omega S_x}$$

And since S_z commutes with itself (the Hamiltonian):

$$\boxed{\frac{dS_z}{dt} = 0}$$

Differentiating again to obtain second-order differential equations:

$$\frac{d^2S_x}{dt^2} = -\omega\left(\frac{dS_y}{dt}\right) \qquad \frac{d^2S_y}{dt^2} = \omega\left(\frac{dS_x}{dt}\right)$$

$$\frac{d^2S_x}{dt^2} = -\omega\left(\omega S_x\right) \qquad \frac{d^2S_y}{dt^2} = \omega\left(-\omega S_y\right)$$

$$\frac{d^2S_x}{dt^2} = -\omega^2 S_x \qquad \frac{d^2S_y}{dt^2} = -\omega^2 S_y$$

These equations have solutions of the form:

$$\boxed{S_x(t) = Ae^{-i\omega t}} \qquad \boxed{S_y(t) = Be^{-i\omega t}}$$

where A and B are constants to be determined by initial conditions.

Since the first derivative of $S_z(t)$ was zero, it is a constant function:

$$\boxed{S_z(t) = C}$$

Problem 2.5

Let $x(t)$ be the coordinate operator for a free particle in one dimension in the Heisenberg picture. Evaluate

$$[x(t), x(0)]$$

The Hamiltonian for the free particle is:

$$H = \frac{p^2}{2m}$$

The Heisenberg equation of motion for the x operator is given by:

$$\frac{dx}{dt} = \frac{1}{i\hbar}[x, H]$$

$$\frac{dx}{dt} = \frac{1}{2i\hbar m}[x, p^2] = \frac{1}{2i\hbar m}(2i\hbar p)$$

$$\frac{dx}{dt} = \frac{p}{m}$$

$$x(t) = \frac{p}{m}t + x(0)$$

where, of course, at $t = 0$, $x(t) = x(0)$.

For the p operator:

$$\frac{dp}{dt} = \frac{1}{i\hbar}[p, H]$$

p commutes with $H \propto p^2$, so $p(t)$ is a constant in time, so $p(t) = p(0)$.

$$[x(t), x(0)] = \left(\frac{p}{m}t + x(0)\right)x(0) - x(0)\left(\frac{p}{m}t + x(0)\right)$$

$$[x(t), x(0)] = \frac{t}{m}p(0)x(0) + x(0)x(0) - \left(\frac{t}{m}x(0)p(0) + x(0)x(0)\right)$$

$$[x(t), x(0)] = \frac{t}{m}\big(p(0)x(0) - x(0)p(0)\big)$$

$$\boxed{[x(t), x(0)] = -\frac{i\hbar t}{m}}$$

Problem 2.12

A one-dimensional simple harmonic oscillator with natural frequency ω is in initial state

$$|\alpha\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{e^{i\delta}}{\sqrt{2}}|1\rangle$$

where δ is real.

a. Find the time-dependent wavefunction $\langle x'|\alpha;t\rangle$ and evaluate the time-dependent expectation values $\langle x\rangle$ and $\langle p\rangle$ in the state $|\alpha;t\rangle$, i.e. in the Schrödinger picture.

Using Equations 2.151 and Equation 2.152:

$$\langle x|0\rangle = \psi_0(x) = \frac{1}{\pi^{1/4}\sqrt{x_0}}e^{-\frac{1}{2}(\frac{x}{x_0})^2}$$

$$\langle x|1\rangle = \psi_1(x) = \left(\frac{1}{\sqrt{2}x_0}\right)\left(x - x_0^2\frac{d}{dx}\right)\left(\frac{1}{\pi^{1/4}\sqrt{x_0}}e^{-\frac{1}{2}(\frac{x}{x_0})^2}\right)$$

$$\psi_1(x) = \left(\frac{1}{\pi^{1/4}\sqrt{2x_0^3}}\right)\left(xe^{\frac{1}{2}(\frac{x}{x_0})^2} + x\left(e^{-\frac{1}{2}(\frac{x}{x_0})^2}\right)\right)$$

$$\boxed{\Psi_1(x,t) = \left(\frac{2}{\pi^{1/4}\sqrt{2x_0^3}}\right)\left(xe^{\frac{1}{2}(\frac{x}{x_0})^2}\right)e^{-i\omega t}}$$

$$\langle x\rangle = \frac{2}{x_0^3\sqrt{\pi}}\int_{-\infty}^{\infty} x^3 e^{-\left(\frac{x}{x_0}\right)^2}dx$$

$$\boxed{\langle x\rangle = 0}$$

$$\langle p\rangle = -i\hbar\frac{2}{x_0^3\sqrt{\pi}}\int_{-\infty}^{\infty} xe^{-\left(\frac{x}{x_0}\right)^2}\frac{d}{dx}\left[xe^{-\left(\frac{x}{x_0}\right)^2}\right]dx$$

$$\langle p\rangle = -i\hbar\frac{2}{x_0^3\sqrt{\pi}}\int_{-\infty}^{\infty} xe^{-\frac{1}{2}\left(\frac{x}{x_0}\right)^2}\left[e^{-\frac{1}{2}\left(\frac{x}{x_0}\right)^2} - \left(\frac{x}{x_0}\right)e^{-\frac{1}{2}\left(\frac{x}{x_0}\right)^2}\right]dx$$

$$\langle p\rangle = -i\hbar\frac{2}{x_0^3\sqrt{\pi}}\int_{-\infty}^{\infty}\left[xe^{-\left(\frac{x}{x_0}\right)^2} - \left(\frac{x^2}{x_0}\right)e^{-\left(\frac{x}{x_0}\right)^2}\right]dx$$

$$\langle p\rangle = -i\hbar\frac{2}{x_0^3\sqrt{\pi}}\left(\frac{\sqrt{\pi}x_0^2}{2}\right)$$

$$\boxed{\langle p\rangle = -\frac{i\hbar}{x_0}}$$

b. Now calculate $\langle x\rangle$ and $\langle p\rangle$ in the Heisenberg picture and compare the results.

Problem 2.16

Consider a one-dimensional simple harmonic oscillator.

a. Using

$$\sqrt{\frac{m\omega}{2\hbar}}\left(x \pm \frac{ip}{m\omega}\right) = \begin{cases} a \\ a^\dagger \end{cases} \qquad \begin{cases} \sqrt{n}\,|n-1\rangle \\ \sqrt{n+1}\,|n+1\rangle \end{cases} = \begin{cases} a \\ a^\dagger \end{cases}$$

evaluate $\langle m|\,x\,|n\rangle$, $\langle m|\,p\,|n\rangle$, $\langle m|\,\{x,p\}\,|n\rangle$, $\langle m|\,x^2\,|n\rangle$ and $\langle m|\,p^2\,|n\rangle$.

The x and p operators can be expressed in terms of creation and annihilation operators as:

$$x\,|n\rangle = \sqrt{\frac{m\omega}{2\hbar}}(a + a^\dagger)\,|n\rangle = \sqrt{\frac{m\omega}{2\hbar}}(\sqrt{n}\,|n-1\rangle + \sqrt{n+1}\,|n+1\rangle)$$

$$p\,|n\rangle = i\sqrt{\frac{m\omega\hbar}{2}}(a^\dagger - a)\,|n\rangle = i\sqrt{\frac{m\omega\hbar}{2}}(\sqrt{n+1}\,|n+1\rangle - \sqrt{n}\,|n\rangle)$$

Hitting this with $\langle m|$ from the left:

$$\langle m|\,x\,|n\rangle = \sqrt{\frac{m\omega}{2\hbar}}(\sqrt{n}\,\langle m|n-1\rangle + \sqrt{n+1}\,\langle m|n+1\rangle)$$

$$\langle m|\,p\,|n\rangle = i\sqrt{\frac{m\omega\hbar}{2}}(\sqrt{n+1}\,\langle m|n+1\rangle - \sqrt{n}\,\langle m|n\rangle)$$

$$\boxed{\langle m|\,x\,|n\rangle = \sqrt{\frac{m\omega}{2\hbar}}(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1})}$$

$$\boxed{\langle m|\,p\,|n\rangle = i\sqrt{\frac{m\omega\hbar}{2}}(\sqrt{n+1}\delta_{m,n+1} - \sqrt{n}\delta_{m,n})}$$

$$\langle m|\,\{x,p\}\,|n\rangle = \langle m|\,(xp+px)\,|n\rangle = i\sqrt{\frac{m\omega\hbar}{2}}\,\langle m|\,x(a^\dagger - a)\,|n\rangle + \sqrt{\frac{m\omega}{2\hbar}}\,\langle m|\,p(a+a^\dagger)\,|n\rangle$$

$$\langle m|\,\{x,p\}\,|n\rangle = i\sqrt{\frac{m\omega\hbar}{2}}\left[\sqrt{n+1}\,\langle m|\,x\,|n+1\rangle - \sqrt{n}\,\langle m|\,x\,|n-1\rangle\right]$$

$$-\sqrt{\frac{m\omega}{2\hbar}}\left[\sqrt{n}\,\langle m|\,p\,|n-1\rangle + \sqrt{n+1}\,\langle m|\,p\,|n+1\rangle\right]$$

After inserting the expressions we found for $\langle m|\,x\,|n\rangle$ and $\langle m|\,p\,|n\rangle$, we obtain another expression in terms of Kronecker deltas:

$$\langle m|\,\{x,p\}\,|n\rangle = i\frac{m\omega}{2}\left[(n+1)\delta_{m,n+1} + \sqrt{(n+1)(n+2)}\delta_{m,n+2} - \sqrt{n(n-1)}\delta_{m,n-1} - n\delta_{n,m}\right]$$

$$-i\frac{m\omega}{2}\left[n\delta_{n,m} - \sqrt{n(n-1)}\delta_{m,n-1} + \sqrt{(n+1)(n+2)}\delta_{m,n+2} - (n+1)\delta_{m,n+1}\right]$$

Which simplifies to:

$$\boxed{\langle m|\,\{x,p\}\,|n\rangle = im\omega\big((n+1)\delta_{m,n+1} - n\delta_{m,n}\big)}$$

The x^2 and p^2 operators can be expanded in terms of creation and annihilation operators as well:

$$x^2\,|n\rangle = \frac{m\omega}{2\hbar}(aa + aa^\dagger + a^\dagger a + a^\dagger a^\dagger)\,|n\rangle$$

$$x^2 \left|n\right\rangle = \frac{\hbar}{2m\omega}\big(\sqrt{n(n-1}\left|n-2\right\rangle + (2n+1)\left|n\right\rangle + \sqrt{(n+1)(n+2)}\left|n+2\right\rangle\big)$$

$$\boxed{\left\langle m\right| x^2 \left|n\right\rangle = \frac{\hbar}{2m\omega}\big(\sqrt{n(n-1}\delta_{m,n-2} + (2n+1)\delta_{m,n} + \sqrt{(n+1)(n+2)}\delta_{m,n+2}\big)}$$

By the same process for p^2:

$$p^2 \left|n\right\rangle = \frac{m\omega\hbar}{2}(a^\dagger a^\dagger - a^\dagger a - aa^\dagger + aa)\left|n\right\rangle$$

$$\boxed{\left\langle m\right| p^2 \left|n\right\rangle = \frac{m\omega\hbar}{2}\big((2n+1)\delta_{m,n} + \sqrt{n(n-1)}\delta_{m,n-2} - \sqrt{(n+1)(n+2)}\delta_{m,n+2}\big)}$$

b. Translated from classical physics, the virial theorem states that

$$\left\langle \frac{p^2}{m} \right\rangle = \langle x \cdot \nabla V\rangle \text{ (3D)} \qquad \text{or} \qquad \left\langle \frac{p^2}{m} \right\rangle = \left\langle x\frac{dV}{dx} \right\rangle \text{ (1D)}$$

Check that the virial theorem holds for the expectation values of the kinetic and potential energy taken with respect to an energy eigenstate.

Using our results for $\left\langle m\right| x \left|n\right\rangle$ and $\left\langle m\right| p^2 \left|n\right\rangle$, we can check both sides:

$$\left\langle \frac{p^2}{2m} \right\rangle = \frac{1}{m}\left\langle n\right| p^2 \left|n\right\rangle$$

$$\left\langle \frac{p^2}{2m} \right\rangle = \frac{1}{m}\frac{m\omega\hbar}{2}(2n+1) = \omega\hbar(n+\frac{1}{2})$$

as expected.

For the Harmonic Oscillator, $V = \frac{1}{2}m\omega^2 x^2$, so $x\frac{dV}{dx} = m\omega^2 x^2$:

$$\left\langle x\frac{dV}{dx} \right\rangle = m\omega^2 \left\langle n\right| x^2 \left|n\right\rangle = m\omega^2 \frac{\hbar}{2m\omega}(2n+1) = \omega\hbar(n+\frac{1}{2})$$

and so the virial theorem from classical physics is satisfied by the expectation values of these quantum operators.