Physics 606

Quantum Mechanics I

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Homework #2

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1 Problem #1

(i) For an arbitrary function $F(z)$ that is expandable as a power series we can calculate the commutation relation of x_i and $G(\mathbf{p})$ where x and p are the position and momentum. We note the expansion

$$F(\mathbf{p}) = \sum_{n=0}^{\infty} a_n \mathbf{p}^n$$

which we can use to find

$$\begin{aligned}
[x_i, F(\mathbf{p})] &= \sum_{n=0}^{\infty} a_n \left[x_i, \mathbf{p}^n\right] \\
&= \sum_{n=0}^{\infty} a_n \left[x_i, p_i^n\right]
\end{aligned}$$

We note that we select the i component of the momentum vector due to the fact that the commutator is zero for all other components. Now we see that

$$\begin{aligned}
[x_i, p_i^n] &= x_i x p_i^n - p_i^n x_i \\
&= (x_i p_i) p_i^{n-1} - p_i^n x_i \\
&= \left(p_i x_i x + [x_i x, p_i]\right) p_i^{n-1} - p_i^n x_i x \\
&= p_i (x_i p_i) p_i^{n-2} + [x_i, p_i] p_i^{n-1} - p_i^n x_i \\
&= p_i (p_i x_i + [x_i, p_i]) p_i^{n-2} + [x_i, p_i] p_i^{n-1} - p_i^n x_i \\
&= p_i^2 x_i p_i^{n-2} + p_i [x_i, p_i] p_i^{n-2} + [x_i, p_i] p_i^{n-1} - p_i^n x_i \\
&= p_i^2 x_i p_i^{n-2} + 2[x_i, p_i] p_i^{n-1} - p_i^n x_i \\
&\ \ \vdots \\
&= p_i^n x_i + n[x_i, p_i] p_i^{n-1} - p_i^n x_i \\
&= n[x_i, p_i] p_i^{n-1} = -i\hbar n p_i^{n-1}
\end{aligned}$$

So our summation becomes

$$[x_i, F(\mathbf{p})] = -i\hbar \sum_{n=0}^{\infty} a_n n p_i^{n-1} = -i\hbar \frac{dF}{dp_i}$$

(ii) We repeat the process above but this time for the commutation $[p_i, G(\mathbf{x})]$ where we note that

$$[p_i, x_i^n] = i\hbar n x^{n-1}$$

by the same process as above. This gives

$$\begin{aligned}
[p_i, G(\mathbf{x})] &= \sum_{n=0}^{\infty} c_n [p_i, x_i^n] \\
&= i\hbar \sum_{n=0}^{\infty} c_n n x^{n-1} \\
&= i\hbar \frac{dG}{dx_i}
\end{aligned}$$

2 Problem #2

(i) Given a free particle inside a one dimensional infinite potential well of width a with a wave function at $t = 0$ given by

$$\Psi(x, t = 0) = \psi_0 = A \sin^3\left(\frac{\pi x}{a}\right)$$

we calculate the wave function for an arbitrary time, t, by projecting the wave function onto the basis of the infinite potential well

$$\Psi(x,t) = \sum_{n=0}^{\infty} c_n \psi_n \exp\left(-i/\hbar E_n t\right)$$

where ψ_n are the eigenfunctions of a free particle in an infinitely deep potential well. We know that ψ_n is given by

$$\psi_n = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{\pi(n+1)x}{a}\right) \tag{2.1}$$

and E_n are the associated eigenvalues given by

$$E_n = \frac{\hbar^2\pi^2(n+1)^2}{2ma^2}.$$

We note that ψ_n forms an orthonormal basis which implies that we can calculate the coefficients c_n from equation 2.1 by

$$c_n = \int \psi_n^* \psi_0 dx$$

$$\Downarrow$$

$$\begin{aligned}
c_n &= \int_0^a \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{\pi(n+1)x}{a}\right) A \sin^3\left(\frac{\pi x}{a}\right) dx \\
&= A\left(\frac{2}{a}\right)^{1/2} \int_0^a \sin\left(\frac{\pi(n+1)x}{a}\right) \sin^3\left(\frac{\pi x}{a}\right) dx \\
&= A\left(\frac{2}{a}\right)^{1/2} \int_0^a \sin\left(\frac{\pi(n+1)x}{a}\right) \sin\left(\frac{\pi x}{a}\right)\left(1 - \cos^2\left(\frac{\pi x}{a}\right)\right) dx \\
&= A\left(\frac{2}{a}\right)^{1/2} \int_0^a \sin\left(\frac{\pi(n+1)x}{a}\right) \sin\left(\frac{\pi x}{a}\right) dx - \int_0^a \sin\left(\frac{\pi(n+1)x}{a}\right) \sin\left(\frac{\pi x}{a}\right) \cos^2\left(\frac{\pi x}{a}\right) dx \\
&= A\left(\frac{2}{a}\right)^{1/2} \int_0^a \sin\left(\frac{\pi(n+1)x}{a}\right) \sin\left(\frac{\pi x}{a}\right) dx - \frac{1}{4}\int_0^a \sin\left(\frac{\pi(n+1)x}{a}\right)\left(\sin\left(\frac{\pi x}{a}\right) + \sin\left(\frac{3\pi x}{a}\right)\right) dx \\
&= A\left(\frac{2}{a}\right)^{1/2} \frac{3}{4}\int_0^a \sin\left(\frac{\pi(n+1)x}{a}\right) \sin\left(\frac{\pi x}{a}\right) dx - \frac{1}{4}\int_0^a \sin\left(\frac{\pi(n+1)x}{a}\right) \sin\left(\frac{3\pi x}{a}\right) dx
\end{aligned}$$

We note that for the right integral is nonzero for only $n = 0$ and the left integral only is nonzero for $n = 2$. This implies that we picked out only two terms for the sum over our basis. So we calculate c_0 by

$$\begin{aligned}
c_0 &= A\left(\frac{2}{a}\right)^{1/2} \frac{3}{4}\int_0^a \sin^2\left(\frac{\pi x}{a}\right) dx \\
&= A\left(\frac{2}{a}\right)^{1/2} \frac{3}{4}\frac{a}{2} = A\left(\frac{2}{a}\right)^{1/2} \frac{3a}{8}
\end{aligned}$$

and then we calculate c_2 by

$$
\begin{aligned}
c_2 &= -A\left(\frac{2}{a}\right)^{1/2}\frac{1}{4}\int_0^a \sin^2\left(\frac{3\pi x}{a}\right)dx \\
&= -A\left(\frac{2}{a}\right)^{1/2}\frac{1}{4}\frac{a}{2} = -A\left(\frac{2}{a}\right)^{1/2}\frac{a}{8}
\end{aligned}
$$

So we can easily write $\Psi(x,t)$ as the sum of two terms

$$
\Psi(x,t) = A\left(\frac{2}{a}\right)^{1/2}\frac{a}{8}\left(3\sin\left(\frac{\pi x}{a}\right)e^{(-iE_0t/\hbar)} - \sin\left(\frac{3\pi x}{a}\right)e^{(-iE_2t/\hbar)}\right)
$$

(ii) For a spherical rotator with an initial wave function at $t=0$ given by

$$
\psi_0(\theta,\phi) = A\cos^2(\theta)
$$

we can find the wave function $\Psi(\theta,\phi,t)$ for an arbitrary time, t, by projecting on the basis of spherical harmonics given by $\psi_{lm} = Y_{lm}(\theta,\phi)$. We note that each ψ_{lm} has an associated energy, E_l, given by

$$
E_l = \frac{\hbar^2 l(l+1)}{2I}
$$

where I is the moment of inertia. This implies that we can construct

$$
\Psi(\theta,\phi,t) = \sum_{l=0}^{\infty} c_l\psi_{lm}e^{-iE_lt/\hbar}
$$

where we calculate c_l by using the initial condition

$$
c_l = \int \psi_{lm}^*\psi_0 dA
$$

We first note that the form of the spherical harmonics is given by

$$
Y_{lm}(\theta,\phi) = Ne^{im\phi}P_l^m(\cos\theta)
$$

where N is a normalization factor and P_l^m are the *Legendre polynomials*. We note that P_l^m form a orthonormal basis therefore we will pick out the specific polynomial that is of the form $\cos^2\theta$ this is the $l=2$, $m=0$ term given by

$$
Y_{20}(\theta,\phi) = \frac{1}{4}\sqrt{\frac{5}{\pi}}\left(3\cos^2\theta - 1\right)
$$

so we can calculate the only coefficient c_2 by

$$
\begin{aligned}
c_2 &= \int_0^{2\pi}\int_0^{\pi}\psi_{20}^*\cos^2\theta\sin\theta d\theta d\phi \\
&= \frac{8}{3}\sqrt{\frac{\pi}{5}}
\end{aligned}
$$

Note that we can test the orthogonality condition of $\cos^2\theta$ by a Mathematica line of code given by `Table[Table[Integrate[SphericalHarmonicY[l, m, [Theta], [Phi]](Cos[[Theta]]^2)* Sin[[Theta]], {[Theta], 0, Pi}, {[Phi], 0, 2 Pi}] , {m, -l, l}] , {l, 0, 20}]` which confirms that c_2 is the only nonzero coefficient. So we have

$$
\Psi(\theta,\phi,t) = \frac{8}{3}\sqrt{\frac{\pi}{5}}Y_{20}(\theta,\phi)e^{-iE_2t/\hbar}
$$

3 Problem #3

For a wave packet at the moment of time, $t = 0$, we are given the wave function of a free particle as

$$\psi_0 = A\exp\left(-\frac{x^2}{2a^2} + i\frac{p_0 x}{\hbar}\right).$$

We note that for a free particle we have a plane wave solution to *Schrödinger's Equation.*

$$\psi_x = A\exp\left(i(px - Et)/\hbar\right)$$

We note that the plane was solution will form our basis, but since this state is a free particle we know that we will have a continuous spectrum. For ease we can work in momentum space such that

$$\Psi(x,t) = \int C(p)\exp\left[i\left(\frac{px}{\hbar} - \frac{p^2}{2\mu\hbar}t\right)\right]dp$$

Note that we replace E with $E = p^2/2\mu$. We can calculate $C(p)$ by the Fourier Transform

$$\begin{aligned}
C(p) &= \int \psi_0 \exp\left(-i\frac{px}{\hbar}\right)dx \\
&= \int A\exp\left(-\frac{x^2}{2a^2} + i\frac{p_0 x}{\hbar}\right)\exp\left(-i\frac{px}{\hbar}\right)dx \\
&= A\int \exp\left(-\frac{x^2}{2a^2} + i\frac{(p_0 - p)x}{\hbar}\right)dx \\
&= A\exp\left(-\frac{a^2(p-p_0)^2}{2\hbar^2}\right)
\end{aligned}$$

So now we can solve for $\Psi(x,t)$ as

$$\begin{aligned}
\Psi(x,t) &= \int C(p)\exp\left[i\left(\frac{px}{\hbar} - \frac{p^2}{2\mu\hbar}t\right)\right]dp \\
&= \int A\exp\left(-\frac{a^2(p-p_0)^2}{2\hbar^2}\right)\exp\left[i\left(\frac{px}{\hbar} - \frac{p^2}{2\mu\hbar}t\right)\right]dp \\
&= \int A\exp\left(-\frac{a^2(p-p_0)^2}{2\hbar^2} + i\frac{px}{\hbar} - i\frac{p^2}{2\mu\hbar}t\right)dp \\
&= \int A\exp\left(-\frac{a^2\mu(p-p_0)^2 + i(\hbar p^2 t - 2\hbar\mu x p)}{2\mu\hbar^2}\right)dp \\
&= \int A\exp\left(-\frac{(a^2\mu - i\hbar t)p^2 - (i2\hbar\mu x)p + a^2\mu(p_0^2 - 2p_0)}{2\mu\hbar^2}\right)dp \\
&= A\exp\left(-\frac{a^2\mu(p_0^2 - 2p_0)}{2\mu\hbar^2}\right)\int\exp\left(-\frac{(a^2\mu - i\hbar t)p^2 - (i2\hbar\mu x)p}{2\mu\hbar^2}\right)dp \\
&= A\exp\left(-\frac{a^2\mu(p_0^2 - 2p_0)}{2\mu\hbar^2}\right)\int\exp\left(-\frac{a^2\mu + it}{2\mu\hbar^2}\left(p^2 - \frac{i2\hbar\mu x}{a^2\mu + it}p\right)\right)dp \\
&= A\exp\left(-\frac{a^2\mu(p_0^2 - 2p_0)}{2\mu\hbar^2}\right)\int\exp\left(-\frac{a^2\mu + it}{2\mu\hbar^2}\left(\left(p - \frac{i\hbar\mu x}{a^2\mu + it}\right)^2 + \left(\frac{\hbar\mu x}{a^2\mu + it}\right)^2\right)\right)dp \\
&= A\exp\left(-\frac{a^2 p_0(p_0 - 2)}{2\hbar^2}\right)\exp\left(-\frac{a^2\mu + it}{2\mu\hbar^2}\left(\frac{\hbar\mu x}{a^2\mu + it}\right)^2\right)\int\exp\left(-\frac{a^2\mu + it}{2\mu\hbar^2}\left(\left(p - \frac{i\hbar\mu x}{a^2\mu + it}\right)^2\right)\right)dp
\end{aligned}$$

We note that the integral over all momentum space yields a factor of π which we absorb into A and a square root the $a^2\mu + it/2\mu\hbar^2$ term so

$$\begin{aligned}
\Psi(x,t) &= A\sqrt{\frac{2\mu\hbar^2}{a^2\mu + it}} \exp\left(-\frac{a^2\mu(p_0^2 - 2p_0)}{2\mu\hbar^2}\right) \exp\left(-\frac{a^2\mu + it}{2\mu\hbar^2}\left(\frac{\hbar\mu x}{a^2\mu + it}\right)^2\right) \\
&= A\sqrt{\frac{2\mu\hbar^2}{a^2\mu + it}} \exp\left(-\frac{a^2\mu(p_0^2 - 2p_0)}{2\mu\hbar^2}\right) \exp\left(-\frac{a^2\mu + it}{2\mu\hbar^2}\frac{\hbar^2\mu^2}{(a^2\mu + it)^2}x^2\right) \\
&= A\sqrt{\frac{2\mu\hbar^2}{a^2\mu + it}} \exp\left(-\frac{a^2\mu(p_0^2 - 2p_0)}{2\mu\hbar^2}\right) \exp\left(-\frac{\mu}{2(a^2\mu + it)}x^2\right) \\
&= A\frac{2\hbar}{\sigma_x(t)} \exp\left(-\frac{a^2\mu(p_0^2 - 2p_0)}{2\mu\hbar^2}\right) \exp\left(-\frac{x^2}{\sigma_x(t)^2}\right)
\end{aligned}$$

We see that we still have a wave packet, but now we have a time dependent variance given by

$$\sigma_x(t)^2 \equiv \frac{2(a^2\mu + it)}{\mu}$$

this implies that as time increases the width of the wave packet increases by

$$< \Delta x(t) >^2 = |\sigma_x(t)^2| = \sqrt{\frac{(2a\mu)^2 + t^2}{\mu^2}}$$