J13Q1 (Solution by Jim Wu)

A quantum particle moves in one dimension with energy as a function of wavenumber $E(k)$. Its momentum is $p = \hbar k$ and is conserved. At time $t = 0$, the wave function $\psi(x, t = 0)$ of this particle is a minimum-uncertainty wave packet centered at the origin ($x = 0$) in real space and with average momentum $\langle p \rangle_{t=0} = \hbar k_0$. Assume that the initial uncertainty $\sqrt{\langle x^2 \rangle_{t=0}} = \sigma$ is large but finite, so the uncertainty in the momentum is small by nonzero. Thus approximate $E(k)$ by its Taylor expansion about k_0 keeping terms only to order $(k - k_0)^2$.

(a) In terms of the given parameters, $E(k_0)$, and $\frac{dE}{dk}$ and $\frac{d^2E}{dk^2}$ evaluated at $k = k_0$ obtain the normalized wave function $\psi(x, t)$ at nonzero times t. Do not make any assumption about the dispersion relation $E(k)$ other than that its first and second derivatives exist and are finite at k_0.

(b) Calculate the expectation values $\langle x \rangle_t$, $\langle p \rangle_t$, $\langle (x - \langle x \rangle_t)^2 \rangle_t$ at nonzero times t. [If you get bogged down: first do this problem assuming $\frac{d^2E}{dk^2} = 0$ before letting it be nonzero.]

Solution:

(a) The minimized-uncertainty wave packet centered around the origin with initial positional uncertainty σ and average momentum $\hbar k_0$ is a gaussian wave function of the form

$$\psi(x, t = 0) = e^{i(\hbar k_0)x/\hbar} \left(\frac{1}{2\pi\sigma^2} \right)^{1/4} e^{-\frac{x^2}{4\sigma^2}} = \frac{1}{\sqrt{\sqrt{2\pi}\sigma}} e^{-\frac{x^2}{4\sigma^2} + ik_0 x}$$

Now, we evolve the wave function over time by applying the unitary time evolution operator $U = e^{-iEt/\hbar}$ where $E = E(k)$ is the energy and is a function of the wave number. Applying this and expanding $E(k)$ around $k = k_0$ up to second order, we have

$$\psi(x, t) = U\psi(x, 0) = \exp\left[-\frac{it}{\hbar} \left(E(k_0) + E'(k_0)(k - k_0) + \frac{1}{2}E''(k_0)(k - k_0)^2 \right) \right] \frac{1}{\sqrt{\sqrt{2\pi}\sigma}} e^{-\frac{x^2}{4\sigma^2} + ik_0 x}$$

Grouping the terms that only depend on k_0 together into a single phase $\phi_0(t)$, we can rewrite the time evolved wave function as

$$\begin{aligned} \psi(x, t) &= \frac{e^{-i\phi_0(t)}}{\sqrt{\sqrt{2\pi}\sigma}} \exp\left[-\frac{it}{\hbar} \left(E'(k_0)k + \frac{1}{2}E''(k_0)k^2 - E''(k_0)k_0 k \right) \right] \exp\left(-\frac{x^2}{4\sigma^2} + ik_0 x \right) \\ &= \frac{e^{-i\phi_0(t)}}{\sqrt{\sqrt{2\pi}\sigma}} \exp\left[-\frac{it}{\hbar} \left(\frac{(E'(k_0) - E''(k_0)k_0)}{\hbar} \hat{p} + \frac{E''(k_0)}{2\hbar^2} \hat{p}^2 \right) \right] \exp\left(-\frac{x^2}{4\sigma^2} + ik_0 x \right) \end{aligned}$$

where I invoked conservation of momentum $p = \hbar k$. Letting

$$A = \frac{(E'(k_0) - E''(k_0)k_0)}{\hbar^2} t \qquad \text{and} \qquad B = \frac{E''(k_0)}{2\hbar^3} t$$

we have

$$\psi(x, t) = \frac{e^{-i\phi_0(t)}}{\sqrt{\sqrt{2\pi}\sigma}} \exp\left[-i(A\hat{p} + B\hat{p}^2) \right] \exp\left(-\frac{x^2}{4\sigma^2} + ik_0 x \right)$$

We will use this last form to simplify the calculations of the position and momentum expectation values.

To find the actual form of the wave function in position space, we first need to apply a Fourier transform on $\psi(x,0)$ into momentum space, apply the time propagator, and then do an inverse Fourier transform to back out $\psi(x,0)$ in position space. But that's too messy and we can find the position and momentum expectation values in a much easier way.

(b) Note that for $t = 0$,

$$\langle x \rangle_{t=0} = 0 \qquad \langle x^2 \rangle_{t=0} = \sigma^2 \qquad \langle p \rangle_{t=0} = \hbar k_0 \qquad \langle p^2 \rangle_{t=0} = \frac{\hbar^2}{4\sigma^2} + \hbar^2 k_0^2$$

where we obtain the final relation from using $\Delta x \Delta p = \hbar/2$ for a minimum uncertainty wave packet.

Now let's start by finding $\langle p \rangle_t$ as this is the simplest. Note that p commutes with the unitary time evolution operator U, which suggests that average momentum does not change with time, hence

$$\boxed{\langle p \rangle_t = \int_{-\infty}^{\infty} \psi^*(x,t)\hat{p}\psi(x,t)\,dx = \hbar k_0}$$

The average position clearly changes as U looks similar to a translation operator in position, however computation of $\langle x \rangle_t$ is a bit more difficult as it does not commute with U:

$$\langle x \rangle_t = \int_{-\infty}^{\infty} \psi^*(x,t)x\psi(x,t)\,dx = \int_{-\infty}^{\infty} \psi^*(x,0)\hat{U}^\dagger \hat{x}\hat{U}\psi(x,0)\,dx$$

Before I proceed, let me make a small digression that will make calculations much simpler. Recall the following commutation relation:

$$[\hat{x}, \hat{F}(p)] = i\hbar \frac{\partial \hat{F}}{\partial p}$$

This can be derived by doing a Taylor expansion of $\hat{F}(p)$ and exploiting the commutation of $[\hat{x}, \hat{p}^n] = i\hbar p^{n-1}$. Now, if $\hat{F}(p)$ is the unitary time evolution operator, then

$$\begin{aligned}
[\hat{x}, \hat{U}(p)] &= i\hbar \frac{\partial}{\partial p} \exp[-i(A\hat{p} + B\hat{p}^2)] \\
&= \hbar(A + 2B\hat{p}) \exp[-i(A\hat{p} + B\hat{p}^2)]
\end{aligned}$$

and therefore,

$$xU = \hbar(A + 2B\hat{p})e^{-i(A\hat{p}+B\hat{p}^2)} + e^{-i(A\hat{p}+B\hat{p}^2)}x = U(\hbar A + 2B\hbar\hat{p} + \hat{x})$$

Notice that the time evolution operator has been moved all the way to the left! This is very useful as the expectation value of the position as a function of time is

$$\begin{aligned}
\langle x \rangle_t &= \int_{-\infty}^{\infty} \psi^*(x,0)\hat{U}^\dagger \hat{x}\hat{U}\psi(x,0)\,dx \\
&= \int_{-\infty}^{\infty} \psi^*(x,0)\hat{U}^\dagger \hat{U}(\hbar A + 2B\hbar\hat{p} + \hat{x})\psi(x,0)\,dx \\
&= \hbar A + 2\hbar B\langle p \rangle_{t=0} + \langle x \rangle_{t=0}
\end{aligned}$$

Substituting in the values for A, B, and the average position and momentum at $t = 0$, we get

$$\langle x\rangle_t = \hbar\left(\frac{(E'(k_0) - E''(k_0)k_0)}{\hbar^2}t\right) + 2\hbar\left(\frac{E''(k_0)}{2\hbar^3}t\right)(\hbar k_0) + 0 = \boxed{\frac{E'(k_0)t}{\hbar}}$$

Checking the limits, we see that at $t = 0$, we get $\langle x\rangle_{t=0} = 0$ as expected. Furthermore, if $E(k) = \hbar\omega(k)$, then $\langle x\rangle_t = \frac{d\omega}{dk}t = v_g t$, where v_g is the group velocity. This suggests that the center of the wave packet moves with velocity v_g, in agreement with our intuition.

Now, let's do the same for $\langle x^2\rangle$. Consider the commutator of x^2 and U:

$$\begin{aligned}
[\hat{x}^2, \hat{U}] &= \hat{x}[\hat{x}, \hat{U}] + [\hat{x}, \hat{U}]\hat{x} \\
&= \hat{x}e^{-i(A\hat{p}+B\hat{p}^2)}(\hbar A + 2\hbar B\hat{p}) + (\hbar A + 2\hbar B\hat{p})\, e^{-i(A\hat{p}+B\hat{p}^2)}\hat{x} \\
&= (\hat{x}\hat{U})(\hbar A + 2\hbar B\hat{p}) + \hat{U}(\hbar A + 2\hbar B\hat{p})\hat{x} \\
&= [\hat{U}(\hbar A + 2B\hbar\hat{p} + \hat{x})](\hbar A + 2\hbar B\hat{p}) + \hat{U}(\hbar A + 2\hbar B\hat{p})\hat{x} \\
&= \hat{U}\left[\hbar^2 A^2 + 4\hbar^2 B^2\hat{p}^2 + 4\hbar^2 AB\hat{p} + 2\hbar A\hat{x} + 2\hbar B(\hat{x}\hat{p} + \hat{p}\hat{x})\right]
\end{aligned}$$

and hence

$$\hat{x}^2\hat{U} = \hat{U}\left[\hbar^2 A^2 + 4\hbar^2 B^2\hat{p}^2 + 4\hbar^2 AB\hat{p} + 2\hbar A\hat{x} + 2\hbar B(\hat{x}\hat{p} + \hat{p}\hat{x}) + \hat{x}^2\right]$$

Therefore, the expectation value of $\langle x^2\rangle$ is

$$\begin{aligned}
\langle x^2\rangle_t &= \int_{-\infty}^{\infty} \psi^*(x,0)\hat{U}^\dagger\hat{x}^2\hat{U}\psi(x,0)\,dx \\
&= \int_{-\infty}^{\infty} \psi^*(x,0)\hat{U}^\dagger\hat{U}\left[\hbar^2 A^2 + 4\hbar^2 B^2\hat{p}^2 + 4\hbar^2 AB\hat{p} + 2\hbar A\hat{x} + 2\hbar B(\hat{x}\hat{p} + \hat{p}\hat{x}) + \hat{x}^2\right]\psi(x,0)\,dx \\
&= \hbar^2 A^2 + 4\hbar^2 B^2\langle p^2\rangle_{t=0} + 4\hbar^2 AB\langle p\rangle_{t=0} + 2\hbar A\langle x\rangle_{t=0} + 2\hbar B\langle\{x,p\}\rangle_{t=0} + \langle x^2\rangle_{t=0}
\end{aligned}$$

where the braces signify the anticommutator. The only term that we do not know is the expectation value

$$\langle\{x,p\}\rangle_{t=0} = \langle xp + px\rangle_{t=0} = \langle 2xp - xp + px\rangle_{t=0} = \langle 2xp - i\hbar\rangle_{t=0} = 2\langle xp\rangle_{t=0} - i\hbar$$

Let's explicitly compute $\langle xp\rangle_{t=0}$:

$$\begin{aligned}
\langle xp\rangle_{t=0} &= \int_{-\infty}^{\infty} \psi^*(x,0)\hat{x}\hat{p}\psi(x,0)\,dx \\
&= \frac{1}{\sqrt{2\pi}\sigma}\int_{-\infty}^{\infty} e^{-\frac{x^2}{4\sigma^2} - ik_0 x}\, x\frac{\hbar}{i}\frac{d}{dx}\left(e^{-\frac{x^2}{4\sigma^2} + ik_0 x}\right)dx \\
&= -\frac{i\hbar}{\sqrt{2\pi}\sigma}\int_{-\infty}^{\infty} e^{-\frac{x^2}{4\sigma^2} - ik_0 x}\, x\left(-\frac{x}{2\sigma^2} + ik_0\right)e^{-\frac{x^2}{4\sigma^2} + ik_0 x}\,dx \\
&= -\frac{i\hbar}{\sqrt{2\pi}\sigma}\int_{-\infty}^{\infty}\left(-\frac{x^2}{2\sigma^2} + ik_0 x\right)e^{-\frac{x^2}{2\sigma^2}}\,dx \\
&= \frac{i\hbar}{2\sqrt{2\pi}\sigma^3}\int_{-\infty}^{\infty} x^2 e^{-\frac{x^2}{2\sigma^2}}\,dx + 0 \\
&= \frac{i\hbar}{2\sqrt{\pi}\sigma^3}\left(\frac{1}{2}\sqrt{\pi 2^3\sigma^6}\right) \\
&= \frac{i\hbar}{2}
\end{aligned}$$

Therefore, $2\langle xp\rangle_{t=0} - i\hbar = 0$ and the expectation value of x^2 is

$$\begin{aligned}
\langle x^2\rangle_t &= \hbar^2 A^2 + 4\hbar^2 B^2 \langle p^2\rangle_{t=0} + 2\hbar^2 AB\langle p\rangle_{t=0} + 2\hbar A\langle x\rangle_{t=0} + \langle x^2\rangle_{t=0} \\
&= \hbar^2 \left(\frac{(E'(k_0) - E''(k_0)k_0)}{\hbar^2} t\right)^2 + 4\hbar^2 \left(\frac{E''(k_0)}{2\hbar^3} t\right)^2 \left(\frac{\hbar^2}{4\sigma^2} + \hbar^2 k_0^2\right) \\
&\quad + 4\hbar^2 \left(\frac{(E'(k_0) - E''(k_0)k_0)}{\hbar^2} t\right)\left(\frac{E''(k_0)}{2\hbar^3} t\right)(\hbar k_0) + 0 + \sigma^2 \\
&= \sigma^2 + \frac{1}{\hbar^2}\left[E'^2(k_0)t^2 + E''^2(k_0)t^2\left(\frac{1}{4\sigma^2} + k_0^2\right)\right]
\end{aligned}$$

This means that the variance in the position is

$$\begin{aligned}
\langle (x - \langle x\rangle_t)^2\rangle_t = \langle x^2\rangle_t - \langle x\rangle_t^2& \\
&= \sigma^2 + \frac{1}{\hbar^2}\left[E'^2(k_0)t^2 + E''^2(k_0)t^2\left(\frac{1}{4\sigma^2} + k_0^2\right)\right] - \frac{E'^2(k_0)t^2}{\hbar^2} \\
&= \boxed{\sigma^2 + \frac{1}{\hbar^2}\left[E''^2(k_0)t^2\left(\frac{1}{4\sigma^2} + k_0^2\right)\right]}
\end{aligned}$$

Again, we can check that at $t = 0$, the variance is σ^2 as expected. Furthermore, the existence of a nonzero second derivative of $E(k)$ tells us that there is dispersion and that the wave should spread out and decrease in amplitude over time.

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