Homework 2 - Wave function

Question 1:

Calculate the inverse Fourier transform for the function

$$\tilde{\psi}(k,t) = e^{-\frac{(k-k_0)^2}{2\sigma} - i(kx_0 + \omega(t)t)},$$

where $\omega(k) = ck$. This is a packet of planar waves with an amplitude that is distributed like a Gaussian.

Solution:

The inverse Fourier transform is

$$\begin{aligned}\psi(x,t) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\tilde{\psi}(k,t)\,e^{ikx}dk\\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}e^{-\frac{(k-k_0)^2}{2\sigma} - ik(x_0 - x + ct)}dk,\end{aligned}$$

completing the square in the power,

$$\begin{aligned}-\frac{(k-k_0)^2}{2\sigma} - ik(x_0 - x + ct) &= -\frac{1}{2\sigma}\left[k^2 - 2kk_0 + k_0^2 + ik2\sigma(x_0 - x + ct)\right]\\ &= -\frac{1}{2\sigma}\left[k^2 - 2k(k_0 - i\sigma(x_0 - x + ct)) + (k_0 - i\sigma(x_0 - x + ct))^2 - (k_0 - i\sigma(x_0 - x + ct))^2 + k_0^2\right]\\ &= -\frac{1}{2\sigma}(k + k_0 - i\sigma(x_0 - x + ct))^2 - ik_0(x_0 - x + ct) - \frac{\sigma}{2}(x_0 - x + ct)^2\end{aligned}$$

then preforming the resulting Gaussian integral leads to

$$\begin{aligned}\psi(x,t) &= \frac{1}{\sqrt{2\pi}}e^{-ik_0(x_0 - x + ct) - \frac{\sigma}{2}(x_0 - x + ct)^2}\int_{-\infty}^{\infty}e^{-\frac{1}{2\sigma}(k + k_0 - i\sigma(x_0 - x + ct))^2}dk\\ &= \frac{e^{-ik_0(x_0 - x + ct)}}{\sqrt{2\pi}}e^{-\frac{\sigma}{2}(x_0 - x + ct)^2}\sqrt{2\pi\sigma}.\end{aligned}$$

Thus

$$\boxed{\psi(x,t) = \sqrt{\sigma}e^{-\frac{\sigma}{2}(ct + x_0 - x)^2 - ik_0(ct + x_0 - x)}},$$

which is a Gaussian that shifts with time.

Question 2:

Prove the following identity

$$\mathcal{F}\left[\frac{d^n f(x)}{dx^n}\right] = (ik)^n\,\mathcal{F}[f(x)],$$

where $f(x)$ is some analytic function and $\mathcal{F}[]$ denotes a Fourier transform of whatever is in the brackets.

Solution:

Looking at $f(x)$ in terms of the k-space basis,

$$f(x) = \frac{1}{\sqrt{2\pi}}\int\tilde{f}(k)\,e^{ikx}dk$$

we see that

$$\frac{d^n}{dx^n} f(x) = \frac{1}{\sqrt{2\pi}} \int (ik)^n \tilde{f}(k) e^{ikx} dk.$$

Now, taking the Fourier transform reads

$$\begin{aligned}
\mathcal{F}\left[\frac{d^n f(x)}{dx^n}\right] &= \frac{1}{2\pi} \int \int (ik)^n \tilde{f}(k) e^{ikx} dk e^{-ik'x} dk' \\
&= \int (ik)^n \tilde{f}(k) dk \underbrace{\frac{1}{2\pi} \int e^{ix(k-k')} dk'}_{\delta(k-k')} \\
&= (ik')^n \tilde{f}(k'),
\end{aligned}$$

hence

$$\boxed{\mathcal{F}\left[\frac{d^n f(x)}{dx^n}\right] = (ik)^n \mathcal{F}[f(x)]}.$$

Question 3:

Given the initial wave function

$$\psi(x,0) = Ae^{-\frac{x^2}{4\sigma^2} + ik_0 x}$$

and the dispersion relation $\omega = \hbar k^2/2m$,

1. Find A.
2. Find $\tilde{\psi}(k)$.
3. Find $\psi(x,t)$.
4. Calculate $\rho(x,t)$.
5. Calculate $\tilde{\rho}(k)$. Show that it is time independent, i.e. $\tilde{\rho}(k,t) = \tilde{\rho}(k)$.
6. Calculate: $\langle x(t) \rangle$, $\langle p(t) \rangle$, $\Delta x(t)$, $\Delta p(t)$, using the definition of mean values $\langle f(x,t) \rangle = \int \rho(x,t) f(x,t) dx$. *Hint: Use $p = \hbar k$.*
7. Calculate the group velocity v_g and the phase velocity v_p.
8. Show that $x_{\max} = \langle x(t) \rangle$ and $\langle x(t) \rangle = v_g t$. what is the meaning of this result?
9. Show that wave function from satisfies Schrodinger's equation for a free particle: $i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}$.

Note: feel free to use any computer program for your calculations.

Solution:

1. Normalizing the inner product yields

$$\langle \psi(x), \psi(x) \rangle = \int_{-\infty}^{\infty} |A|^2 e^{-\frac{x^2}{8\sigma^2}} dx = |A|^2 \sigma\sqrt{2\pi} = 1 \quad \rightarrow \quad \boxed{|A| = \left(\sigma\sqrt{2\pi}\right)^{-1/2}}.$$

2. Taking the Fourier transform of $\psi(x,0)$ yields

$$\begin{aligned}
\tilde{\psi}(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} Ae^{-\frac{x^2}{4\sigma^2} + ik_0 x} e^{-ikx} dx \\
&= \frac{1}{\sqrt{\sigma}(2\pi)^{3/4}} \int_{-\infty}^{\infty} e^{-\frac{1}{4\sigma^2}\left(x^2 - 4\sigma^2 i(k_0-k)x\right)} dx \\
&= \frac{e^{-\sigma^2(k_0-k)^2}}{\sqrt{\sigma}(2\pi)^{3/4}} \int_{-\infty}^{\infty} e^{-\frac{1}{4\sigma^2}\left(x^2 - 2\sigma^2 i(k_0-k)\right)^2} dx
\end{aligned}$$

$$\boxed{\tilde{\psi}(k) = \left(\frac{2}{\pi}\right)^{1/4} \sqrt{\sigma} e^{-\sigma^2(k_0-k)^2}}.$$

3. Taking the inverse Fourier transform, with the propagator and defining $\tau = \hbar t/2m$, reads

$$-\left(\sigma^2 + i\tau\right)\left(k - \frac{2\sigma^2 k_0 + ix}{\sigma^2 + i\tau}k\right)^2 + \frac{1}{4}\frac{\left(2\sigma^2 k_0 + ix\right)^2}{\sigma^2 + i\tau} - \sigma^2 k_0^2$$

$$\begin{aligned}
\psi(x,t) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\tilde{\psi}(k)\, e^{i(kx-\omega t)}dk \\
& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left(\frac{2}{\pi}\right)^{1/4}\sqrt{\sigma}e^{-\sigma^2(k_0-k)^2}e^{i(kx-\omega t)}dk \\
&= \frac{\sqrt{\sigma}}{2^{1/4}\pi^{3/4}}\int_{-\infty}^{\infty} e^{-\sigma^2\left(k^2-2kk_0+k_0^2\right)}e^{i\left(kx-\tau k^2\right)}dk \\
&= \frac{\sqrt{\sigma}}{2^{1/4}\pi^{3/4}}\int_{-\infty}^{\infty} e^{-\left(\sigma^2+i\tau\right)\left(k^2-\frac{2\sigma^2k_0+ix}{\sigma^2+i\tau}k\right)-\sigma^2k_0^2}dk \\
&= \frac{\sqrt{\sigma}}{2^{1/4}\pi^{3/4}}e^{\frac{\left(2\sigma^2k_0+ix\right)^2}{4\left(\sigma^2+i\tau\right)}-\sigma^2k_0^2}\int_{-\infty}^{\infty} e^{-\left(\sigma^2+i\tau\right)\left(k-\frac{2\sigma^2k_0+ix}{2\left(\sigma^2+i\tau\right)}\right)^2}dk \\
&= \frac{\sqrt{\sigma}}{2^{1/4}\pi^{3/4}}e^{\frac{\left(2\sigma^2k_0+ix\right)^2}{4\left(\sigma^2+i\tau\right)}-\sigma^2k_0^2}\sqrt{\frac{\pi}{\sigma^2+i\tau}} \\
&= \frac{1}{(2\pi)^{1/4}}\sqrt{\frac{\sigma}{\sigma^2+i\tau}}e^{\frac{\left(2\sigma^2k_0+ix\right)^2}{4\left(\sigma^2+i\tau\right)}-\sigma^2k_0^2}
\end{aligned}$$

leading to

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

4. The probability density is

$$\begin{aligned}
\rho &= \psi(x,t)\,\psi^*(x,t) \\
&= \frac{1}{(2\pi)^{1/4}}\sqrt{\frac{\sigma}{\sigma^2+i\tau}}e^{\frac{\left(2\sigma^2k_0+ix\right)^2}{4\left(\sigma^2+i\tau\right)}-\sigma^2k_0^2}\frac{1}{(2\pi)^{1/4}}\sqrt{\frac{\sigma}{\sigma^2-i\tau}}e^{\frac{\left(2\sigma^2k_0-ix\right)^2}{4\left(\sigma^2-i\tau\right)}-\sigma^2k_0^2} \\
&= \frac{\sigma}{(2\pi)^{1/2}}\sqrt{\frac{1}{\sigma^4+\tau^2}}e^{-\frac{\sigma^2(x-2k\tau)^2}{2\left(\sigma^4+\tau^2\right)}},
\end{aligned}$$

hence

$$\boxed{\rho(x,t) = \frac{\sigma}{(2\pi)^{1/2}}\sqrt{\frac{1}{\sigma^4+(\hbar t/2m)^2}}e^{-\frac{\sigma^2(x-k\hbar t/m)^2}{2\left(\sigma^4+\hbar^2t^2/4m^2\right)}}}.$$

5. Since the time dependence is expressed by a phase in the k-space

$$\tilde{\psi}(k,t) = \left(\frac{2}{\pi}\right)^{1/4}\sqrt{\sigma}e^{-\sigma^2(k_0-k)^2}e^{-i\omega t},$$

it is clear that the probability density will be time independent

$$\boxed{\tilde{\rho}(k,t) = \tilde{\psi}(k,t)\,\tilde{\psi}^*(k,t) = \left(\frac{2}{\pi}\right)^{1/2}\sigma e^{-2\sigma^2(k_0-k)^2}}.$$

6. Let us evaluate the expectation values

$$\begin{aligned}
\langle x(t)\rangle &= \int_{-\infty}^{\infty} x\rho(x,t)\,dx \\
&= \frac{\sigma}{(2\pi)^{1/2}}\sqrt{\frac{1}{\sigma^4+\tau^2}}\int_{-\infty}^{\infty} xe^{-\frac{\sigma^2(x-2k\tau)^2}{2\left(\sigma^4+\tau^2\right)}}dx,
\end{aligned}$$

changing variables to $\xi = x - 2k\tau$, $d\xi = dx$ we have

$$\begin{aligned}
\langle x(t)\rangle &= \frac{\sigma}{(2\pi)^{1/2}}\sqrt{\frac{1}{\sigma^4+\tau^2}}\int_{-\infty}^{\infty}(\xi + 2k\tau)\, e^{-\frac{\sigma^2\xi^2}{2(\sigma^4+\tau^2)}}\, d\xi \\
&= \frac{\sigma}{(2\pi)^{1/2}}\sqrt{\frac{1}{\sigma^4+\tau^2}}\left[\underbrace{\int_{-\infty}^{\infty}\xi e^{-\frac{\sigma^2\xi^2}{2(\sigma^4+\tau^2)}}\, d\xi}_{0} + \underbrace{\int_{-\infty}^{\infty} 2k\tau e^{-\frac{\sigma^2\xi^2}{2(\sigma^4+\tau^2)}}\, d\xi}_{2k\tau\sqrt{2\pi\frac{\sigma^4+\tau^2}{\sigma^2}}}\right],
\end{aligned}$$

thus

$$\boxed{\langle x(t)\rangle = 2k\tau = \frac{k\hbar}{m}t}.$$

In the same manner

$$\begin{aligned}
\langle p(t)\rangle &= \hbar\int_{-\infty}^{\infty} k\tilde{\rho}(k)\, dk \\
&= \hbar\int_{-\infty}^{\infty} k\left(\frac{2}{\pi}\right)^{1/2}\sigma e^{-2\sigma^2(k-k_0)^2}\, dk,
\end{aligned}$$

changing variables to $\xi = k - k_0$, $d\xi = dk$ we have

$$\begin{aligned}
\langle p(t)\rangle &= \hbar\int_{-\infty}^{\infty}(\xi + k_0)\left(\frac{2}{\pi}\right)^{1/2}\sigma e^{-2\sigma^2\xi^2}\, d\xi \\
&= \hbar\left(\frac{2}{\pi}\right)^{1/2}\sigma\left[\underbrace{\int_{-\infty}^{\infty}\xi e^{-2\sigma^2\xi^2}\, d\xi}_{0} + \underbrace{k_0\int_{-\infty}^{\infty} e^{-2\sigma^2\xi^2}\, d\xi}_{k_0\sqrt{\pi/2\sigma^2}}\right],
\end{aligned}$$

thus

$$\boxed{\langle p(t)\rangle = \hbar k_0}.$$

Whereas

$$\begin{aligned}
\left\langle x^2\right\rangle &= \int_{-\infty}^{\infty} x^2\rho(x,t)\, dx \\
&= \frac{1}{(2\pi)^{1/2}\Sigma(\tau)}\int_{-\infty}^{\infty} x^2 e^{-\frac{(x-2k\tau)^2}{2\Sigma^2(\tau)}}\, dx,
\end{aligned}$$

where $\Sigma^2(\tau) \equiv \frac{\sigma^4+\tau^2}{\sigma^2}$, changing variables to $\xi = x - 2k\tau$,

$$\begin{aligned}
\left\langle x^2\right\rangle &= \frac{1}{(2\pi)^{1/2}\Sigma(\tau)}\int_{-\infty}^{\infty}\left(\xi^2 + \cancel{4k\tau\xi} + 4k^2\tau^2\right) e^{-\frac{\xi^2}{2\Sigma^2(\tau)}}\, d\xi \\
&= \frac{1}{(2\pi)^{1/2}\Sigma(\tau)}\int_{-\infty}^{\infty}\left(\xi^2 + 4k^2\tau^2\right) e^{-\frac{\xi^2}{2\Sigma^2(\tau)}}\, d\xi.
\end{aligned}$$

Recalling that

$$\int_{-\infty}^{\infty}\xi^2 e^{-\alpha\xi^2}\, d\xi = -\frac{\partial}{\partial\alpha}\int_{-\infty}^{\infty} e^{-\alpha\xi^2}\, d\xi = -\frac{\partial}{\partial\alpha}\sqrt{\pi/\alpha} = \frac{1}{2}\sqrt{\pi}\alpha^{-3/2},$$

we have

$$\begin{aligned}
\left\langle x^2\right\rangle &= \frac{1}{(2\pi)^{1/2}\Sigma(\tau)}\left[\frac{1}{2}\sqrt{\pi}\Sigma^3 + 4k^2\tau^2\sqrt{2\pi\Sigma^2}\right] \\
&= \Sigma^2 + 4k^2\tau^2.
\end{aligned}$$

Thus

$$\boxed{\Delta x\left(t\right)=\sqrt{\left\langle x^{2}\right\rangle -\left\langle x\right\rangle ^{2}}=\sqrt{\Sigma^{2}+4k^{2}\tau^{2}-\left(2k\tau\right)^{2}}=\Sigma=\frac{\sqrt{\sigma^{4}+\hbar^{2}t^{2}/4m}}{\sigma}}.$$

Similarly, we have

$$\left\langle p^{2}\right\rangle =\frac{\hbar^{2}}{4\sigma^{2}}+\hbar k_{0},$$

since we expect

$$\boxed{\Delta p\left(t\right)=\sqrt{\left\langle p^{2}\right\rangle -\left\langle p\right\rangle ^{2}}=\frac{\hbar}{2\sigma}}.$$

7. Using the expressions for velocity and group velocities we find

$$\boxed{v_{g}=\frac{\partial\omega}{\partial k}=\frac{\hbar k}{m}},$$

and

$$\boxed{v_{p}=\frac{\omega}{k}=\frac{\hbar k}{2m}}.$$

8. Since our probability distribution is Gaussian, it is immediate to see that

$$\frac{d\rho\left(x_{\max},t\right)}{dx}=0$$

satisfies $x_{\max}=\left\langle x\left(t\right)\right\rangle$, while the conclusion from our results for $\left\langle x\left(t\right)\right\rangle$ and v_{g} imply that $\left\langle x\left(t\right)\right\rangle =v_{g}t$. This means that the probability density for the position of the particle at time t is a Gaussian that propagates in time with velocity v_{g}.

9. Let us look at the k-space instead,

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^{2}}{2m}\frac{\partial^{2}\psi}{\partial x^{2}}\quad\rightarrow\quad i\hbar\left(-i\omega\right)\tilde{\psi}\left(k\right)=-\frac{\hbar^{2}}{2m}\left(ikx\right)^{2}\tilde{\psi}\left(k\right)$$

$$i\hbar\left(-i\omega\right)\cancel{\tilde{\psi}\left(k\right)}=-\frac{\hbar^{2}}{2m}\left(ik\right)^{2}\cancel{\tilde{\psi}\left(k\right)}\quad\rightarrow\quad\omega=\frac{\hbar k^{2}}{2m},$$

which means that our wave function indeed solves the Schrodinger equation.

Question 4:

Show that for the internal product

$$\left\langle \Psi_{1},\Psi_{2}\right\rangle =\int_{\Omega}\Psi_{1}^{*}\Psi_{2}d\alpha\left(x\right),$$

where Ψ_{i} are normalizable wave-functions, Ω is the sample space and $\alpha\left(x\right)$ is a real measure, the following statements hold:

- $\left\langle \Psi_{1},\Psi_{2}\right\rangle =\left\langle \Psi_{2},\Psi_{1}\right\rangle ^{*}$
- $\left\langle c\Psi_{1},\Psi_{2}\right\rangle =c^{*}\left\langle \Psi_{1},\Psi_{2}\right\rangle$
- $\left\langle \Psi_{1},c\Psi_{2}\right\rangle =c\left\langle \Psi_{1},\Psi_{2}\right\rangle$
- $\left\langle \Psi_{1}+\Psi_{2},\Psi_{3}\right\rangle =\left\langle \Psi_{1},\Psi_{3}\right\rangle +\left\langle \Psi_{2},\Psi_{3}\right\rangle$

Solution:

- Looking at the inner product

$$\left\langle \Psi_{1},\Psi_{2}\right\rangle =\int\Psi_{1}^{*}\Psi_{2}d^{3}x=\int\left(\Psi_{1}\Psi_{2}^{*}\right)^{*}d^{3}x=\left\langle \Psi_{2},\Psi_{1}\right\rangle .$$

- Looking at the inner product
$$\langle c\Psi_1, \Psi_2\rangle = \int (c\Psi_1)^* \Psi_2 d^3x = c^* \int \Psi_1^* \Psi_2 d^3x = c^* \langle \Psi_1, \Psi_2\rangle .$$
- Looking at the inner product
$$\langle \Psi_1, c\Psi_2\rangle = \int \Psi_1^* (c\Psi_2) d^3x = c \int \Psi_1^* \Psi_2 d^3x = c \langle \Psi_1, \Psi_2\rangle .$$
- Looking at the inner product
$$\langle \Psi_1 + \Psi_2, \Psi_3\rangle = \int (\Psi_1 + \Psi_2)^* \Psi_3 d^3x = \int (\Psi_1^* + \Psi_2^*) \Psi_3 d^3x = \langle \Psi_1, \Psi_3\rangle + \langle \Psi_2, \Psi_3\rangle .$$

Question 5:

Find the Fourier transform of the Gaussian $g(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{x^2}{2\sigma^2}}$, and show that $\Delta x \Delta k = 1$.

Solution:

Taking the Fourier transform of $g(x)$ yields
$$\begin{aligned}\tilde{g}(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(x) e^{-ikx} dx \\ &= \frac{1}{2\pi\sigma} \int_{-\infty}^{\infty} e^{-\frac{x^2}{2\sigma^2}} e^{-ikx} dx.\end{aligned}$$
Looking at the power of the exponent we can write
$$-\frac{1}{2\sigma^2}\left(x^2 + 2i\sigma^2 kx\right) = -\frac{1}{2\sigma^2}\left(x^2 + 2i\sigma^2 kx - \sigma^4 k^2\right) - \frac{\sigma^2 k^2}{2},$$
which leads to
$$\tilde{g}(k) = \frac{e^{-\sigma^2 k^2/2}}{2\pi\sigma} \underbrace{\int_{-\infty}^{\infty} e^{-\frac{u^2}{2\sigma^2}} du}_{I},$$
where we defined $u = x + i\sigma^2 k$. we are left with a simple Gaussian integral I which can be solved as follows
$$I^2 = \left(\int_{-\infty}^{\infty} e^{-\frac{x^2}{2\sigma^2}} dx\right)^2 = \int_{-\infty}^{\infty} e^{-\frac{x^2}{2\sigma^2}} dx \int_{-\infty}^{\infty} e^{-\frac{y^2}{2\sigma^2}} dy = \int_{-\infty}^{\infty} e^{-\frac{x^2+y^2}{2\sigma^2}} dxdy$$
moving to polar coordinates
$$I^2 = \int_0^{2\pi} \int_0^{\infty} e^{-\frac{r^2}{2\sigma^2}} r dr d\varphi = \pi \int_0^{\infty} e^{-\frac{\xi}{2\sigma^2}} d\xi = 2\pi\sigma^2,$$
where we defined $\xi = r^2$ hence $d\xi = 2rdr$, which gives $I = \sqrt{2\pi\sigma^2}$.
Therefore
$$\boxed{\tilde{g}(k) = \frac{e^{-\sigma^2 k^2/2}}{\sqrt{2\pi}}}.$$
Calculating the square root of the variance $\Delta x \equiv \sqrt{\langle x^2\rangle - \langle x\rangle^2}$ of both results we see that
$$\langle x\rangle = \int_{-\infty}^{\infty} x \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{x^2}{2\sigma^2}} dx = 0,$$
where the integral vanishes as it is symmetric and the integrand is anti-symmetric.
$$\langle x^2\rangle = \int_{-\infty}^{\infty} x^2 \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{x^2}{2\sigma^2}} dx$$

defining $\alpha = \frac{1}{2\sigma^2}$ we can write

$$\begin{aligned}\left\langle x^2 \right\rangle &= -\frac{1}{\sigma\sqrt{2\pi}} \frac{d}{d\alpha} \int_{-\infty}^{\infty} e^{-\alpha x^2} dx \\ &= -\frac{1}{\sigma\sqrt{2\pi}} \frac{d}{d\alpha} \sqrt{\pi/\alpha} \\ &= \frac{1}{\sigma 2\sqrt{2}} \left(2\sigma^2\right)^{3/2} \\ &= \sigma^2.\end{aligned}$$

Therefore

$$\Delta x = \sigma.$$

A similar calculation for Δk yields

$$\Delta k = \frac{1}{\sigma},$$

therefore

$$\boxed{\Delta x \Delta k = 1}.$$