Homework 3 - Fourier Transform and Wave Function

Question 1:

Show that $a_n \sin\frac{\pi n x}{L}$ and $b_n \cos\frac{\pi n x}{L}$ form an orthogonal basis in the domain $[-L, L]$. Normalize the basis by finding the appropriate a_n and b_n.

Solution:

Taking the inner product for all combinations we find

$$\begin{aligned}
\left\langle a_m \sin\frac{\pi m x}{L},\, a_n \sin\frac{\pi n x}{L}\right\rangle &= \int_{-L}^{L} a_m^* \sin\frac{\pi m x}{L} a_n \sin\frac{\pi n x}{L} dx \\
&= a_m^* a_n \int_{-L}^{L} \frac{1}{2}\left[\cos\left(\frac{\pi x}{L}(m-n)\right) - \cos\left(\frac{\pi x}{L}(m+n)\right)\right] dx \\
\text{if } n \neq m \text{ then: } &= \frac{1}{2} a_m^* a_n \left[\frac{L}{\pi(m-n)}\sin\left(\frac{\pi x}{L}(m-n)\right) - \frac{L}{\pi(m+n)}\sin\left(\frac{\pi x}{L}(m+n)\right)\right]_{-L}^{L}
\end{aligned}$$

which leads to terms proportional to $\sin(\pi(m \pm n)) = 0$.

$$\begin{aligned}
\text{if } n = m \text{ then: } &= a_m^* a_n \int_{-L}^{L} \frac{1}{2}\left[1 - \cos\left(\frac{2\pi n x}{L}\right)\right] dx \\
&= a_m^* a_n \frac{1}{2}\left[x - \cancel{\frac{L}{2\pi n}\sin\left(\frac{2\pi n x}{L}\right)}\right]_{-L}^{L} \\
&= a_m^* a_n L,
\end{aligned}$$

thus the two are orthogonal,

$$\boxed{\left\langle a_m \sin\frac{\pi m x}{L},\, a_n \sin\frac{\pi n x}{L}\right\rangle = L a_m^* a_n \delta_{nm}} = L\left|a_n\right|^2.$$

Requiring orthonormality we find

$$\boxed{|a_n| = L^{-1/2}}.$$

Next is

$$\begin{aligned}
\left\langle b_m \cos\frac{\pi m x}{L},\, b_n \cos\frac{\pi n x}{L}\right\rangle &= \int_{-L}^{L} b_m^* \cos\frac{\pi m x}{L} b_n \cos\frac{\pi n x}{L} dx \\
&= b_m^* b_n \int_{-L}^{L} \frac{1}{2}\left[\cos\left(\frac{\pi x}{L}(m-n)\right) + \cos\left(\frac{\pi x}{L}(m+n)\right)\right] dx \\
\text{if } n \neq m \text{ then: } &= \frac{1}{2} b_m^* b_n \left[\frac{L}{\pi(m-n)}\sin\left(\frac{\pi x}{L}(m-n)\right) + \frac{L}{\pi(m+n)}\sin\left(\frac{\pi x}{L}(m+n)\right)\right]_{-L}^{L}
\end{aligned}$$

which leads to terms proportional to $\sin(\pi(m \pm n)) = 0$.

$$\begin{aligned}
\text{if } n = m \text{ then: } &= b_n^* b_n \int_{-L}^{L} \frac{1}{2}\left[1 + \cos\left(\frac{2\pi n x}{L}\right)\right] dx \\
&= \left|b_n\right|^2 \frac{1}{2}\left[x + \cancel{\frac{L}{2\pi n}\sin\left(\frac{2\pi n x}{L}\right)}\right]_{-L}^{L} \\
&= \left|b_n\right|^2 L,
\end{aligned}$$

thus the two are orthogonal,

$$\boxed{\left\langle b_m \cos\frac{\pi m x}{L}, b_n \cos\frac{\pi n x}{L}\right\rangle = L b_m^* b_n \delta_{nm}} = L\left|b_n\right|^2.$$

Requiring orthonormality we find

$$\boxed{|b_n| = L^{-1/2}}.$$

And last is the cross term

$$\begin{aligned}\left\langle a_m \sin\frac{\pi m x}{L}, b_n \cos\frac{\pi n x}{L}\right\rangle &= \int_{-L}^{L} a_m^* \sin\frac{\pi m x}{L} b_n \cos\frac{\pi n x}{L} dx \\ &= a_m^* b_n \int_{-L}^{L} \frac{1}{2}\left[\sin\left(\frac{\pi x}{L}(m+n)\right) + \sin\left(\frac{\pi x}{L}(m-n)\right)\right] dx = 0,\end{aligned}$$

where we used the fact that this is a symmetric integral over a sum of antisymmetric functions and thus it vanishes - indicating that the two sets are orthogonal.

Question 2:

Find the Fourier coefficients for the function $f(x) = 1$ in the domain $[-\pi, \pi]$.

Solution:

Expanding $f(x)$ into Fourier series we have

$$f(x) = \sum_n c_n e^{inx},$$

where

$$c_n = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} e^{-inx} dx.$$

If $n = 0$ we find

$$\boxed{c_0 = 1},$$

if $n \neq 0$ then,

$$\boxed{c_n = \frac{1}{in\sqrt{2\pi}}\left(e^{in\pi} - e^{-in\pi}\right) = \sqrt{2\pi}\frac{\sin \pi n}{\pi n} = 0 \quad \forall n \in \text{int}}.$$

Question 3:

Prove the following identities for the Dirac delta function:

1. Show that $\delta(x) = \frac{d\Theta(x)}{dx}$, where

$$\Theta(x) = \begin{cases} 1 & , \text{ for } 0 < x \\ 0 & , \text{ for } 0 \geq x \end{cases}$$

   is the Heaviside step function.

2. Show that

$$\int_{-\infty}^{\infty} \frac{d\delta(x - x_0)}{dx} f(x)\, dx = -\left.\frac{df(x)}{dx}\right|_{x=x_0} = -f'(x_0).$$

3. If $f(x_0) = 0$ and $f'(x_0) \neq 0$, then

$$\delta[f(x)] = \frac{\delta(x - x_0)}{|f'(x_0)|}.$$

Solution:

1. Taking the derivative of the Heaviside step function can be explicitly as the limit

$$\frac{d\Theta(x)}{dx} = \lim_{\varepsilon \to 0} \frac{\Theta(x+\varepsilon) - \Theta(x-\varepsilon)}{2\varepsilon},$$

plugging this expression into the generic integral over a function $f(x)$ we find

$$\begin{aligned}\int_{-\infty}^{\infty} f(x) \frac{d\Theta(x)}{dx} dx &= \lim_{\varepsilon \to 0} \int_{-\infty}^{\infty} f(x) \frac{\Theta(x+\varepsilon) - \Theta(x-\varepsilon)}{2\varepsilon} dx \\ &= \lim_{\varepsilon \to 0} \left[\int_{-\varepsilon}^{\infty} \frac{f(x)}{2\varepsilon} dx - \int_{\varepsilon}^{\infty} \frac{f(x)}{2\varepsilon} dx \right] \\ &= \lim_{\varepsilon \to 0} \int_{-\varepsilon}^{\varepsilon} \frac{f(x)}{2\varepsilon} dx,\end{aligned}$$

since $\int_{-\varepsilon}^{\varepsilon} f(x)\,dx = 2\varepsilon f(0)$, on an infinitesimal interval (i.e. the value of the function times the interval), we get

$$\boxed{\int_{-\infty}^{\infty} f(x) \frac{d\Theta(x)}{dx} dx = f(0)},$$

proving that $d\Theta(x)/dx$ operates just as $\delta(x)$ does.

2. Starting from the left side

$$\begin{aligned}\int_{-\infty}^{\infty} \frac{d\delta(x-x_0)}{dx} f(x)\,dx &= \int_{-\infty}^{\infty} \frac{d}{dx}\left[\delta(x-x_0) f(x)\right] dx - \int_{-\infty}^{\infty} \delta(x-x_0) \frac{df(x)}{dx} dx \\ &= \cancel{\left[\delta(x-x_0) f(x)\right]_{-\infty}^{\infty}} - \left.\frac{df(x)}{dx}\right|_{x=x_0},\end{aligned}$$

where we used integration by parts and the fact that $\delta(x-x_0)$ vanishes anywhere but at $x = x_0$, for the boundary term, and the definition of $\delta(x-x_0)$ for the second integral term, which yields

$$\boxed{\int_{-\infty}^{\infty} \frac{d\delta(x-x_0)}{dx} f(x)\,dx = -\left.\frac{df(x)}{dx}\right|_{x=x_0} = -f'(x_0)}.$$

3. Rearranging the equation into

$$|f'(x_0)|\,\delta[f(x)] = \delta(x-x_0),$$

and defining $y = f(x)$ or $x = f^{-1}(y)$, hence $f(x_0) \equiv y_0 = 0$ or $f^{-1}(0) = x_0$, we have

$$dy = f'(x)\,dx \quad \to \quad dx = \frac{dy}{|f'[f^{-1}(y)]|}.$$

Now let us show that the left hand side of the equation above operates as $\delta(x-x_0)$ on some function $g(x)$,

$$\begin{aligned}\int_{-\infty}^{\infty} |f'(x_0)|\,\delta[f(x)]\,g(x)\,dx &= |f'(x_0)| \int_{-\infty}^{\infty} \delta(y)\,g\left(f^{-1}(y)\right) \frac{dy}{|f'[f^{-1}(y)]|} \\ &= |f'(x_0)| \frac{g\left(f^{-1}(0)\right)}{|f'[f^{-1}(0)]|} \\ &= |f'(x_0)| \frac{g(x_0)}{|f'(x_0)|} \\ &= g(x_0).\end{aligned}$$

This proves that

$$\boxed{|f'(x_0)|\,\delta[f(x)] = \delta(x-x_0)}.$$

Question 4:

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 5:

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

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

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

$$\begin{aligned}\tilde{\psi}(k)&=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}Ae^{-\frac{x^2}{4\sigma^2}+ik_0x}e^{-ikx}dx\\&=\frac{1}{\sqrt{\sigma}(2\pi)^{3/4}}\int_{-\infty}^{\infty}e^{-\frac{1}{4\sigma^2}\left(x^2-4\sigma^2i(k_0-k)x\right)}dx\\&=\frac{e^{-\sigma^2(k_0-k)^2}}{\sqrt{\sigma}(2\pi)^{3/4}}\int_{-\infty}^{\infty}e^{-\frac{1}{4\sigma^2}\left(x^2-2\sigma^2i(k_0-k)\right)^2}dx\end{aligned}$$

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

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

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

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

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

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

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

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

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

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

Similarly, we have

$$\left\langle p^2\right\rangle = \frac{\hbar^2}{4\sigma^2} + \hbar k_0,$$

since we expect

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

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

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

satisfies $x_{\max} = \langle x(t)\rangle$, while the conclusion from our results for $\langle x(t)\rangle$ and v_g imply that $\langle x(t)\rangle = v_g t$. 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,

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

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

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

Question 6:

Show that for the internal product

$$\langle \Psi_1, \Psi_2 \rangle = \int_\Omega \Psi_1^* \Psi_2 d\alpha\left(x\right),$$

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:

- $\langle \Psi_1, \Psi_2 \rangle = \langle \Psi_2, \Psi_1 \rangle^*$
- $\langle c\Psi_1, \Psi_2 \rangle = c^* \langle \Psi_1, \Psi_2 \rangle$
- $\langle \Psi_1, c\Psi_2 \rangle = c \langle \Psi_1, \Psi_2 \rangle$
- $\langle \Psi_1 + \Psi_2, \Psi_3 \rangle = \langle \Psi_1, \Psi_3 \rangle + \langle \Psi_2, \Psi_3 \rangle$

Solution:

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

Bonus

Question 7:

Derive the Fourier series for the function $f\left(x\right) = x^2$ in the domain $[-\pi, \pi]$. Use this to prove that

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}.$$

Solution:

Expanding $f\left(x\right)$ into Fourier series we have

$$f\left(x\right) = \frac{1}{\sqrt{2\pi}} \sum_n c_n e^{inx},$$

where

$$c_n = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} x^2 e^{-inx} dx.$$

If $n = 0$ we find

$$c_0 = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} x^2 dx = \sqrt{2\pi}\frac{\pi^2}{3},$$

if $n \neq 0$ then,

$$\begin{aligned}
c_n &= -\frac{1}{\sqrt{2\pi}}\frac{d^2}{dn^2}\int_{-\pi}^{\pi} e^{-inx}dx \\
&= \frac{1}{\sqrt{2\pi}}\frac{d^2}{dn^2}\left[\frac{1}{in}\left(e^{-in\pi}-e^{in\pi}\right)\right] \\
&= \frac{1}{\sqrt{2\pi}}\frac{d}{dn}\left[\frac{1}{in^2}\left(e^{in\pi}-e^{-in\pi}\right)-\frac{\pi}{n}\left(e^{in\pi}+e^{-in\pi}\right)\right] \\
&= \frac{1}{\sqrt{2\pi}}\frac{d}{dn}\left[\frac{2}{n^2}\sin(n\pi)-\frac{2\pi}{n}\cos(n\pi)\right] \\
&= \sqrt{\frac{2}{\pi}}\left[\left(\frac{\pi^2}{n}-\frac{2}{n^3}\right)\cancel{\sin(n\pi)}+\frac{2\pi}{n^2}\underbrace{\cos(n\pi)}_{(-1)^n}\right] \\
&= \frac{2\sqrt{2\pi}}{n^2}(-1)^n .
\end{aligned}$$

Therefore, the Fourier series is

$$\begin{aligned}
f(x) &= \frac{1}{\sqrt{2\pi}}\sum_n c_n e^{inx} \\
&= \frac{\pi^2}{3}+\sum_{n\neq 0}\frac{2}{n^2}(-1)^n e^{inx} \\
&= \frac{\pi^2}{3}+\sum_{n=1}^{\infty}\frac{2}{n^2}(-1)^n\left(e^{inx}+e^{-inx}\right),
\end{aligned}$$

or simply

$$\boxed{f(x)=\frac{\pi^2}{3}+\sum_{n=1}^{\infty}\frac{4}{n^2}(-1)^n\cos(nx)}.$$

Now let us take its value at $x=\pi$,

$$\pi^2=\frac{\pi^2}{3}+\sum_{n=1}^{\infty}\frac{4}{n^2}(-1)^n\underbrace{\cos(n\pi)}_{(-1)^n}=\frac{\pi^2}{3}+\sum_{n=1}^{\infty}\frac{4}{n^2}\quad\rightarrow\quad\boxed{\frac{\pi^2}{6}=\sum_{n=1}^{\infty}\frac{1}{n^2}}.$$

Question 8:

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

$$\begin{aligned}
\tilde{g}(k) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(x)e^{-ikx}dx \\
&= \frac{1}{\sqrt{2\pi}}\frac{1}{\sigma\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-\frac{x^2}{2\sigma^2}}e^{-ikx}dx.
\end{aligned}$$

Looking at the power of the exponent we can write

$$-\frac{1}{2\sigma^2}\left(x^2+2i\sigma^2kx\right)=-\frac{1}{2\sigma^2}\left(x^2+2i\sigma^2kx-\sigma^4k^2\right)-\frac{\sigma^2k^2}{2},$$

which leads to

$$\tilde{g}(k)=\frac{e^{-\sigma^2k^2/2}}{2\pi\sigma}\underbrace{\int_{-\infty}^{\infty}e^{-\frac{u^2}{2\sigma^2}}du}_{I},$$

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

$$I^2 = \int_0^{2\pi} \int_0^{\infty} e^{-\frac{r^2}{2\sigma^2}} rdrd\varphi = \pi \int_0^{\infty} e^{-\frac{\xi}{2\sigma^2}} d\xi = 2\pi\sigma^2,$$

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.

$$\left\langle x^2 \right\rangle = \int_{-\infty}^{\infty} x^2 \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{x^2}{2\sigma^2}} dx$$

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

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

Question 9:

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

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

hence

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