The Fourier Transform and wave-packets

The objective of this class is to get you familiar with the tools needed to describe the wave-function of simple systems with a single particle. The main tool that we will use is the Fourier Transform.

Course Book Chapters: Chapter 2 and annex B

Additional material: A very detailed introductory discussion of this material is also present in the Cohen-Tannouji Chapter 1 (and complements A_3 and A_4).

1 Prerequisites

1.1 The space of $p-$integrable functions $L^p(S)$

We wish to give a formal definition of the space containing all possible wave-functions. We have already discussed that physical wave-functions are those that have a bounded integral over the whole space such that we can interpret their square value as a probability density, and the two definitions you find below are simply a formal way to impose such condition.

Given a complex function

$$f : \mathcal{S} \to \mathbb{C}$$

the Lebesgue-p norm of the function, $\|f\|_p$ is

$$\|f\|_p = \left(\int_S |f(\mu)|^p d\mu \right)^{\frac{1}{p}}. \tag{1}$$

Note: we are usually interested in the $2-$norm, as it is what allows us to normalize a wave-function to have a valid probability density. We adopt the standard convention of taking $\|f\| \equiv \|f\|_2$, and only denoting non L^2 norms.

We define $L^p(S)$ to be the space of functions with a bounded $p-$norm

$$L^p := \{ f : S \to \mathcal{C} \;\mid\; \|f\|_p < \infty \} \tag{2}$$

$$= \left\{ f : S \to \mathcal{C} \;\mid\; \left(\int_S |f(\mu)|^p d\mu \right)^{\frac{1}{p}} < \infty \right\} \tag{3}$$

Note: While this definition is general, we are generally interested in $L^2(\mathbb{R})$ spaces as they will be those of wave-functions with a bounded integral over the real axis and can therefore represent a particle in 1-Dimensional space, or $L^2(\mathbb{R}^3)$ for a particle in the physical 3-Dimensional space.

1.2 The wave-function

The state of a particle in a 1-Dimensional space $\mathbb{R}$ is encoded into the time-dependent wave-function $\psi(x,t)$. If we attempt to measure the position of the particle, the probability density to measure it at the point x at time t is $p(x,t) = |\psi(x,t)|^2$.

Requiring that this probability density be physical, we ask that at every time t the wave-function be $\psi \in L^2(\mathbb{R})$, that means have a bounded integral over the whole space x, namely

$$\int_{\mathbb{R}} |\psi(x,t)|^2 dx < \infty$$

The space $L^2(\mathbb{R})$ is called the space of *square-integrable functions over* $\mathbb{R}$. *In the lecture number 5 we will discuss the fact that this space is a particular kind of vector space, an Hilbert space. For that reason, physicists often call the space of wave-functions the Hilbert space.*

1.3 Plane waves

The *matter wave* (or, wavefunction) of a particle with momentum p and energy ω propagating in the *free space* is:

$$\psi_p(x,t) = \exp\left[i(\frac{p}{\hbar}x - \omega_p t)\right] \tag{4}$$

It is easy to show (can you?) that this function is not square-integrable so it's not a valid *wave-function*.

1.4 The Fourier Transform

The Fourier transform $\mathcal{F}$ is a *function map* that associates functions in $L^2(\mathbb{R})$ to functions in $L^2(\mathbb{R})$. More formally,

$$\begin{aligned} \mathcal{F} : L^2(\mathbb{R}) &\to L^2(\mathbb{R}) \\ \psi &\to \varphi = \mathcal{F}(\psi) \end{aligned}$$

where the fourier transform φ of ψ is defined as

$$\varphi(p) = (\mathcal{F}(\psi))(p) \equiv \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \psi(x) e^{-ipx/\hbar} dx. \tag{5}$$

We can also define the *inverse-Fourier transform* to be a function map from $L^2(\mathbb{R})$ into $L^2(\mathbb{R})$, defined as:

$$\begin{aligned} \mathcal{F}^{-1} : L^2(\mathbb{R}) &\to L^2(\mathbb{R}) \\ \mathcal{F}(\psi) &\to \psi \end{aligned}$$

and the functional definition will follow to be:

$$\psi(x) = (\mathcal{F}^{-1}(\varphi))(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \varphi(p) e^{ipx/\hbar} dp. \tag{6}$$

Note: the choice for p as the dependent variable for th transform is completely arbitray, we could also have called it x' or anything else. But with this particular definition p has the dimensions of a momentum, and therefore we pick p. The motivation will become evident later on.

We can verify the following relationships (using the definition $\varphi = \mathcal{F}(\psi)$)

- Linearity : $\mathcal{F}(\lambda\psi_1 + \mu\psi_2) = \lambda\mathcal{F}(\psi_1) + \mu\mathcal{F}(\psi_2)$
- Translation :

$$\mathcal{F}\left(\psi(x - x_0)\right)(p) = \varphi(p) e^{-ipx_0/\hbar} \tag{7}$$

$$\mathcal{F}^{-1}\left(\varphi\right)(p - p_0) = \psi(x) e^{ip_0 x/\hbar} \tag{8}$$

- Dilation: $\mathcal{F}(\psi)(ax) = \frac{1}{|a|}\varphi(p/a)$ with $a \neq 0$
- Conjugation : $\mathcal{F}(\psi^\star)(x) = \varphi^\star(-p)$
- Parseval-Plancherel Relation :

$$\int_{-\infty}^{+\infty} \psi_1^\star(x)\psi_2(x) dx = \int_{-\infty}^{+\infty} \varphi_1^\star(p)\varphi_2(p) dp \tag{9}$$

The Fourier transform therefore preserves the Hermitian inner product: it is an isometry.

- Differentiation :

$$\mathcal{F}\left(\frac{d^n\psi}{dx^n}\right) = \left(\frac{ip}{\hbar}\right)^n \varphi(p) \tag{10}$$

$$\mathcal{F}^{-1}\left(\frac{d^n\varphi}{dp^n}\right) = \left(\frac{-ix}{\hbar}\right)^n \psi(x) \tag{11}$$

Note: the fourier transform is well-defined for arbitrary functions $\psi \in C^\alpha(\mathbb{R})$, not necessarily continuous at all orders or square integrable. However, in that case the Fourier transform is not an endomorphism and the image space can be much more complicated. A good example is the Fourier transform of a plane wave, which is a dirac-delta, a functional in the space of distributions, which you will study in some later course next year.

2 Excercises

2.1 Excercise 1: Properties of the Fourier Transform

Using the definitions of the Fourier transform given above, prove the following properties:

Q1 **Translation:** if $\tilde{\psi}(x) = \psi(x - x_0)$ then $\mathcal{F}(\tilde{\psi})(p) = e^{-i\frac{p}{\hbar}x_0}\mathcal{F}(\psi)(p)$

Applying the definitions, we have

$$\tilde{\varphi}(p) = \mathcal{F}(\tilde{\psi})(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}\tilde{\psi}(x)e^{-ipx/\hbar}dx.$$

and substituting the definition of $\tilde{\psi}(x)$ into that we obtain

$$\tilde{\varphi}(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}\psi(x - x_0)e^{-ipx/\hbar}dx$$

and performing the change of variables $\tilde{x} = x - x_0$ we get:

$$\begin{aligned}\tilde{\varphi}(p) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}\psi(\tilde{x})e^{-ip\tilde{x}/\hbar}e^{-ipx_0/\hbar}dx \\ &= \frac{e^{-ipx_0/\hbar}}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty}\psi(\tilde{x})e^{-ip\tilde{x}/\hbar}d\tilde{x} \\ &= e^{-ipx_0/\hbar}\varphi(p)\end{aligned}$$

which proves the translation property.

Q2 **Dilation:** if $\tilde{\psi}(x) = \psi(ax)$ then $\mathcal{F}(\tilde{\psi})(p) = \frac{1}{|a|}\mathcal{F}(\psi)(\frac{p}{a})$

Given that $\tilde{\psi}(x) = \psi(ax)$, let's find the Fourier transform $\mathcal{F}(\tilde{\psi})(p)$. Recall the definition of the Fourier transform:

$$\mathcal{F}(\tilde{\psi})(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\tilde{\psi}(x)e^{-i\frac{p}{\hbar}x}dx. \tag{12}$$

Now substitute $\tilde{\psi}(x)$ with $\psi(ax)$:

$$\mathcal{F}(\tilde{\psi})(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi(ax)e^{-i\frac{p}{\hbar}x}dx. \tag{13}$$

Perform a change of variables with $u = ax$, which implies $x = \frac{u}{a}$ and $dx = \frac{1}{|a|}du$:

$$\begin{aligned}\mathcal{F}(\tilde{\psi})(p) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi(u)e^{-i\frac{p}{\hbar}\frac{u}{a}}\frac{du}{|a|} &(14)\\ &= \frac{1}{|a|\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi(u)e^{-i\frac{p}{a\hbar}u}du &(15)\\ &= \frac{1}{|a|}\mathcal{F}(\psi)(\frac{p}{a}) = \frac{1}{|a|}\varphi(\frac{p}{a}) &(16)\end{aligned}$$

which proves the dilation property.

Appearance of the Modulus of a:
During the proof of the dilation property, we performed a change of variables with $u = ax$. The Jacobian determinant of this transformation is given by:

$$J = \frac{du}{dx} = a. \tag{17}$$

When changing variables in an integral, we must take into account the absolute value of the Jacobian determinant:

$$dx = \frac{1}{|a|} du. \tag{18}$$

The modulus of a appears in the result because it is the absolute value of the Jacobian determinant, which determines how the integral scales under the change of variables. This scaling factor ensures that the integral remains invariant under transformations that change the direction of the axis (i.e., when a is negative).

Q3 **Differentiation** prove that

$$\mathcal{F}\left(\frac{d^n\psi}{dx^n}\right)(p) = \left(\frac{ip}{\hbar}\right)^n \varphi(p) \tag{19}$$

$$\mathcal{F}^{-1}\left(\frac{d^n\varphi}{dp^n}\right)(x) = \left(\frac{-ix}{\hbar}\right)^n \psi(x) \tag{20}$$

Applying the definition of the fourier transform

$$\mathcal{F}\left(\frac{d^n\psi}{dx^n}\right)(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \frac{d^n\psi}{dx^n} e^{-i\frac{p}{\hbar}x} dx.$$

Integrate by parts once, you obtain

$$\mathcal{F}\left(\frac{d^n\psi}{dx^n}\right)(p) = \frac{1}{\sqrt{2\pi\hbar}} \left[\left(\frac{d^{n-1}\psi(x)}{dx^{n-1}} e^{-i\frac{p}{\hbar}x}\right|_{\infty}^{\infty} - \frac{1}{\sqrt{2\pi\hbar}} \left(-i\frac{p}{\hbar}\right) \int_{-\infty}^{\infty} \frac{d^{n-1}\psi}{dx^{n-1}} e^{-i\frac{p}{\hbar}x} dx$$

we notice that the first term must be zero assuming that the wave-function is well behaved at $x \to \pm\infty$ and goes to zero with its derivatives faster than any other polynomial (it's a function from the Schwartz space). Then

$$\mathcal{F}\left(\frac{d^n\psi}{dx^n}\right)(p) = \left(-i\frac{p}{\hbar}\right) \mathcal{F}\left(\frac{d^{n-1}\psi}{dx^{n-1}}\right)(p)$$

and therefore by applying this recurrent relation n times we find that

$$\begin{aligned}\mathcal{F}\left(\frac{d^n\psi}{dx^n}\right)(p) &= \left(\frac{ip}{\hbar}\right)^n \mathcal{F}[\psi](p) \\ &= \left(\frac{ip}{\hbar}\right)^n \varphi(p).\end{aligned}$$

We leave the other proof as an unproven excercise.

Q4 **Conjugation** prove that

$$\mathcal{F}\left(\psi^{\star}\right)(p)=\varphi^{\star}(-p)$$

Starting (again) from the definition, we find

$$\begin{aligned}\mathcal{F}\left(\psi^{\star}\right)(p) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi^{\star}(x)e^{-i\frac{p}{\hbar}x}dx \\ &= \left(\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi^{(}x)e^{i\frac{p}{\hbar}x}dx\right)^{\star} \\ &= \left(\mathcal{F}[\psi](-p)\right)^{\star} \\ &= \varphi^{\star}(-p)\end{aligned}$$

Q5 Use the previous properties to prove the **Parseval-Plancherel** formula.

We want to prove that

$$\int_{-\infty}^{+\infty}\psi_1^{\star}(x)\psi_2(x)dx=\int_{-\infty}^{+\infty}\varphi_1^{\star}(p)\varphi_2(p)dp$$

where $\psi_1(x)$ and $\psi_2(x)$ are two functions with Fourier transforms $\varphi_1(p)$ and $\varphi_2(p)$, respectively. To prove this theorem, let's start with the left hand side, and substitute the fourier transform of ψ_2:

$$\int_{-\infty}^{\infty}\psi_1^{*}(x)\left(\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\varphi_2(p)e^{i\frac{p}{\hbar}x}dp\right)dx.$$

We can switch the order of the two integrals:

$$\begin{aligned}&=\int_{-\infty}^{\infty}\varphi_2(p)\left(\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi_1^{*}(x)e^{i\frac{p}{\hbar}x}dx\right)dp \\ &=\int_{-\infty}^{\infty}\varphi_2(p)\left(\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi_1(x)e^{-i\frac{p}{\hbar}x}dx\right)^{\star}dp.\end{aligned}$$

Now, recognize that the inner integral is the Fourier transform of $\psi_1(x)$:

$$\int_{-\infty}^{\infty}\varphi_2(p)\varphi_1^{*}(p)dp.$$

which proves the theorem

2.2 Excercise 2: Plane-wave decomposition

Consider Schroedinger's Equation

$$i\hbar\nabla_t\psi(x,t) = -\frac{\hbar^2}{2m}\nabla_x^2\psi(x,t); \tag{21}$$

last week you have seen that it is solved by the *plane wave*

$$\psi_p(x,t) = e^{i\frac{p}{\hbar}x-\omega_p t} \qquad \text{where} \qquad \omega_p = \frac{\hbar p^2}{2m} \tag{22}$$

and according to the De-Broglie relationship $E(p) = \frac{\omega_p}{\hbar}$ we get that $E(p) = \frac{p^2}{2m}$ as we expect from classical mechanics.

Q1 Is a plane-wave a valid wave-function to describe a particle in 1 dimension? (think about the probability to detect the particle...)

No, because it's norm is infinite.

We will now look at a more general expression of a wave-function that is physical and can be interpreted as describing the state of a particle. Consider a wave-function $\psi(x,t)$ obtained by the inverse Fourier-Transform of $\varphi(p,t)$, namely

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{\mathbb{R}}\varphi(p,t)e^{i\frac{p}{\hbar}x}dp \tag{23}$$

Q2 Derive the differential equation that $\varphi(p,t)$ must respect assuming that Schroedinger's equation must be respected.

Let's compute the Fourier transform of both sides of the Schroedinger's equation:

$$i\hbar\mathcal{F}\left[\frac{d}{dt}\psi\right](p,t) = -\frac{\hbar^2}{2m}\mathcal{F}\left[\nabla_x^2\psi\right](p,t),$$

as the derivative in time acts on a different free variable than the Fourier Transform on x, we can simply replace $\mathcal{F}\left[\nabla_t\psi\right](p,t)$ with $\nabla_t\varphi(p,t)$. For the right hand side, instead, we use the properties demonstrated earlier and we obtain

$$\begin{aligned} i\hbar\frac{d}{dt}\varphi(p,t) &= -\frac{\hbar^2}{2m}\left(i\frac{p}{\hbar}\right)^2\varphi(p,t) \\ &= \frac{p^2}{2m}\varphi(p,t) \end{aligned}$$

And this differential equation is solved by integration by parts, as doing

$$i\hbar\frac{d\varphi(p,t)}{\varphi(p,t)} = \frac{p^2}{2m}dt$$

and integrating

$$i\hbar\int_{\varphi(p,0)}^{\varphi(p,t)}\frac{d\varphi(p,t)}{\varphi(p,t)}=\frac{p^2}{2m}\int_0^t dt$$

leads to

$$i\hbar(\log\varphi(p,t)-\log\varphi(p,0)=\frac{p^2}{2m}t$$

and by taking the exponential of both sides we get

$$\varphi(p,t)=\varphi(p,0)\exp\left[-\frac{i}{\hbar}\frac{p^2}{2m}t\right]=\varphi(p,0)\exp\left[-i\frac{E(p)}{\hbar}t\right]$$

The point above can be solved by substituting eq. (23) into eq. (21) and Fourier transforming both the right and left hand side of the resulting equation. You will obtain a new differential equation where on the left hand side you have a ∇_t but on the right hand side you no longer have ∇_x.

Q3 Considering the differential equation you obtained at the previous question, verify that

$$\varphi(p,t)=\varphi(p,0)e^{-i\frac{E(p)}{\hbar}t} \tag{24}$$

using the definition of the energy coming from the De-Broglie relationship.

The proof is trivial by inserting the definition in the differential equation. Moreover, above we found the solution analytically which also proves this point. We simply used $E(p)=\frac{p^2}{2m}$ which is the kinetic energy of a free particle.

Q4 Assuming the definition of the wave-function (eq. (23)) and the expression of its Fourier transform that we just derived (eq. (24)), derive an expression for $\psi(x,t)$. Once you did that, can you relate the expression you found to plane waves and give an intuitive understanding of what is that you have obtained?

By using the definition of the fourier transform

$$\psi(x,t)=\frac{1}{\sqrt{2\pi\hbar}}\int_{\mathbb{R}}\varphi(p,t)e^{i\frac{p}{\hbar}x}dp$$

and substituting eq. (24) we get

$$\psi(x,t)=\frac{1}{\sqrt{2\pi\hbar}}\int_{\mathbb{R}}\varphi(p,0)e^{-i(\frac{E(p)}{\hbar}t-\frac{p}{\hbar}x)}dp$$

which is a linear combination of plane waves with amplitudes $\varphi(p,0)$.

In few words, up to this point you should have understood that we have *decomposed the wavefunction into a (continuous) sum of plane waves.*

Q5 Assuming that the wave-function is correctly normalised, meaning that

$$\|\psi\|_2^2 = \int_{\mathbb{R}} |\psi(x,t)|^2 dx = 1$$

can you use the properties of the Fourier Transform to prove that the same normalisation applies to $\|\varphi\|$? Can you use this to interpret what $\varphi(p,t)$ is, and its relationship to $\psi(x,t)$?

$\|\psi\|_2^2 = \|\varphi\|_2^2$ follows trivially from the Parcel Plancherel theorem. This means that the Fourier Transform is an isometry for the wave-functions, and therefore it simply represents a change of basis.

You should have understood by now that a single plane wave is not a valid wave-function as it is not $L^2(\mathbb{R})$. However, it is possible to show that a superposition of plane waves can be a valid wave-function thanks to intereference, and the amplitudes for every plane waves of momentum p are given by the fourier transform.

Q6 *To conclude, we will try to derive a connection between Classical Mechanics and Quantum Mechanics (for the curious, we will be looking at a special case of the Ehrenfest Theorem).* Assuming only the Schroedinger's Equation eq. (21), prove that

$$\frac{d\langle x\rangle}{dt} = \frac{\langle p\rangle}{m}. \tag{25}$$

Is there a similar equation in classical mechanics?

We will consider a more general version of the Schroedinger's Equation where we also account for an external potential, namely,

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t).$$

you can simply put $V(x) = 0$ to find again the equation we worked with until now.

To compute the time derivative of $\langle x\rangle$, start with its definition:

$$\langle x\rangle = \int_{-\infty}^{\infty} \psi^*(x,t)x\psi(x,t)dx.$$

Take the time derivative:

$$\frac{d\langle x\rangle}{dt} = \int_{-\infty}^{\infty}\left(\frac{\partial\psi^*}{\partial t}x\psi + \psi^* x\frac{\partial\psi}{\partial t}\right)dx.$$

Now, substitute the time derivatives from Schrödinger's equation and its complex conjugate:

$$\frac{d\langle x\rangle}{dt} = \frac{i}{\hbar}\int_{-\infty}^{\infty}\left(\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2} + V\psi^*\right)x\psi - \psi^* x\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi\right)\right)dx.$$

where the opposite sign between the two terms arises from the conjugation of i and we have assumed that the potential is real valued so $V^\star(x) = V(x)$. It is easy to see that the potential terms cancel out, and we are left with

$$\begin{aligned}\frac{d\langle x\rangle}{dt} &= \frac{i}{\hbar}\int_{-\infty}^{\infty}\left(\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2}\right)x\psi - \psi^* x\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}\right)\right)dx \\ &= -\frac{i\hbar}{2m}\int_{-\infty}^{\infty}\left(\left(\frac{\partial^2\psi^*}{\partial x^2}\right)x\psi - \psi^* x\left(\frac{\partial^2\psi}{\partial x^2}\right)\right)dx\end{aligned}$$

Integrate the remaining terms by parts:

$$\begin{aligned}\int_{-\infty}^{\infty}\left(\frac{\partial^2\psi^*}{\partial x^2}\right)x\psi &= \left[\frac{\partial\psi^*(x)}{\partial x}x\psi(x)\right|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\left(\frac{\partial\psi^\star(x)}{\partial x}\right)\left(\psi(x) + x\frac{\partial\psi(x)}{\partial x}\right)dx \\ &= -\int_{-\infty}^{\infty}\left(\frac{\partial\psi^\star(x)}{\partial x}\right)\psi(x)dx - \int_{-\infty}^{\infty}\left|\frac{\partial\psi^\star(x)}{\partial x}\right|^2 x dx\end{aligned}$$

where we have used in the second line the fact that the wavefunction and its derivatives go to zero at infinity. Substituting back into the original equation we get

$$\begin{aligned}\frac{d\langle x\rangle}{dt} = -\frac{i\hbar}{2m}&\left(-\int_{-\infty}^{\infty}\left(\frac{\partial\psi^\star(x)}{\partial x}\right)\psi(x)dx - \int_{-\infty}^{\infty}\left|\frac{\partial\psi^\star(x)}{\partial x}\right|^2 x dx\right) + \\ &\frac{i\hbar}{2m}\left(-\int_{-\infty}^{\infty}\left(\frac{\partial\psi^\star(x)}{\partial x}\right)\psi(x)dx - \int_{-\infty}^{\infty}\left|\frac{\partial\psi^\star(x)}{\partial x}\right|^2 x dx\right)\end{aligned}$$

and i can rewrite it as:

$$\begin{aligned}\frac{d\langle x\rangle}{dt} = \frac{i\hbar}{2m}&\left(\int_{-\infty}^{\infty}\left(\frac{\partial\psi^\star(x)}{\partial x}\right)\psi(x)dx - \int_{-\infty}^{\infty}\psi^\star(x)\left(\frac{\partial\psi(x)}{\partial x}\right)dx\right) + \\ &\frac{i\hbar}{2m}\left(\int_{-\infty}^{\infty}\left|\frac{\partial\psi^\star(x)}{\partial x}\right|^2 x dx - \int_{-\infty}^{\infty}\left|\frac{\partial\psi^\star(x)}{\partial x}\right|^2 x dx\right)\end{aligned}$$

and the last term is 0, while the first term can be manipulated by using the Parcel Plancherel theorem obtaining

$$\frac{d\langle x\rangle}{dt} = \frac{1}{m}\int_{-\infty}^{\infty}\varphi^\star(p)p\varphi(p) = \frac{\langle p\rangle}{m}$$

2.3 Excercise 3: Gaussian wave packet

The initial state at $t = 0$ of our wave-function $\psi(x,t)$ satisfies the differential equation (where we assume that $\psi(x) = \psi(x, t = 0)$ and that where $\sigma_x \in \mathbb{R}, \sigma_x > 0$

$$\frac{d\psi}{dx}(x) = -\frac{x}{2\sigma_x^2}\psi(x) \tag{26}$$

Q1 Solve the differential equation and determine $\psi(x)$ up to a costant value ψ_0

We use the separation of variables to get the differential equation

$$\int_{\psi_0}^{\psi(x)} \frac{d\psi(x)}{\psi(x)} = -\frac{1}{2\sigma_x^2}\int_0^x x dx$$

which leads to

$$\log\psi(x) - \log\psi_0 = -\frac{x^2}{4\sigma_x^2}$$

and following an exponentiation we get

$$\psi(x) = \psi_0 \exp\left[-\frac{x^2}{4\sigma_x^2}\right]$$

Q2 What should be the constant value ψ_0 to ensure that the wave-function is physical and can be interpreted as the state of a particle?

We need to compute

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = |\psi_0|^2 \int_{-\infty}^{\infty} \exp\left[-\frac{x^2}{2\sigma_x^2}\right]$$
$$= |\psi_0|^2 \sqrt{2\pi}\sigma_x$$

therefore to get a proper normalization we must impose

$$|\psi_0| = \left(\sqrt{2\pi}\sigma_x\right)^{-1/2}$$

In the following, consider

$$\psi(x) = (\sqrt{2\pi}\sigma_x)^{-\frac{1}{2}} \exp\left[\frac{x^2}{-4\sigma_x^2}\right] \tag{27}$$

where $\sigma_x \in \mathbb{R}, \sigma_x > 0$

Q3 What is the average position of the particle $\langle x\rangle$ and the variance of the position Δx at $t = 0$?

We computed those quantities for the gaussian in PC1. We have $\langle x\rangle = 0$ and $(\Delta x)^2 = \sigma_x^2$

Q4 Find the expression for the Fourier Transform of the wave-function at $t = 0$, $\varphi(p) = \mathcal{F}(\psi)(p)$, using the definition $\sigma_p = \hbar/2\sigma_x$. (Note: You can brute force the integral, but this will not be very simple with your current knowledge of math tricks. What follows are a few hints for a simpler derivation.)

- Take the derivatives $\frac{d}{dx}$ of both sides of eq. (27), and write an expression in the form of $\frac{d\psi(x)}{dx} = f(x, \psi(x))$
- Replace the occurences of $\psi(x)$ with some functions of $\varphi(p)$ by using the two Differentiation relations of the Fourier transform and anti-transform.
- use the definition $\sigma_p = \hbar/2\sigma_x$
- you should get a differential equation for $d\varphi(p)/dp \propto p\varphi(p)$. You recently solved a very similar equation. Can you use that to say what is the shape of the solution to this differential equation?

We start from the differential equation satisfied by the gaussian, namely eq. (26) (which is what you obtain from the first step of the hints) then, we Fourier transform both sides of the ODE,

$$\mathcal{F}\left[\frac{d\psi}{dx}\right](p) = -\frac{1}{2\sigma_x^2}\mathcal{F}\left[x\psi(x)\right] \tag{28}$$

$\mathcal{F}\left[\frac{d\psi}{dx}\right](p) = i\frac{p}{\hbar}\varphi(p)$ because of the properties we already derived. We now try to find an expression for $\mathcal{F}\left[x\psi(x)\right](p)$. We start from eq. (11), namely

$$\mathcal{F}^{-1}\left(\frac{d^n\varphi}{dp^n}\right) = \left(\frac{-ix}{\hbar}\right)^n \psi$$

and we invert it to obtain

$$x\psi = i\hbar\mathcal{F}^{-1}\left[\frac{d\varphi}{dp}\right].$$

Substituting this into $\mathcal{F}\left[x\psi(x)\right]$ we get

$$\begin{aligned}\mathcal{F}\left[x\psi(x)\right](p) &= i\hbar\mathcal{F}\left[\mathcal{F}^{-1}\left[\frac{d\varphi}{dp}\right]\right](p)\\ &= i\hbar\frac{d\varphi}{dp}(p).\end{aligned}$$

And by substituting everything back into the eq. (28) we obtain

$$i\frac{p}{\hbar}\varphi(p) = -\frac{1}{2\sigma_x^2}i\hbar\frac{d\varphi}{dp}(p)$$

and after some manipulation

$$\frac{d\varphi}{dp}(p) = -\frac{p}{2}\frac{4\sigma_x^2}{\hbar^2}\varphi(p)$$

and defining $\sigma_p = \hbar/2\sigma_x$

$$\frac{d\varphi}{dp}(p) = -\frac{p}{2\sigma_p^2}\varphi(p).$$

This equation has the same form as the eq. (26), with the only exception that $\psi(x) \to \varphi(p)$, $\sigma_x \to \sigma_p$. Therefore its solution is also a gaussian, and we can interpret this as the fact that the Fouerier Transform of a gaussian is a gaussian with a related variance.

Q5 We multiply the state $\psi(x)$ of eq. (27) by $\exp\left[i\frac{p_0}{\hbar}x\right]$. Considering the new state

$$\tilde{\psi}(x) = \psi(x)\exp\left[i\frac{p_0}{\hbar}x\right] \tag{29}$$

what is its Fourier transform $\tilde{\varphi}(p) = \mathcal{F}(\tilde{\psi})(p)$? What is the maximum of $\varphi(p)$? What is the average value of the momentum $\langle p\rangle$?

If we take $\tilde{\psi}(x) = \psi(x)e^{i\frac{p_0}{\hbar}x}$, we can notice that this is the fourier transform of a translated function $\varphi(p-p_0)$.

Si the Fourier transform will be a translated gaussian:

$$\mathcal{F}[\psi(x)e^{i\frac{p_0}{\hbar}x}](p) = \varphi_0\exp\left[-\frac{(p-p_0)^2}{4\sigma_p^2}\right] \tag{30}$$

and the expectation value of the momentum will be $\langle p\rangle = p_0$

By now you should have noticed that we have $\Delta x = \sigma_x$ and $\Delta p = \sigma_p$ therefore $\Delta x\Delta p = \frac{\hbar}{2}$

Q6 Assuming the expression for $\tilde{\varphi}(p) = \tilde{\varphi}(p, t = 0)$ corresponding to a gaussian wave-packet at $t = 0$, determine the expression of $\tilde{\psi}(x, t)$ at all times. (Hint: substitute $\tilde{\varphi}(p)$ into the solution to the Schroedinger's equation for a superposition of many plane waves, eq. (24), and anti-transform.)

Q7 We now consider the square-amplitude

$$|\psi(x,t)|^2 = \frac{1}{\sqrt{2\pi}\sigma^2(t)}\exp\left[-\frac{\left(x-\frac{p_0}{m}t\right)^2}{2\sigma^2(t)}\right], \tag{31}$$

where the variance of this gaussian is given by

$$\sigma^2(t) = \sigma_x^2 + \frac{\hbar^2t^2}{4m^2\sigma_x^2}. \tag{32}$$

Can you easily write the evolution of $\langle x\rangle(t)$? Also derive an expression for the variance of the position $(\Delta x)^2$ as a function of the uncertainty of the speed of the particle, $(\Delta v)^2$ (where $v = p/m$). Do you understand what is happening? Thinking about the uncertainty principle and remembering that gaussians have the property $\Delta x\Delta p = \hbar/2$, can you give an intuitive understanding of how this is related to the uncertainty in the momentum?

The average position is $\langle x\rangle(t) = \frac{p_0}{m}t$, which means the particle is advancing along the x axis with momentum p_0 and speed p_0/m. The uncertainty of the position is increasing linearly in time (the variance increases quadratically). This is essential to ensure that the Heisenberg equation is verified at all times, as you could use a time of flight measurement to determine the position with increasing precision at later times.

2.4 Excercise 4: Heisenberg Inequality

We will be deriving the Heisenberg Uncertainty relation from the Fourier Transform. Consider a wave-function $\psi(x)$ and its Fourier transform $\varphi(p)$, and assume that $\langle x\rangle = 0$ and $\langle p\rangle = 0$ for simplicity.

Q1 Derive an expression for the variances $(\Delta x)^2$ and $(\Delta p)^2$ as a function of $\psi(x)$ and $d\psi(x)/dx$ using the properties of the Fourier Transform.

We have $\langle x\rangle = 0$ therefore $(\Delta x)^2 = \langle x^2\rangle$ and the same for the momentum.

$$(\Delta x)^2 = \int_{\mathbb{R}} x^2 |\psi(x)|^2 dx$$

For the momentum I will use the relation that $p\varphi(p) = -i\hbar\mathcal{F}[\frac{d\psi}{dx}](p)$,

$$\begin{aligned}(\Delta p)^2 &= \int_{\mathbb{R}} p^2 |\varphi(p)|^2 dp \\ &= \int_{\mathbb{R}} (p\varphi(p))^\star (p\varphi(p)) dp \\ &= \hbar^2 \int_{\mathbb{R}} (\mathcal{F}\left[\frac{d\psi}{dx}\right](p))^\star (\mathcal{F}\left[\frac{d\psi}{dx}\right](p)) dp\end{aligned}$$

and applying the Plancherel theorem we get

$$(\Delta p)^2 = \hbar^2 \int_{\mathbb{R}} \left|\frac{d\psi(x)}{dx}\right|^2 dx$$

We now introduce the function where $\lambda \in \mathbb{R}$

$$I(\lambda) = \int_{-\infty}^{\infty} \left| x\psi(x) + \lambda \frac{d\psi(x)}{dx}\right|^2 dx \tag{33}$$

Q2 Rewrite the Integral $I(\lambda)$ as a polynomial of (Δx), (Δp) and λ.

$$\begin{aligned}I(\lambda) &= \int_{\mathbb{R}} x^2|\psi(x)|^2 dx + \lambda^2 \int_{\mathbb{R}} \left|\frac{d\psi(x)}{dx}\right|^2 dx + \lambda \int_{\mathbb{R}} x\left(\psi^\star(x)\frac{d\psi(x)}{dx} + \frac{d\psi^\star(x)}{dx}\psi(x)\right) dx \\ &= (\Delta x)^2 + \lambda^2 \frac{(\Delta p)^2}{\hbar^2} - \lambda\end{aligned}$$

where we have replaced the definition obtained in Q1, and the last term is integrated by parts and gives -1 assuming the wave-function is normalised and goes to zero at infinity:

$$\begin{aligned}\int_{\mathbb{R}} x\left(\psi^\star(x)\frac{d\psi(x)}{dx} + \frac{d\psi^\star(x)}{dx}\psi(x)\right) dx &= \int_{\mathbb{R}} x\frac{d}{dx}\left(\psi^\star(x)\psi(x)\right) dx \\ &= \left[x|\psi(x)|^2\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} |\psi(x)|^2 dx\right.\end{aligned}$$

Q3 Can you say something about the sign of $I(\lambda)$ and its relationship to Herisenberg's uncertainty principle?

Considering

$$I(\lambda) = \lambda^2 \frac{(\Delta p)^2}{\hbar^2} - \lambda + (\Delta x)^2$$

which has a discriminant

$$\Delta = 1 - \frac{4}{\hbar^2}(\Delta x)^2(\Delta p)^2$$

As the Integrand of $I(\lambda)$ is an absolute value, it is positive, therefore $I(\lambda) \geq 0$, meaning that $\Delta \leq 0$, and therefore

$$(\Delta x)^2(\Delta p)^2 \geq \left(\frac{\hbar}{2}\right)^2$$

which is the uncertainty principle.

Q3 What must be the physical dimension of λ? If you replace in the expression for I the formulas for the uncertainities you derived in Q1 you will obtain a differential equation for $\psi(x)$. What form does this differential equation take when the Heisenberg inequality is an equality? What is the solution?

You can notice that the integrand is 0 when the differential equation

$$\frac{d\psi(x)}{dx} = -\frac{1}{\lambda} x\psi(x) \tag{34}$$

which we have seen several times today, and it has as a solution a gaussian. Therefore we can say that $I(\lambda) = 0$ if $\psi(x)$ is a gaussian.