# Physics 438A – Lecture #5
# Wave Mechanics for 1D Motion

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## 1 Position-Space Wave Functions

The observables considered so far have all been assumed to exhibit discrete eigenvalue spectra. In quantum mechanics, however, there are observables with continuous eigenvalues. Furthermore, observables can have portions of their spectra that are discrete and portions that are continuous. When the spectrum is continuous, there are infinitely many eigenvectors, and the associated vector space has infinite dimension. Thankfully, much of the intuition we've gained by working with finite-dimensional vector spaces will carry over in a relatively straightforward way. I'll be sure to point out the important differences as we go.

Consider a non-relativistic particle moving in one dimension. We assume that we can measure its position anywhere along the $x$ axis. It is therefore natural to introduce an orthonormal set of position eigenstates $|\xi\rangle$ such that

$$\hat{x}|\xi\rangle = x|\xi\rangle \tag{1.1}$$

where $\hat{x}$ is the position operator and the value of $x$ runs over all possible values of the position of the particle, that is, from $-\infty$ to $\infty$. From postulate #3, we may write a general state vector describing the particle as a superposition of position states such that

$$|\psi\rangle = \sum_i \langle\xi_i|\psi\rangle|\xi_i\rangle$$

and it follows that the probability of finding the particle at a particular location $x_i$ is

$$p(x_i) = |\langle\xi_i|\psi\rangle|^2.$$

Unfortunately, since $x$ lies in a continuum, there are infinitely many positions the particle could have, so the probability of obtaining exactly one position out of infinitely many is zero. This is easier to illustrate if we imagine that a quantum particle can occupy only a discrete set of positions $x_i$, each separated by $\Delta x$ such that $\Delta x = x_{i+1} - x_i = x_i - x_{i-1}$, etc. Within some range of length $L \gg \Delta x$, we expect the total probability of finding the particle to be nonzero. Let $N$ be the number of discrete positions in the range of length $L$ such that

$N\Delta x = L$. The probability the particle will be found at a particular position is proportional to $1/N$. In the continuum limit, $N \to \infty$ and $\Delta x \to 0$, so the probability of finding the particle at just one location vanishes.

Assuming the total probability to find the particle in the range $(0, L)$ is some nonzero constant that is independent of our course-graining procedure, then

$$\sum_{i=1}^{N} |\langle \xi_i|\psi\rangle|^2 = \sum_{i=1}^{N} \Delta x \ \left[\frac{|\langle \xi_i|\psi\rangle|^2}{\Delta x}\right] = \text{constant}$$

Look closely at the term in brackets. In both the numerator and the denominator, we have quantities that scale like $1/N$, so in the limit $N \to \infty$, we're left with a constant value. Furthermore, the summation above becomes an integral in the continuum limit.

In order to make use of this result in a mathematically consistent way, we need to redefine our position eigenstates. They will still be orthogonal, but no longer normalized in the familiar sense. We simultaneously require

$$|x\rangle = \lim_{\Delta x \to 0} \frac{|\xi\rangle}{\sqrt{\Delta x}}$$

and for the completeness relation to remain valid. In other words,

$$\sum_i |\xi_i\rangle\langle\xi_i| = \sum_i \Delta x \ |x_i\rangle\langle x_i| = \mathbb{1}$$

and in the limit $\Delta x \to 0$ (or $N \to \infty$),

$$\int_{-\infty}^{\infty} dx \ |x\rangle\langle x| = \mathbb{1} \tag{1.2}$$

So far so good, but now it looks like the inner product $\langle x|x\rangle \to \infty$ when $\Delta x \to 0$. This might be a problem for the finite-dimensional vector spaces we've been working with, but it actually works in the vector space of *functions*. Consider "inserting the completion relation" into the inner product of $|x\rangle$ with an arbitrary ket $|\psi\rangle$:

$$\begin{aligned}\langle x|\psi\rangle &= \langle x|\left(\int_{-\infty}^{\infty} dx' \ |x'\rangle\langle x'|\right)|\psi\rangle \\ &= \int_{-\infty}^{\infty} dx' \ \langle x|x'\rangle\langle x'|\psi\rangle \qquad (1.3)\end{aligned}$$

The quantity $\langle x|\psi\rangle$ is the projection of $|\psi\rangle$ onto the basis ket $|x\rangle$. For a fixed state $|\psi\rangle$, the quantity $\langle x|\psi\rangle$ depends on the value of $x$ much like a function. In fact, we define

$$\psi(x) = \langle x|\psi\rangle \tag{1.4}$$

and call it the **wave function** for purely historical reasons. You'll have to excuse the abuse of notation taking place, where $\psi$ appears as a label inside the ket and as a function. It will be clear from context which object you are working with.

Eq. 1.3 can now be written as

$$\psi(x) = \int_{-\infty}^{\infty} dx' \ \langle x|x'\rangle\psi(x') \tag{1.5}$$

which is (nearly) a defining property of a mathematical object called the *Dirac delta function*. Hence,

$$\langle x|x'\rangle = \delta(x' - x) \tag{1.6}$$

where $\delta(x' - x)$ is the delta function defined as the generalized function (a distribution) on the real numbers, whose value is zero everywhere except where $x = x'$, and whose integral over the entire real line is equal to one:

$$\int_{-\infty}^{\infty} dx' \ \delta(x' - x) = 1 \tag{1.7}$$

Eq. 1.6 is a generalized form of orthonormality suited for continuous variables. It reflects the fact that states like $|x\rangle$ are non-normalizable limits, yet they form a complete basis in the sense of distributions, allowing us to expand and reconstruct functions using integrals.

We can now define the inner product over wave functions by integrating over $x$. Beginning with the inner product of $|\phi\rangle$ with $|\psi\rangle$, we insert the completeness relation:

$$\langle\phi|\psi\rangle = \int_{-\infty}^{\infty} dx \ \langle\phi|x\rangle\langle x|\psi\rangle = \int_{-\infty}^{\infty} dx \ \phi^*(x)\psi(x) \tag{1.8}$$

and in particular,

$$\langle\psi|\psi\rangle = \int_{-\infty}^{\infty} dx \ \psi^*(x)\psi(x) = \int_{-\infty}^{\infty} dx \ |\psi(x)|^2 \tag{1.9}$$

A normalized wave function has the property

$$\int_{-\infty}^{\infty} dx \ |\psi(x)|^2 = 1 \tag{1.10}$$

We identify the quantity $dx\ |\psi(x)|^2$ as the probability of finding the particle between $x$ and $x + dx$. The probability to find the particle in the range $[a, b]$ is given by

$$P(a < x < b) = \int_a^b dx\ |\psi(x)|^2 \tag{1.11}$$

**Example 1.1: Position-space wavefunction**

At time $t = 0$, a particle has an associated wavefunction

$$\psi(x) = \begin{cases} A(x/a) & 0 \le x < a \\ A(b-x)/(b-a) & a \le x \le b \\ 0 & \text{otherwise} \end{cases}$$

where $A, a$, and $b$ are all positive constants. (a) Normalize $\psi$ by finding an appropriate value for $A$. (b) Where is the particle most likely to be found at $t = 0$? (c) What is the probability of finding the particle to the left of $a$? (d) What is the expectation value of $x$?

**Solution:** (a) Normalize by taking the square-modulus of the wavefunction and setting the integral equal to one.

$$1 = \int_0^b dx\ |\psi(x)|^2 = \int_0^a \frac{A^2}{a^2} x^2 dx + \int_a^b A^2 \frac{(b-x)^2}{(b-a)^2} dx$$

$$1 = A^2 \cdot \frac{a}{3} + A^2 \cdot \frac{(b-a)}{3} = A^2 \cdot \frac{b}{3}$$

Hence, $A = \sqrt{3/b}$ is a suitable choice for the constant $A$. (b) The particle is most likely to be found wherever $|\psi(x)|^2$ has a maximum. In this case, that corresponds to $x = a$ where $|\psi(a)|^2 = 3/b$. (c) The probability to find the particle to the left of $a$ is

$$P(x < a) = \int_0^a |\psi(x)|^2 dx = \int_0^a \frac{3}{b} \cdot \frac{x^2}{a^2} dx = \frac{a}{b}$$

Notice if $a = b$, then the probability of finding the particle to the left of $a$ is 1 since the wavefunction is zero for $x > a$. If $b = 2a$, then the probability of finding the particle to the left of $a$ is 0.5; the wavefunction is symmetric about $x = a$. (d) To find the expectation value of $\hat{x}$, apply the definition and use the completeness relation:

$$\begin{aligned}
\langle \hat{x} \rangle = \langle \psi | \hat{x} | \psi \rangle &= \langle \psi | \hat{x} \left( \int_{-\infty}^{\infty} dx \; |x\rangle\langle x| \right) |\psi\rangle \\
&= \int_{-\infty}^{\infty} dx \; \psi^*(x) x \psi(x) \\
&= \int_0^a \frac{3}{b} \cdot \frac{x^3}{a^2} dx + \int_a^b \frac{3}{b} \cdot \frac{(b-x)^2 x}{(b-a)^2} dx \\
&= \frac{3a^2}{4b} + \frac{a}{2} - \frac{3a^2}{4b} + \frac{b}{4} \\
&= \frac{a}{2} + \frac{b}{4}
\end{aligned}$$

When $b = 2a$, the wavefunction (and corresponding probability distribution) is symmetric about $x = a$, which is the most probable location to find the particle. It therefore makes sense that $x = a$ would also be the expectation value of $\hat{x}$. Note, however, that the most probable location and the expectation value do not necessarily coincide. For instance, when $a = b$, the most likely place to find the electron is still $x = a$, but the expectation value of $\hat{x}$ is $3a/4$ since the wavefunction is asymmetric (we would say it is left-skewed).

## 2 Translations in Quantum Mechanics

Mirroring our study of rotations in Lecture #4, we postulate the existence of a unitary operator $T$ acting on state vectors that corresponds to a translation along one dimension of 3D Euclidean space. If we denote the operator that translates a state by an amount $a$ as $T(a)$, then its action on a position eigenstate is defined by

$$T(a)|x\rangle = |x + a\rangle$$

Applying two translations in opposite directions should bring us back to the same point:

$$T(a)T(-a)|x\rangle = T(a)|x - a\rangle = |x\rangle$$

Thus, $T(-a)T(a) = I$, and since $T^\dagger(a)T(a) = \mathbb{1}$,

$$T^\dagger(a) = T(-a)$$

Because performing a translation by $a$ followed by translation by $b$ is equivalent to a translation by $a + b$, the translation operators satisfy

$$T(a+b) = T(a)T(b) = T(b)T(a)$$

We can now examine how the position operator transforms under translation. Acting with $T(a)$ shifts the position eigenvalues by $a$

$$T^\dagger(a)\hat{x}T(a) = \hat{x} + a\mathbb{1} = \hat{x} + a$$

where we have used a shorthand notation suppressing the identity operator.

Let us now see how the translation operator acts on wave functions. The position representation of a state is $\langle x|\psi\rangle$. Acting with $T(a)$ gives

$$\langle x|T(a)|\psi\rangle = \psi(x-a)$$

showing explicitly that $T(a)$ shifts the argument of the wave function to the right by $a$.

## 2.1 Momentum Operator

Consider an infinitesimal translation by $\delta x$

$$T(\delta x) = \mathbb{1} - \frac{i}{\hbar}\hat{p}_x \delta x \tag{2.1}$$

where the operator $\hat{p}_x$ is called the generator of translations such that any finite translation may be written as

$$T(a) = \exp\left(-\frac{i}{\hbar}\hat{p}_x a\right) \tag{2.2}$$

When a classical system is invariant under translations along some axis, the linear momentum about that axis is conserved. Likewise, when the Hamiltonian for a quantum system commutes with the generator of translation along some axis, the expectation value of the generator is conserved. We define the $x$-component of **linear momentum** of a quantum particle as the generator of translation $\hat{p}_x$ along the $x$ axis. In other words,

$$\hat{p}_x = i\hbar \left. \frac{\partial T(x)}{\partial x} \right|_{x=0} \tag{2.3}$$

where the factor of $i$ ensures that $\hat{p}_x$ is self-adjoint[1] and the factor of $\hbar$ is included so that $\hat{p}_x$ has the correct units and corresponds to classical momentum in the appropriate limit.

So far we've been working with operators on the vector space of kets. It will often be convenient to work directly with operators on the space of wave functions. For instance, the position operator can act directly on the wave function $\psi(x)$ as

$$\hat{x}\psi(x) \equiv \langle x|\hat{x}|\psi\rangle = x\psi(x) \tag{2.4}$$

The momentum operator can also act directly on the space of wave functions. Start by considering an infinitesimal translation by $\delta x$ and Taylor expand the wave function to leading order in $\delta x$:

$$\langle x|T(\delta x)|\psi\rangle = \psi(x - \delta x) \approx \psi(x) - \frac{d\psi}{dx}\delta x$$

Expanding the left-hand side to leading order,

$$\langle x|T(\delta x)|\psi\rangle = \langle x|\psi\rangle + \frac{1}{i\hbar}\langle x|\hat{p}_x|\psi\rangle\delta x$$

Hence, the action of the momentum operator can also be written as

$$\hat{p}_x\psi(x) \equiv \langle x|\hat{p}_x|\psi\rangle = -i\hbar\frac{\partial\psi(x)}{\partial x} \tag{2.5}$$

Please excuse the abuse of notation, but it's extremely common and it should be clear from context whether the operator is acting on state vectors or wave functions directly.

## 2.2 Physical Wave Functions

In the quantum mechanics of a non-relativistic particle, certain mathematical conditions must be satisfied to define position $\hat{x}$ and momentum $\hat{p}_x$ operators as self-adjoint operators on a suitable space of wave functions.

[1] We'll see very soon that a mere factor of $i$ is actually not enough to ensure that momentum is self-adjoint.

1. Wave functions must be square-integrable:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx < \infty \tag{2.6}$$

This ensures inner products are well-defined and wave functions can be normalized.

2. Wave functions must vanish at infinity, i.e. $\psi(x) \to 0$ as $x \to \pm\infty$.

Condition #1 is pretty clear, but the reason we impose condition #2 mostly has to do with the status of momentum as a valid observable in quantum theory. If $\hat{p}_x$ is self-adjoint, then $\langle f|\hat{p}_x|g\rangle^* = \langle g|\hat{p}_x|f\rangle$ for any two functions $f$ and $g$. Let's see if this holds:

$$\langle g|\hat{p}_x|f\rangle = \int_{-\infty}^{\infty} dx\ \langle g|\hat{p}_x|x\rangle\langle x|f\rangle = \int_{-\infty}^{\infty} dx\ \left(i\hbar\frac{dg^*(x)}{dx}\right) f(x)$$

$$\langle f|\hat{p}_x|g\rangle^* = \int_{-\infty}^{\infty} dx\ \left(-i\hbar\frac{df(x)}{dx}\right) g^*(x) = -i\hbar f(x)g^*(x)\Big|_{-\infty}^{\infty} + i\hbar\int_{-\infty}^{\infty} dx\ \frac{dg^*(x)}{dx}f(x)$$

For arbitrary functions $f$ and $g$, $\langle f|\hat{p}_x|g\rangle^* \neq \langle g|\hat{p}_x|f\rangle$, so the momentum operator is not self-adjoint! Condition #2 ensures the boundary term vanishes so that momentum is an observable for all physical wave functions–those that may correspond to a particle with position and momentum.

## 2.3 Canonical Commutation Relation

Given a wave function $\psi(x)$, we can easily find the commutator of $\hat{x}$ and $\hat{p}_x$:

$$\begin{aligned}
[\hat{x},\hat{p}_x]\psi(x) &= \hat{x}\hat{p}_x\left[\psi(x)\right] - \hat{p}_x\hat{x}\left[\psi(x)\right] \\
&= -i\hbar x\frac{\partial\psi(x)}{\partial x} + i\hbar\frac{\partial(x\psi(x))}{\partial x} \\
&= -i\hbar x\frac{\partial\psi(x)}{\partial x} + i\hbar\frac{\partial\psi(x)}{\partial x} + i\hbar\psi(x) \\
&= i\hbar\psi(x)
\end{aligned}$$

Hence,

$$[\hat{x},\hat{p}_x] = i\hbar\mathbb{1} = i\hbar \tag{2.7}$$

where it's common to drop the identity operator. Any two observables that satisfy the commutation relation $[A,B] = i\hbar$ are said to be conjugate to one another.

## 2.4 Ehrenfest's Theorem

A non-relativistic particle constrained to move along one dimension of space is essentially a model defined by the Hamiltonian

$$H = \frac{\hat{p}_x^2}{2m} + V(\hat{x}) \tag{2.8}$$

where the first term is the kinetic energy operator and $V(\hat{x})$ is the potential energy operator that models a particle's interaction with its environment—a very large subsystem whose motion/dynamics can be neglected. The potential energy operator $V(\hat{x})$ is a function of the position operator $\hat{x}$ and it multiplies the position-space wave function $\psi(x)$ by the corresponding scalar potential energy function evaluated at position $x$. In other words,

$$V(\hat{x})\psi(x) = V(x)\psi(x) \tag{2.9}$$

For example, $V(\hat{x}) = \frac{1}{2}k\hat{x}^2$ is the potential energy operator for a Hooke's law force; $V(\hat{x})$ can generally be written as a linear combination of monomials $\hat{x}^n$ where $n$ is an integer.

The expectation value of the position operator changes over time in a way that matches the definition of momentum in classical mechanics. Observe that

$$\frac{d\langle\hat{x}\rangle}{dt} = \frac{i}{\hbar}\langle[H, \hat{x}]\rangle = \frac{i}{2m\hbar}\langle[\hat{p}_x^2, x]\rangle$$

The commutator is found by expanding in terms of the canonical commutation relation:

$$\begin{aligned}
[\hat{p}_x^2, x] &= \hat{p}_x\hat{p}_x\hat{x} - \hat{x}\hat{p}_x\hat{p}_x \\
&= \hat{p}_x\hat{p}_x\hat{x} - \hat{p}_x\hat{x}\hat{p}_x + \hat{p}_x\hat{x}\hat{p}_x - \hat{x}\hat{p}_x\hat{p}_x \\
&= \hat{p}_x[\hat{p}_x, \hat{x}] + [\hat{p}_x, \hat{x}]\hat{p}_x \\
&= -2i\hbar\hat{p}_x
\end{aligned}$$

Hence,

$$\frac{d\langle\hat{x}\rangle}{dt} = \frac{\langle\hat{p}_x\rangle}{m} \tag{2.10}$$

which is the result of classical mechanics. This is yet another example of Ehrenfest's theorem, which states that the expectation values of quantum mechanical operators for position and momentum obey equations of motion analogous to classical mechanics.

The equation of motion for the expectation value of momentum is given by

$$\frac{d\langle \hat{p}_x \rangle}{dt} = \frac{i}{\hbar}\langle [H, \hat{p}_x] \rangle = \frac{i}{\hbar}\langle [V(\hat{x}), \hat{p}_x] \rangle$$

where the commutator $[V(\hat{x}, \hat{p}_x)]$ can be evaluated with an arbitrary wave function $\psi(x)$:

$$\Big(V(\hat{x})\hat{p}_x\Big)\psi(x) = -i\hbar V(x)\psi'(x)$$

$$\Big(\hat{p}_x V(\hat{x})\Big)\psi(x) = \hat{p}_x\Big(V(x)\psi(x)\Big) = -i\hbar V'(x)\psi(x) - i\hbar V(x)\psi'(x)$$

$$[V(\hat{x}), \hat{p}_x]\psi(x) = i\hbar V'(x)\psi(x)$$

where we've used prime notation to denote derivatives with respect to $x$. Hence,

$$\frac{d\langle \hat{p}_x \rangle}{dt} = \frac{i}{\hbar}\left\langle i\hbar \frac{\partial V}{\partial x} \right\rangle = \left\langle -\frac{\partial V(\hat{x})}{\partial x} \right\rangle \tag{2.11}$$

which is the analog of Newton's second law in quantum mechanics. Note that to evaluate the commutator leading to Eq. (2.10), I used an "algebraic method" consisting of algebraic manipulations involving commutators and the canonical commutation relation. On the other hand, I used a trial wave function to evaluate $[V(\hat{x}), \hat{p}_x]$ directly. The point is that there's more than one way to skin a cat, whether it's dead or alive...

## 2.5 Definite-Energy States

Substituting Eq. (2.8) into the Schrödinger equation (postulate #5),

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = \left(\frac{\hat{p}_x^2}{2m} + V(\hat{x})\right)|\psi(t)\rangle$$

We can turn this into a partial differential equation for the wave function $\psi(x, t)$ which is the projection of $|\psi\rangle$ in the position basis. The Schrödinger equation for $\psi(x, t)$ is

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x)\psi(x,t) \tag{2.12}$$

Historically, this was the first "Schrödinger equation" and people will often call it the time-dependent Schrödinger equation for obvious reasons. It is a linear, first-order in time, second-order in space partial differential equation (PDE).

In the next few lectures, we're going to solve for the time evolution of wave functions describing a single particle in various potentials. We found in our first introduction to quantum dynamics that it was convenient to express the state vector in the energy eigenbasis, where the Hamiltonian takes a diagonal form. Let $E$ be the energy eigenvalue corresponding to an energy eigenfunction $\psi_E(x,t)$. The eigenvalue equation for the Hamiltonian is

$$H(x)\psi_E(x,t) = i\hbar\frac{\partial\psi_E(x,t)}{\partial t} = E\psi_E(x,t) \tag{2.13}$$

This first-order differential equation has the general solution

$$\psi_E(x,t) = \psi(x)e^{-iEt/\hbar} \tag{2.14}$$

where $\psi(x)$ is a normalized wave function of $x$ only, so we'll refer to it as the "time-independent wave function." Eq. (2.14) describes a **definite-energy state**. Substituting the definite energy state into the time-dependent Schrödinger equation, we obtain the so-called "time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \tag{2.15}$$

Comparing with Eq. (2.12), you'll see that our notation is getting sloppy, but it's very common so we might as well get used to it. It will be clear from context whether we're dealing with a time-dependent or time-independent wave function.

# 3 Momentum-Space Wave Functions

In position space, we describe the quantum state of a particle using a wave function $\psi(x)$ whose squared magnitude $|\psi(x)|^2$ gives the probability density for finding the particle near position $x$. It can often be useful to consider the *momentum representation*, where the wave function is written in terms of eigenvalues of the momentum operator. Given the position-space wave function $\psi(x)$, we can obtain the momentum-space wave function by a change of basis between the eigenstates of position and those of momentum.

## 3.1 Momentum Eigenfunctions

Let $\psi_{x'}(x)$ denote a position eigenstate wave function $\langle x|x'\rangle$ (eigenfunction for short). We've already seen that position eigenstates are in fact delta functions:

$$\hat{x}\psi_{x'}(x) = x'\psi_{x'}(x) = x'\langle x|\psi_{x'}\rangle = x'\delta(x'-x) \Rightarrow \psi_{x'}(x) = \delta(x'-x) \tag{3.1}$$

Now we search for position-space momentum eigenfunctions

$$\hat{p}_x \psi_{p_x}(x) = p_x \psi_{p_x}(x) \tag{3.2}$$

where

$$\psi_{p_x}(x) = \langle x|p_x\rangle \quad \text{and} \quad \hat{p}_x|p_x\rangle = p_x|p_x\rangle$$

Eq. (3.2) leads to a first-order differential equation for $\psi_{p_x}(x)$

$$-i\hbar \frac{\partial \psi_{p_x}(x)}{\partial x} = p_x \psi_{p_x}(x)$$

which has the general solution

$$\psi_{p_x}(x) = A e^{ip_x x/\hbar} \tag{3.3}$$

where $A$ is a constant to be determined. Neither the position eigenfunctions nor the momentum eigenfunctions are normalizable–they are not square integrable and the momentum eigenfunctions do not vanish at infinity. We can assume that momentum eigenstates form a complete basis, so for any state vector $|\psi\rangle$ corresponding to a physical wave function,

$$\begin{aligned}
\langle p_x|\psi\rangle &= \langle p_x| \left( \int_{-\infty}^{\infty} dp'_x \; |p'_x\rangle\langle p'_x| \right) |\psi\rangle \\
&= \int_{-\infty}^{\infty} dp'_x \; \langle p_x|p'_x\rangle\langle p'_x|\psi\rangle \\
\psi(p_x) &= \int_{-\infty}^{\infty} dp'_x \; \langle p_x|p'_x\rangle \psi(p'_x)
\end{aligned}$$

It follows that momentum eigenstates must be Dirac orthonormal in the sense that

$$\langle p_x|p'_x\rangle = \delta(p'_x - p_x) \tag{3.4}$$

This constraint allows us to determine the constant $A$ in Eq. (3.3). Using completeness of the position eigenstates,

$$\begin{aligned}
\langle p_x|p'_x\rangle &= \int_{-\infty}^{\infty} dx \; \langle p_x|x\rangle\langle x|p'_x\rangle \\
&= \int_{-\infty}^{\infty} dx \; \psi_{p_x}(x)\psi_{p'_x}(x)
\end{aligned}$$

$$= \int_{-\infty}^{\infty} dx \ |A|^2 e^{i(p_x - p'_x)x/\hbar}$$

At this point, we must make use of a mathematical identity from complex analysis:

$$\int_{-\infty}^{\infty} dx \ e^{ix(k'-k)} = 2\pi\delta(k'-k) \tag{3.5}$$

We'll call this the "integral representation of the Dirac delta function." Hence,

$$\langle p_x | p'_x \rangle = 2\pi\hbar \ |A|^2 \ \delta(p'_x - p_x)$$

There is technically ambiguity in the phase of $A$, but nonetheless if we choose

$$A = \frac{1}{\sqrt{2\pi\hbar}}$$

then our momentum eigenstates will be Dirac-orthornormal. Finally, we have

$$\psi_{p_x}(x) = \langle x | p_x \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ip_x x/\hbar} \tag{3.6}$$

Momentum eigenfunctions do not belong to the space of "physical wave functions" that we discussed earlier. They are not square-integrable, and hence they are non-normalizable. They do however form a complete basis for wave functions in the sense that any wave function may be written as a linear superposition of the momentum eigenfunctions. In the space of physical wave functions, the momentumm operator is self-adjoint and has a complete set of orthonormal eigenstates which are normalized in a distributional sense by the delta function.

## 3.2 Fourier Transform

Position and momentum eigenstates satisfy integral completeness

$$\int_{-\infty}^{\infty} dp_x \ |p_x\rangle\langle p_x| = \mathbb{1} \qquad \text{and} \qquad \int_{-\infty}^{\infty} dx \ |x\rangle\langle x| = \mathbb{1}$$

Given a quantum system in the state $|\psi\rangle$, we can determine the position-space wave function or the momentum-space wave function as

$$\psi(x) = \langle x|\psi\rangle \qquad \text{and} \qquad \tilde{\psi}(p_x) = \langle p_x|\psi\rangle \tag{3.7}$$

where a tilde is added over the momentum-space wave function for notational convenience. It will often be useful or necessary to go from one representation directly to the other. Given the completeness of momentum states,

$$\psi(x) = \int_{-\infty}^{\infty} dp_x \langle x|p_x\rangle\langle p_x|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp_x \; \tilde{\psi}(p_x) e^{ip_x x/\hbar} \tag{3.8}$$

and from completeness of position states,

$$\tilde{\psi}(p_x) = \int_{-\infty}^{\infty} dx \langle p_x|x\rangle\langle x|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx \; \psi(x) e^{-ip_x x/\hbar} \tag{3.9}$$

The latter equation is called the *Fourier transform* of the function $\psi(x)$, and we interpret this as a change of basis from "position space" to "momentum space." The first expression is the inverse Fourier transform in the sense that substituting $\tilde{\psi}(p_x)$ from the second expression should result in the identity operation:

$$\begin{aligned}
\psi(x) &= \int \frac{dp_x}{\sqrt{2\pi\hbar}} e^{-ip_x x/\hbar} \left\{ \int \frac{dx'}{\sqrt{2\pi\hbar}} e^{-ip_x x'/\hbar} \psi(x') \right\} \\
&= \int dx' \int \frac{dp_x}{2\pi\hbar} e^{ip_x(x-x')/\hbar} \psi(x') \\
&= \int dx' \delta(x'-x)\psi(x') \\
&= \psi(x)
\end{aligned}$$

For example, the Fourier transform of the momentum eigenfuction in position space should give the momentum eigenfunction in momentum space:

$$\tilde{\psi}_{p'_x}(p_x) = \int \frac{dx}{2\pi\hbar} e^{i(p'_x - p_x)x/\hbar} = \delta(p'_x - p_x)$$

## 3.3 Operators in Momentum Space

Nearly all observables we care about will be expressible in terms of position and momentum. We should know how those operators work in momentum space. For instance, we cannot apply $\hat{p}_x = i\hbar\partial/\partial x$ to the wave function $\tilde{\psi}(p_x)$ since there simply is no $x$ dependence.

**Momentum Operator in Momentum Space**

Dirac notation and completeness are especially helpful here.

$$\hat{p}_x \tilde{\psi}(p_x) = \langle p_x | \hat{p}_x | \psi \rangle = \int_{-\infty}^{\infty} dx \; \langle p_x | x \rangle \langle x | \hat{p}_x | \psi \rangle$$

This equation is basically the Fourier transform of the position-space wave function $\hat{p}_x \psi(x)$. Using the position-space momentum operator, we apply integration by parts and eliminate the boundary term since $\psi(x) \to 0$ at $x \to \pm\infty$:

$$\begin{aligned}
\hat{p}_x \tilde{\psi}(p_x) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx \left( -i\hbar \frac{\partial \psi(x)}{\partial x} \right) e^{-ip_x x/\hbar} \\
&= \underbrace{\frac{-i\hbar}{\sqrt{2\pi\hbar}} \psi(x) e^{-ip_x x/\hbar} \Big|_{-\infty}^{\infty}}_{\text{boundary term} \to 0} - (-i\hbar)(-ip_x/\hbar) \underbrace{\frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx \; \psi(x) e^{-ip_x x/\hbar}}_{\tilde{\psi}(p_x)} \\
&= p_x \tilde{\psi}(p_x)
\end{aligned}$$

Hence, in the momentum representation, the momentum operator returns the value of momentum, just like the position operator in position space.

**Position Operator in Momentum Space**

Now consider the position operator in position space. Using Dirac notation,

$$\hat{x} \tilde{\psi}(p_x) = \langle p_x | \hat{x} | \psi \rangle = \int_{-\infty}^{\infty} dx \; \langle p_x | x \rangle \langle x | \hat{x} | \psi \rangle$$

which says the position operator in momentum space is the Fourier transform of the position operator in position space. Use the position operator in position space and observe the integrand is a total derivative with respect to $p_x$:

$$\begin{aligned}
\hat{x} \tilde{\psi}(p_x) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx \; x \psi(x) e^{-ip_x x/\hbar} \\
&= i\hbar \frac{\partial}{\partial p_x} \left\{ \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx \; \psi(x) e^{-ip_x x/\hbar} \right\} \\
&= i\hbar \frac{\partial \tilde{\psi}(p_x)}{\partial p_x}
\end{aligned}$$

The position operator in momentum space acts almost like the momentum operator in position space, but with an overall minus sign. To summarize,

| Position Space | Momentum Space |
|---|---|
| $\hat{x} = x$ | $\hat{x} = i\hbar\dfrac{\partial}{\partial p_x}$ |
| $\hat{p}_x = -i\hbar\dfrac{\partial}{\partial x}$ | $\hat{p}_x = p_x$ |

**Example 3.1: Momentum-Space Wave Function**

At a particular moment in time, a localized particle is described by the position-space wave function

$$\psi(x) = \begin{cases} A, & -a < x < a \\ 0, & \text{otherwise} \end{cases}$$

where $A$ and $a$ are positive real constants. Find the momentum-space wave function.

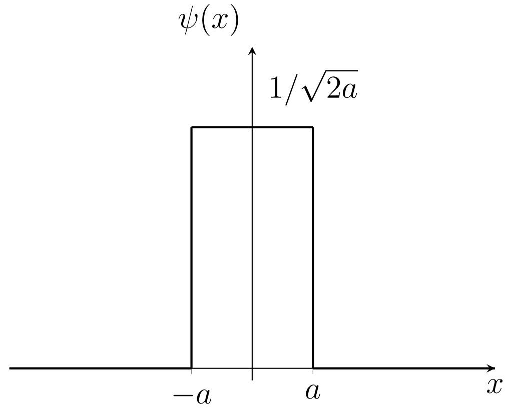
**Solution:** First we need to normalize the wave function:

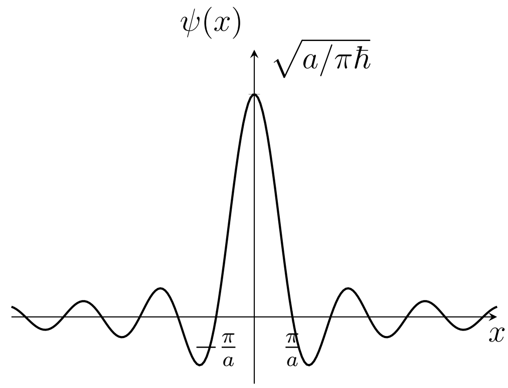
$$1 = \int_{-\infty}^{\infty} dx\ |\psi(x)|^2 = \int_{-a}^{a} dx\ A^2 = (2a)A^2 \Rightarrow A = \frac{1}{\sqrt{2a}}$$

Now we can calculate the momentum-space wave function:

$$\tilde{\psi}(p_x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx\ \psi(x)e^{-ip_x x/\hbar} = \frac{1}{\sqrt{4\pi\hbar a}}\int_{-a}^{a} dx\ e^{-ip_x x/\hbar}$$

$$\tilde{\psi}(p_x) = \frac{1}{\sqrt{4\pi\hbar a}}\frac{2\hbar\sin(p_x a/\hbar)}{p_x} = \sqrt{\frac{\hbar}{\pi a}}\frac{\sin(p_x a/\hbar)}{p_x}$$



# 4 Quantum Dynamics of a Free Particle

Newton's first law states that a free particle–one that is absent of any applied forces–will travel in a straight line at constant speed. The probabilistic nature of quantum dynamics immediately calls for revision; if we can't know for certain where a free particle will move in a short time interval, the velocity is simply undefined.

Consider a particle moving in a constant potential, and for the sake of simplicity, let $V = 0$. The Hamiltonian is then

$$H = \frac{\hat{p}_x^2}{2m}$$

and since $\hat{p}_x$ is Hermitian, it follows that the energy of a free particle must be non-negative:

$$\langle\psi|H|\psi\rangle = \frac{1}{2m}\langle\psi|\hat{p}_x^2|\psi\rangle = \frac{1}{2m}\left\|\hat{p}_x\psi\right\|^2 \geq 0$$

The time-independent Schrödinger equation for the definite-energy wave function $\psi(x)$ is

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi \tag{4.1}$$

where $k = \pm\sqrt{2mE}/\hbar$. Clearly $\psi(x)$ is an eigenstate of $\hat{p}_x$ since $[H, \hat{p}_x] = 0$. Hence,

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{ip_x x/\hbar} \tag{4.2}$$

where $p_x = \hbar k = \pm\sqrt{2mE}$. We know these functions are not square-integrable and don't represent physical wave functions on their own, but they can be combined to produce physical wave functions. In fact, the most general solution to the time-dependent Schrödinger equation for a free particle is

$$\psi(x,t) = \int_{-\infty}^{\infty} \frac{dp_x}{\sqrt{2\pi\hbar}}\tilde{\psi}(p_x)e^{i(kx-\omega(k)t)} \tag{4.3}$$

where $\omega(k) = E/\hbar = \hbar k^2/2m$. This is a superposition of complex waves, each of the form $e^{i(kx-\omega t)}$, weighted by the amplitude $\tilde{\psi}(p_x)$. Each wave has a well-defined **wavevector** $k$ and **angular frequency** $\omega$, which are related to the momentum and energy of the particle via de Broglie's relations:

$$p_x = \hbar k \quad \text{and} \quad E = \hbar\omega \tag{4.4}$$

There are two ways to justify the general solution given by Eq. (4.3). We could substitute directly into the Schrödinger equation, or we can build up the superposition using orthonormality and completeness. The momentum eigenstates are also the eigenstates of the

Hamiltonian. Hence,

$$H|p_x\rangle = \frac{\hbar^2 k^2}{2m}|p_x\rangle \quad \text{where } \hbar k = \sqrt{2mE}$$

Since the momentum eigenstates are complete, we can write any initial state vector as

$$|\psi(0)\rangle = \int_{-\infty}^{\infty} dp_x \; |p_x\rangle\langle p_x|\psi(0)\rangle = \int_{-\infty}^{\infty} dp_x \; \tilde{\psi}(p_x)|p_x\rangle$$

The time-evolved state vector is

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle = \int_{-\infty}^{\infty} dp_x \; \tilde{\psi}(p_x)e^{-i\omega(k)t}|p_x\rangle$$

where $\omega(k)$ is defined above. The time-dependent wave function in the position basis is

$$\psi(x,t) = \langle x|\psi(t)\rangle = \int_{-\infty}^{\infty} dp_x \; \tilde{\psi}(p_x)e^{-i\omega(k)t}\langle x|p_x\rangle = \int_{-\infty}^{\infty} \frac{dp_x}{\sqrt{2\pi\hbar}}\tilde{\psi}(p_x)e^{i(kx-\omega(k)t)}$$

Here's another argument in terms of wave functions–in case that appeals to you. Since the Hamiltonian is diagonal in the momentum basis, it is useful to consider its momentum representation. For a momentum-space wave function $\tilde{\psi}(p_x,t)$,

$$H\tilde{\psi}(p_x,t) = \frac{\hat{p}_x^2}{2m}\tilde{\psi}(p_x,t) = \frac{p_x^2}{2m}\tilde{\psi}(p_x,t)$$

The time-dependent Schrödinger equation for $\tilde{\psi}(p_x)$ is

$$i\hbar\frac{\partial\tilde{\psi}(p_x,t)}{\partial t} = \frac{p_x^2}{2m}\tilde{\psi}(p_x,t)$$

and the solution is

$$\tilde{\psi}(p_x,t) = \tilde{\psi}(p_x,0)e^{-i\omega t}$$

where $\omega = p_x^2/2m\hbar$. Hence, the momentum-space probability distribution remains constant:

$$|\tilde{\psi}(p_x,t)|^2 = |\tilde{\psi}(p_x,0)|^2$$

The position-space wave function is then given by the inverse Fourier transform of $\tilde{\psi}(p_x)$.

## 4.1 Phase and Group Velocity

Consider a single complex wave $e^{i(kx-\omega t)} = e^{i\phi}$. The **phase** $\phi = kx - \omega t$ is constant along points were $x/t = \omega/k$. Thus, we define the **phase velocity** as

$$v_{\text{phase}} = \frac{\omega}{k} \tag{4.5}$$

The phase velocity of a non-relativistic particle with definite energy and momentum is

$$v_{\text{phase}} = \frac{\omega}{k} = \frac{E}{p_x} = \frac{p_x}{2m} \tag{4.6}$$

This is not the classical particle velocity. Instead, it's the speed at which the wave crests move, but not necessarily the speed at which the particle or its probability density moves.

A more physically meaningful quantity is the group velocity, which tells us how the envelope of a wave packet (and thus the probability distribution) propagates. This is particularly relevant when $\tilde{\psi}(p_x)$ is peaked sharply around some value of $p_x = \hbar k$. As we'll explain soon, the **group velocity** is defined as

$$v_{\text{group}} = \frac{d\omega}{dk} \tag{4.7}$$

The group velocity of a non-relativistic particle with definite energy and momentum is

$$v_{\text{group}} = \frac{d\omega}{dk} = \frac{dE}{dp_x} = \frac{p_x}{m} \tag{4.8}$$

This is exactly the classical velocity of a particle with momentum $p_x$ and mass $m$. We say it's the rate at which the wave packet moves. To understand this result, let's assume the wave packet is nearly sinusoidal in the sense that $\tilde{\psi}(p_x)$ is sharply peaked around some value $p_{x0} = \hbar k_0$. The angular frequency depends on the wavenumber, and we call this *dispersion.* The dispersion relation is $\omega(k)$. When the wave packet is nearly sinusoidal, the angular frequency will vary slightly from $\omega_0 = \omega(k_0)$, and we can Taylor expand to first order since $\Delta k = k - k_0$ is small. Hence,

$$\omega(k) \approx \omega(k_0) + \left.\frac{d\omega}{dk}\right|_{k_0} (k - k_0) + \mathcal{O}(\Delta k^2) = \omega_0 + v_g \Delta k + \mathcal{O}(\Delta k^2)$$

Changing variables to $\Delta k$, the wave packet is

$$\psi(x,t) \approx e^{i(k_0 x - \omega_0 t)} \int \frac{d(\Delta p_x)}{\sqrt{2\pi\hbar}} \tilde{\psi}(p_{x0} + \Delta p_x) e^{i\Delta p_x (x - v_g t)/\hbar}$$

$$= e^{i(k_0 x - \omega_0 t)} f(x - v_g t)$$

where the first term is a complex wave with phase velocity $\omega_0/k$ and the second term is a function with a fixed shape moving with the group velocity $v_g$. Generally speaking, the dispersion relation describes the spreading of a wave packet over time, since different $k$ components will move at different speeds. We can analyze this effect by keeping the second order term in the series expansion for the angular frequency $\omega(k)$:

$$\omega(k) \approx \omega(k_0) + \left.\frac{d\omega}{dk}\right|_{k_0} (k - k_0) + \frac{1}{2} \left.\frac{d^2\omega}{dk^2}\right|_{k_0} (k - k_0)^2 + \mathcal{O}(\Delta k^3)$$

$$= \omega_0 + v_g \Delta k + \alpha \Delta k^2$$

where $\alpha = \frac{1}{2} \frac{d^2\omega}{dk^2}\big|_{k_0}$. The resulting wave packet is

$$\psi(x,t) \approx e^{i(k_0 x - \omega_0 t)} \int \frac{d(\Delta p_x)}{\sqrt{2\pi\hbar}} \tilde{\psi}(p_{x0} + \Delta p_x) e^{i\Delta p_x [x - (v_g + \alpha \Delta k) t]/\hbar}$$

Since different $k$ components move at different group speeds, we can no longer think of the integral as a function describing a fixed shape moving at speed $v_g$. Instead, the wave packet spreads out over time. By dimensional analysis, the spreading is proportional to

$$\Delta x \propto \alpha \Delta k t = \frac{1}{2} \left.\frac{d^2\omega}{dk^2}\right|_{k_0} \Delta k t = \frac{\Delta p_x t}{m}$$

The spreading increases over time, is greater for $k$ components further from $k_0$, and it depends on the mass–the rate of spreading is evidently slower for an object with larger mass.

The "quantum revision" to Newton's first law might be something like: in the absence of external forces, the momentum-space distribution of a quantum particle remains constant, while its position-space distribution spreads over time. In other words, a free particle moves with constant *average momentum*, but its position becomes increasingly uncertain as its wave function spreads. As soon as a position measurement is made on the particle, it will spontaneously "localize," but we'll lose knowledge of the momentum.

## 4.2 Free Gaussian Wave Packet

Consider a free particle with a normalized initial wave function given by

$$\psi(x,0) = \left(\frac{1}{2\pi\sigma_x^2}\right)^{1/4} \exp\left(-\frac{x^2}{4\sigma_x^2}\right) \tag{4.9}$$

where $\sigma_x$ is a positive constant. The probability distribution $|\psi(x)|^2$ is called a Gaussian or normal distribution. In order to verify that the wave function is normalized, we need to use the following integral identity, which I'll state without proof but you can find many online:

$$\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} dx\; e^{-x^2} = 1 \tag{4.10}$$

Normalization can be demonstrated by applying a change of variables where $u = x/\sqrt{2}\sigma_x$.

$$\begin{aligned}
\int_{-\infty}^{\infty} dx\; |\psi(x)|^2 &= \left(\frac{1}{2\pi\sigma_x^2}\right)^{1/2} \int_{-\infty}^{\infty} dx\;\; \exp\left(-\frac{x^2}{2\sigma_x^2}\right) \\
&= \left(\frac{1}{2\pi\sigma_x^2}\right)^{1/2} \sqrt{2}\sigma_x \int_{-\infty}^{\infty} du\; e^{-u^2} \\
&= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} du\; e^{-u^2} \\
&= 1
\end{aligned}$$

### 4.2.1 Uncertainty Principle

According to the uncertainty principle, the product of uncertainties in position and momentum for a quantum particle in any state must satisfy the inequality

$$\Delta p_x \Delta x \geq \frac{1}{2}|\langle[\hat{x},\hat{p}_x]\rangle| = \frac{\hbar}{2} \tag{4.11}$$

As it turns out, the Gaussian wave function is a *minimum uncertainty state.* The expectation value of position in the state $\psi(x)$ is

$$\langle\hat{x}\rangle = \int_{-\infty}^{\infty} dx\; x|\psi(x)|^2 = 0$$

since $x$ is an odd function about $x = 0$ and the Gaussian distribution is even. To compute the uncertainty in position, we need to compute the expectation value of $\hat{x}^2$, which is

$$\langle \hat{x}^2 \rangle = \int_{-\infty}^{\infty} dx\ x^2 |\psi(x)|^2 = \sigma_x^2 \tag{4.12}$$

and you can verify this with integration by parts or using a fun little trick. First apply the same change of variables as before with $u = x/\sqrt{2}\sigma_x$:

$$\int_{-\infty}^{\infty} dx\ x^2 |\psi(x)|^2 = \frac{2\sigma^2}{\sqrt{\pi}} \int_{-\infty}^{\infty} du\ u^2 e^{-u^2}$$

Observe that the integral may be written in a strange but strategic form

$$\int_{-\infty}^{\infty} du\ u^2 e^{-u^2} = \int_{-\infty}^{\infty} du\ \left( -\frac{\partial}{\partial z} e^{-u^2 z} \right)_{z=1}$$

In this form, we can make use of Eq. (4.10) to compute the integral above:

$$\begin{aligned}
\int_{-\infty}^{\infty} du\ u^2 e^{-u^2} &= \int_{-\infty}^{\infty} du\ \left( -\frac{\partial}{\partial z} e^{-u^2 z} \right)_{z=1} \\
&= -\frac{d}{dz} \left[ \int du\ e^{u^2 z} \right]_{z=1} \\
&= -\frac{d}{dz} \left( \sqrt{\frac{\pi}{z}} \right)_{z=1} \\
&= \frac{\sqrt{\pi}}{2}
\end{aligned}$$

Now that we've verified the expectation value of $\hat{x}^2$, it follows that the initial uncertainty in the position is

$$\Delta x = \sqrt{\langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2} = \sigma_x \tag{4.13}$$

In order to compute the uncertainty in momentum, it will be easier to compute the momentum-space wave function $\tilde{\psi}(p_x)$. As an added benefit, this will allow us to solve for the time-evolved wave function $\psi(x, t)$ later on. Applying the Fourier transform,

$$\tilde{\psi}(p_x) = \left( \frac{1}{2\pi(\hbar/2\sigma_x)^2} \right)^{1/4} \exp\left( -\frac{p_x^2}{4(\hbar/2\sigma_x)^2} \right) \tag{4.14}$$

After some calculations, we learn that the Fourier transform of a Gaussian function is itself a Gaussian function. In this form, we can immediately identify the expectation values of $\hat{p}_x$ and $\hat{p}_x^2$ by analogy with the position-space wave function. The expectation value of $\hat{p}_x$ is zero, and the expectation value of $\hat{p}_x^2$ is $(\hbar/2\sigma_x)^2$. Hence, the uncertainty in momentum is

$$\Delta p_x = \frac{\hbar}{2\sigma_x} \tag{4.15}$$

and the product of uncertainties in position and momentum is

$$\Delta p_x \Delta x = \frac{\hbar}{2} \tag{4.16}$$

Note that the uncertainty in momentum is inversely related to the uncertainty in the position. An initial wave function with a large spread in position will have a narrow spread in momentum. As time goes on, we expect the spread in position to grow while the spread in momentum remains constant (the momentum-space distribution is stationary).

### 4.2.2 Time-Dependent Wave Function

Given the initial wave function in Eq. (4.9), the time-dependent wave function for the free particle is given by the general solution

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp_x \ \tilde{\psi}(p_x) e^{i(kx-\omega t)}$$

where $k = p_x/\hbar$ and $\omega = E/\hbar = p_x^2/2m\hbar$. Inserting $\tilde{\psi}(p_x)$, we have

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \left(\frac{1}{2\pi(\hbar/2\sigma_x)^2}\right)^{1/4} \int_{-\infty}^{\infty} dp_x \ \exp\left(-\frac{\sigma_x^2 p_x^2}{\hbar^2} + \frac{ip_x x}{\hbar} - \frac{ip_x^2 t}{2m\hbar}\right)$$

The integral may look intimidating, but we can easily extend the identity in Eq. (4.10) to handle any quadratic function by simply completing the square in the argument of the exponential. This leads to a more generally applicable integral identity:

$$\int_{-\infty}^{\infty} dx \ e^{-(ax^2+bx+c)} = \sqrt{\frac{\pi}{a}} e^{(b^2/4a)-c} \tag{4.17}$$

For the situation at hand, the argument of the exponential can be written as

$$-\frac{\sigma_x^2 p_x^2}{\hbar^2} + \frac{ip_x x}{\hbar} - \frac{ip_x^2 t}{2m\hbar} = -\sigma_x^2 \left(1 + \frac{i\hbar t}{2m\sigma_x^2}\right) \frac{p_x^2}{\hbar^2} + ix\frac{p_x}{\hbar}$$

Hence, the time-dependent wave function is

$$\psi(x,t) = \left(\frac{1}{2\pi\sigma_x^2(1+it/\tau)}\right)^{1/4} \exp\left(-\frac{x^2}{4\sigma_x^2(1+it/\tau)}\right) \tag{4.18}$$

where we've defined a time scale $\tau$ over which the wave function changes appreciably:

$$\tau = \frac{2m\sigma_x^2}{\hbar} \tag{4.19}$$

We can more easily obtain a physical interpretation of the wave function by computing the probability distribution:

$$|\psi(x,t)|^2 = \frac{1}{\sqrt{2\pi\sigma_x^2(1+t^2/\tau^2)}} \exp\left(-\frac{x^2}{2\sigma_x^2(1+t^2/\tau^2)}\right) \tag{4.20}$$

The probability distribution spreads out over time in a way that can be quantified by the uncertainty in position:

$$\Delta x(t) = \sigma_x\sqrt{1+t^2/\tau^2} \tag{4.21}$$

Evidently, $\tau$ gives us the time scale over which the probability distribution changes significantly. Notice the spreading will happen faster for less massive particles that are highly localized in their initial state. After a time interval much larger than $\tau$, i.e. $t \gg \tau$, the uncertainty in $\hat{x}$ is approximately

$$\Delta x_{t\gg\tau} \approx \frac{\sigma_x t}{\tau} = \frac{\hbar t}{2m\sigma_x} = \frac{\Delta p_x t}{m}$$

which matches the result of our dimensional argument in Section 4.1.