Wave Mechanics

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1 The time-dependent Schrödinger equation

We have seen how the time-dependent Schrodinger equation,

$$-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\Psi + V\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{1}$$

follows as a non-relativistic version of the Klein-Gordon equation. In wave mechanics, the function Ψ is called the *wave function*, although we will shortly see that its generalization is called the *state* of the system. Next, we look at its interpretation and solution.

1.1 Conservation of $\psi^*\psi$

There is a conservation law associated with the Schruodinger equation. Multiplying eq.(1) by the complex conjugate wave function, Ψ^*, we have

$$-\frac{\hbar^2}{2m}\Psi^*\boldsymbol{\nabla}^2\Psi + V\Psi^*\Psi = i\hbar\Psi^*\frac{\partial\Psi}{\partial t}$$

and the complex conjugate of this is

$$-\frac{\hbar^2}{2m}\Psi\boldsymbol{\nabla}^2\Psi^* + V\Psi^*\Psi = -i\hbar\Psi\frac{\partial\Psi^*}{\partial t}$$

Taking the difference of these gives

$$\begin{aligned}
-\frac{\hbar^2}{2m}\Psi^*\boldsymbol{\nabla}^2\Psi + V\Psi^*\Psi + \frac{\hbar^2}{2m}\Psi\boldsymbol{\nabla}^2\Psi^* - V\Psi^*\Psi &= i\hbar\Psi^*\frac{\partial\Psi}{\partial t} + i\hbar\Psi\frac{\partial\Psi^*}{\partial t} \\
\frac{\hbar^2}{2m}\left(\Psi\boldsymbol{\nabla}^2\Psi^* - \Psi^*\boldsymbol{\nabla}^2\Psi\right) &= i\hbar\frac{\partial}{\partial t}\left(\Psi^*\Psi\right) \\
\boldsymbol{\nabla}\cdot\left(-\frac{i\hbar}{2m}\left(\Psi\boldsymbol{\nabla}\Psi^* - \Psi^*\boldsymbol{\nabla}\Psi\right)\right) &= \frac{\partial}{\partial t}\left(\Psi^*\Psi\right)
\end{aligned}$$

Now define

$$\begin{aligned}
\rho &\equiv \Psi^*\Psi \\
\mathbf{J} &\equiv \frac{i\hbar}{2m}\left(\Psi\boldsymbol{\nabla}\Psi^* - \Psi^*\boldsymbol{\nabla}\Psi\right)
\end{aligned}$$

so that

$$\frac{\partial\rho}{\partial t} + \boldsymbol{\nabla}\cdot\mathbf{J} = 0$$

This is the continuity equation, and it shows that the integral of ρ over a volume V is conserved to the extent that no current $\mathbf{J}$ flows across the boundary of V. Specifically, consider

$$\begin{aligned}
\frac{d}{dt}\int_V \rho(\mathbf{x},t)\, d^3x &= \int_V \frac{\partial\rho}{\partial t} d^3x \\
&= -\int_V \boldsymbol{\nabla}\cdot\mathbf{J} d^3x \\
&= -\oint_S \mathbf{n}\cdot\mathbf{J} d^2x
\end{aligned}$$

We see that any change in $\int_V \rho(\mathbf{x},t)$ is exactly given by the flux of the current $\mathbf{J}$ across the boundary.

We interpret this integral as the probability of finding the particle described by ρ in the volume V, giving $\rho = \Psi^*\Psi$ the interpretation of a probability density. Further justification for this interpretation is given below. Since the wave function Ψ vanishes at infinity, the integral of $\rho = \Psi^*\Psi$ over all space is strictly constant. This represents the probability of finding the particle *somewhere*. In keeping with the requirments of probability, we agree to *normalize* the wave function so that this integral is one:

$$\int_{all\ space} \rho(\mathbf{x},t)\, d^3x = \int_{all\ space} \Psi^*\Psi d^3x = 1$$

1.2 Separation of the time variable and superposition

The most common approach to a solution, which works when the potential depends on position only, is separation of the time variable. Let the wave function, $\Psi(\mathbf{x},t)$ be written as a product,

$$\Psi(\mathbf{x},t) = \psi(\mathbf{x})\, T(t)$$

Substituting, we have

$$\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi(\mathbf{x}) + V(\mathbf{x})\,\psi(\mathbf{x})\right) T(t) = i\hbar\psi(\mathbf{x})\,\frac{dT(t)}{dt}$$

so dividing by Ψ we have

$$\frac{1}{\psi(\mathbf{x})}\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi(\mathbf{x}) + V(\mathbf{x})\,\psi(\mathbf{x})\right) = \frac{i\hbar}{T(t)}\frac{dT(t)}{dt}$$

Since the left side depends only on $\mathbf{x}$ and the right only on t, each side must equal some constant, which (using some foresight) we call E. Then we have two equations,

$$\begin{aligned}
-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi_E(\mathbf{x}) + V(\mathbf{x})\,\psi_E(\mathbf{x}) &= E\psi_E(\mathbf{x}) \\
-\frac{i}{\hbar}ET(t) &= \frac{dT(t)}{dt}
\end{aligned}$$

The first is the stationary state Schrödinger equation, while the second is immediately integrated to give

$$T(t) = e^{-\frac{i}{\hbar}Et}$$

There is no obvious restriction on the separation constant, E, but there will be in bound states: not every value of E will be consistent with the boundary conditions. We will see this effect shortly.

Suppose all values of the energy are allowed. Then for each value of E, we have a solution of the form,

$$\Psi_E(\mathbf{x},t) = \psi_E(E,\mathbf{x})\, e^{-\frac{i}{\hbar}Et} \tag{2}$$

Since the time-dependent Schrödinger equation is linear, any superposition of these is allowed. The general solution is an *arbitrary linear combination* of these particular ones. Introducing arbitrary amplitudes $A(E)$ for each energy of wave function, we have the general solution,

$$\Psi(\mathbf{x},t) = \int_{-\infty}^{\infty} A(E)\,\psi_E(E,\mathbf{x})\,e^{-\frac{i}{\hbar}Et}dE \tag{3}$$

Notice that while each Ψ_E oscillates with the single frequency $\omega = \frac{E}{\hbar}$, in the superposition the time behavior may become quite complex.

When we deal with bound states, so that the wave function must satisfy boundary conditions at a finite distance, the allowed energies will be discrete. Let n label the state with energy E_n, so we may write the stationary state solution as $\psi_n(\mathbf{x})$. Now the solution is a linear combination over all n,

$$\Psi(\mathbf{x},t) = \sum_{n=0}^{\infty} A_n\psi_n(E_n,\mathbf{x})\,e^{-\frac{i}{\hbar}E_nt} \tag{4}$$

where again, the constants A_n are arbitrary.

2 The time-independent Schrödinger equation

Once we have separated the time dependence, we still have a differential equation for the spatial dependence of the wave function. The remaining equation is the *stationary state Schrödinger equation*,

$$-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi_E(\mathbf{x}) + V(\mathbf{x})\,\psi_E(\mathbf{x}) = E\psi_E(\mathbf{x}) \tag{5}$$

The name stationary state refers to the fact that solutions for a single eigenvalue E have trivial time dependence,

$$\Psi = A\psi_E(\mathbf{x})\,e^{-\frac{i}{\hbar}Et}$$

with a probability density that is stationary,

$$\rho(\mathbf{x},t) = \Psi^*\Psi = |A|^2\,\psi_E^*(\mathbf{x})\,\psi_E(\mathbf{x})$$

The presence of the familiar Laplacian $\boldsymbol{\nabla}^2$ tells us to expect unique solutions once we impose boundary conditions. A linear differential operator $\mathcal{L}$ acting on a function which return a constant α times the function,

$$\mathcal{L}f = \alpha f$$

is called an *eigenvalue equation*, and the constant α is called the *eigenvalue*. Eq.(5) has this form where the linear differential operator is the Hamiltonian (in operator form) and *the energy E is the eigenvalue*. In general, we write operators with a hat, so the Hamiltonian operator is

$$\hat{H} = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(\mathbf{x})$$

and the time-dependent Schrödinger equation is

$$\hat{H}\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

The stationary state Schrödinger equation is the eigenvalue equation

$$\hat{H}\Psi = E\Psi$$

2.1 Boundary conditions

Suppose we have a boundary at $\mathbf{x}_0$ on a boundary surface S. Integrate eq.(5) from an infinitesimal distance ε on one side of the boundary to a distance ε on the other side, with $\mathbf{n}$ the unit normal to the boundary.

$$
\begin{aligned}
0 &= \int_{\mathbf{x}_0-\varepsilon\mathbf{n}}^{\mathbf{x}_0+\varepsilon\mathbf{n}} \left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi_E + V(\mathbf{x})\,\psi_E - E\psi_E\right) d\varepsilon' \\
&= \int_{\mathbf{x}_0-\varepsilon\mathbf{n}}^{\mathbf{x}_0+\varepsilon\mathbf{n}} \left(-\frac{\hbar^2}{2m}\left(\nabla_\parallel^2 + \boldsymbol{\nabla}_\perp^2\right)\psi_E + V(\mathbf{x})\,\psi_E - E\psi_E\right) d\varepsilon' \\
&= \int_{\mathbf{x}_0-\varepsilon\mathbf{n}}^{\mathbf{x}_0+\varepsilon\mathbf{n}} \left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi_E}{\partial\varepsilon'^2} - \frac{\hbar^2}{2m}\boldsymbol{\nabla}_\perp^2\psi_E + V(\mathbf{x})\,\psi_E - E\psi_E\right) d\varepsilon' \\
&= -\frac{\hbar^2}{2m}\left(\frac{\partial\psi_E}{\partial\varepsilon}(\mathbf{x}_0+\varepsilon\mathbf{n}) - \frac{\partial\psi_E}{\partial\varepsilon}(\mathbf{x}_0-\varepsilon\mathbf{n})\right) + \left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}_\perp^2\psi_E(\mathbf{x}_0) + V(\mathbf{x}_0)\,\psi_E(\mathbf{x}_0) - E\psi_E(\mathbf{x}_0)\right) 2\varepsilon
\end{aligned}
$$

Setting

$$
\begin{aligned}
\frac{\partial\psi_E}{\partial\varepsilon_+} &= \lim_{\varepsilon\longrightarrow 0}\frac{\partial\psi_E}{\partial\varepsilon}(\mathbf{x}_0+\varepsilon\mathbf{n}) \\
\frac{\partial\psi_E}{\partial\varepsilon_-} &= \lim_{\varepsilon\longrightarrow 0}\frac{\partial\psi_E}{\partial\varepsilon}(\mathbf{x}_0-\varepsilon\mathbf{n})
\end{aligned}
$$

and taking the $\varepsilon \to 0$ limit shows that $\frac{\partial\psi_E}{\partial\varepsilon_+} = \frac{\partial\psi_E}{\partial\varepsilon_-}$ so that the first derivative must be continuous across the boundary.

Returning to the general expression and integrating again,

$$
\begin{aligned}
0 &= \int_{\mathbf{x}_0-\varepsilon\mathbf{n}}^{\mathbf{x}_0+\varepsilon\mathbf{n}} \left[-\frac{\hbar^2}{2m}\left(\frac{\partial\psi_E}{\partial\varepsilon'}(\mathbf{x}_0+\varepsilon'\mathbf{n}) - \frac{\partial\psi_E}{\partial\varepsilon'}(\mathbf{x}_0-\varepsilon'\mathbf{n})\right) + \left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}_\perp^2\psi_E(\mathbf{x}_0) + V(\mathbf{x}_0)\,\psi_E(\mathbf{x}_0) - E\psi_E(\mathbf{x}_0)\right) 2\varepsilon'\right] d\varepsilon' \\
&= -\frac{\hbar^2}{2m}\left(\psi_E(\mathbf{x}_0+\varepsilon\mathbf{n}) - \psi_E(\mathbf{x}_0-\varepsilon\mathbf{n})\right) + \left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}_\perp^2\psi_E(\mathbf{x}_0) + V(\mathbf{x}_0)\,\psi_E(\mathbf{x}_0) - E\psi_E(\mathbf{x}_0)\right)\varepsilon^2
\end{aligned}
$$

Again taking $\varepsilon \to 0$, we see that $\psi_+(\mathbf{x}_0) = \psi_-(\mathbf{x}_0)$. Therefore, at a boundary both the wave function and its first derivative must be continuous:

$$
\begin{aligned}
\psi_+(\mathbf{x}_0) &= \psi_-(\mathbf{x}_0) \\
\frac{\partial\psi_E}{\partial\varepsilon_+} &= \frac{\partial\psi_E}{\partial\varepsilon_-}
\end{aligned}
\tag{6}
$$

There is an exception to this if the potential diverges at the boundary, since then the potential term in the first limit may be finite,

$$
\infty > \left|\lim_{\varepsilon\longrightarrow 0} 2\varepsilon V(\mathbf{x}_0)\,\psi_E(\mathbf{x}_0)\right| > 0
$$

In such cases, the first derivative may have a discontinuity. This happens with infinite square well potentials and with delta function potentials. The additional constraint needed to determine the solution is generally provided by the vanishig of the wave function beyond the infinite barrier. While these examples are obviously idealizations, they often reveal certain quantum properties correctly, and in a simpler context.

3 Vacuum solution in one dimension

We may use the boundary conditions to construct a wide range of quantum mechanical solutions. For example, any piecewise constant potential is easily handled.

In 1-dimension, eq.(5) reduces to

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

We will consider several one-dimensional solutions; here we explore a free Gaussian wave packet in detail.

3.1 Free particle

3.1.1 Plane waves

If there is no potential, the Schrödinger equation reduces to

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_E(x)}{dx^2} = E\psi_E(x)$$

This has simple oscillatory form. If we define $k = +\sqrt{\frac{2mE}{\hbar^2}}$ then we have

$$\frac{d^2\psi_E}{dx^2} + k^2\psi_E = 0$$

with solutions

$$\psi_E = \frac{A}{\sqrt{2\pi}}e^{ikx} + \frac{B}{\sqrt{2\pi}}e^{-ikx}$$

where $A(E)$ and $B(E)$ are arbitrary and the $\sqrt{2\pi}$ factor is chosen for later convenience. When we impose boundary conditions, some linear combinations of these will be ruled out, but the appropriate conditions depend on our interpretation of these solutions.

To see what the solutions mean, we look at the time-dependent eigenfunctions

$$\Psi_E(x,t) = Ae^{\frac{i}{\hbar}(\hbar kx - Et)} + Be^{-\frac{i}{\hbar}(\hbar kx + Et)}$$

We can extract the energy and momentum associated with this state by acting with the energy and momentum operators. Consider the right moving wave given by setting $B = 0$. We have

$$\begin{aligned}
\hat{H}\Psi_E(x,t) &= i\hbar\frac{\partial}{\partial t}\Psi_E(x,t) \\
&= E\Psi_E(x,t) \\
\hat{p}\Psi_E(x,t) &= -i\hbar\frac{d}{dx}\Psi_E(x,t) \\
&= \hbar k\Psi_E(x,t)
\end{aligned}$$

To extract just the eigenvalues, multiply by Ψ and integrate,

$$\begin{aligned}
\int_V \Psi_E^*\hat{H}\Psi_E dx &= E\int_V \Psi_E^*\Psi_E dx \\
&= E\int_V \rho dx
\end{aligned}$$

The integral on the right is conserved throughout the evolution. If we take the volume V to include all space available to the particle, then there can be no flux across the boundary and the integral is constant.

These plane wave solutions are not normalizable over the whole real line. Instead, we may use a "box" normalization. Normalized on a box of length L,

$$\begin{aligned}
1 &= |A|^2 \int_0^L e^{-\frac{i}{\hbar}(\hbar kx - Et)} e^{\frac{i}{\hbar}(\hbar kx - Et)} dx \\
1 &= |A|^2 L \\
A &= \frac{1}{\sqrt{L}}
\end{aligned}$$

Then

$$\int_0^L \Psi_E^* \hat{H} \Psi_E dx = E$$

Similarly,

$$\int_0^L \Psi_E^* \hat{p} \Psi_E dx = \hbar k$$

so we recover the de Broglie and Planck relations for a plane wave $e^{i(kx-\omega t)} = e^{\frac{i}{\hbar}(px-Et)}$. These integrals are called *expectation values.*

Since $\int_V \rho$ is conserved, we may evaluate it at any time. Quite generally, choosing the initial time, we see that

$$\int_V \Psi^* \Psi dx = \int_V \psi^* \psi dx$$

so normalizing the stationary state solution is sufficient to normalize the full time-dependent solution.

3.1.2 Superposition

As noted above, the plane wave solution cannot satisfy the normalization condition, since

$$\begin{aligned}
\int_V \Psi_E^* \Psi_E dx &= \int_V e^{-\frac{i}{\hbar}(px-Et)} e^{\frac{i}{\hbar}(px-Et)} dx \\
&= V
\end{aligned}$$

which diverges if V is an unbounded region. This leads us to an additional condition. We will restrict our attention to those solutions of the Schrödinger equation which are *square integrable*, meaning that $\int_V \Psi_E^* \Psi_E dx$ is bounded. The sum of any linear combination of a finite number of square integrable functions is also square integrable, as well as a well-defined set of infinite combinations.

Returning our attention to the general solution for a free particle, we display a class of square-integrable solutions. First, notice that since $E = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m} > 0$ we can label states by k instead of E, and integrate over all k rather than positive E,

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{ikx} dk$$

We now need only choose $A(k)$ so that

$$1 = \int_V \psi^* \psi dx$$

$$
\begin{aligned}
&= \frac{1}{2\pi}\int_V dx \left(\int_{-\infty}^{\infty} A^*(q)\,e^{-iqx}dq\right)\left(\int_{-\infty}^{\infty} A(k)\,e^{+ikx}dk\right) \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} dq \int_{-\infty}^{\infty} dk A^*(q)\,A(k)\int_V dx e^{i(k-q)x} \\
&= \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dq A^*(k)\,A(q)\,\delta(q-k) \\
&= \int_{-\infty}^{\infty} dk\,|A(k)|^2
\end{aligned}
$$

Therefore, any function $A(k)$ satisfying

$$
\int_{-\infty}^{\infty} dk\,|A(k)|^2 = 1 \tag{7}
$$

gives an allowed superposition state.

Example: Gaussian wave packet Consider a Gaussian superposition in momentum space (since $p = \hbar k$), $A(k) = Ae^{-\frac{(k-k_0)^2}{4\sigma^2}}$ for any constants A, σ. Normalizing this, we require

$$
\begin{aligned}
1 &= \int_{-\infty}^{\infty} dk\,|A(k)|^2 \\
&= A^2\int_{-\infty}^{\infty} e^{-\frac{(k-k_0)^2}{2\sigma^2}}dk
\end{aligned}
$$

To integrate the Gaussian, let $y = \frac{k-k_0}{\sqrt{2\sigma^2}}$ so we have

$$
\int_{-\infty}^{\infty} e^{-\frac{(k-k_0)^2}{2\sigma^2}}dk = \sqrt{2\sigma^2}\int_{-\infty}^{\infty} e^{-y^2}dy
$$

then defining $I = \int_{-\infty}^{\infty} e^{-y^2}dy$ consider I^2

$$
\begin{aligned}
I^2 &= \int_{-\infty}^{\infty} e^{-y^2}dy\int_{-\infty}^{\infty} e^{-z^2}dz \\
&= \int_0^{2\pi}\int_0^{\infty} e^{-r^2}r\,d\theta\,dr \\
&= 2\pi\int_0^{\infty} e^{-r^2}r\,dr
\end{aligned}
$$

where we convert the integral over the yz plane to polar coordinates. Then letting $\chi = r^2$, the integral is trivial

$$
I^2 = \pi\int_0^{\infty} e^{-\chi}d\chi = \pi
$$

so that $I=\sqrt{\pi}$. Returning to the normalization,

$$\int_{-\infty}^{\infty} e^{-\frac{(k-k_0)^2}{2\sigma^2}}dk=\sqrt{2\pi\sigma^2}$$

and we choose $A=\frac{1}{(2\pi\sigma^2)^{1/4}}$. With this choice $A(k)$ satisfies the normalization condition, eq.(7), guaranteeing that the corresponding wave function is normalized.

The normalized state itself is therefore

$$\psi(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left(\frac{1}{(2\pi\sigma^2)^{1/4}}e^{-\frac{(k-k_0)^2}{4\sigma^2}}\right)e^{ikx}dk$$

To see the spatial form of wave function, we carry out this Gaussian integral. Expanding the exponent,

$$\begin{aligned}\psi(x) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left(\frac{1}{(2\pi\sigma^2)^{1/4}}e^{-\frac{(k-k_0)^2}{4\sigma^2}}\right)e^{ikx}dk\\ &= \frac{1}{\sqrt{2\pi}}\frac{1}{(2\pi\sigma^2)^{1/4}}\int_{-\infty}^{\infty}\exp\left(-\frac{1}{4\sigma^2}\left(k^2-2kk_0+k_0^2\right)+ikx\right)dk\\ &= \frac{1}{\sqrt{2\pi}}\frac{1}{(2\pi\sigma^2)^{1/4}}\int_{-\infty}^{\infty}\exp\left(-\left(\frac{1}{4\sigma^2}k^2-\left(\frac{1}{2\sigma^2}k_0-ix\right)k+\frac{1}{4\sigma^2}k_0^2\right)\right)dk\end{aligned}$$

we complete the square,

$$\begin{aligned}\frac{1}{4\sigma^2}k^2-\left(\frac{1}{2\sigma^2}k_0-ix\right)k+\frac{1}{4\sigma^2}k_0^2 &= \left(\frac{1}{2\sigma}k-\sigma\left(\frac{1}{2\sigma^2}k_0-ix\right)\right)^2-\sigma^2\left(\frac{1}{2\sigma^2}k_0-ix\right)^2+\frac{1}{4\sigma^2}k_0^2\\ &= y^2-\sigma^2\left(\frac{1}{2\sigma^2}k_0-ix\right)^2+\frac{1}{4\sigma^2}k_0^2\\ &= y^2-\frac{1}{4\sigma^2}k_0^2+ik_0x+\sigma^2x^2+\frac{1}{4\sigma^2}k_0^2\\ &= y^2+ik_0x+\sigma^2x^2\end{aligned}$$

where we have defined a new integration variable

$$\begin{aligned}y &\equiv \frac{1}{2\sigma}k-\sigma\left(\frac{1}{2\sigma^2}k_0-ix\right)\\ dy &= \frac{1}{2\sigma}dk\end{aligned}$$

The wave function now becomes

$$\begin{aligned}\psi(x) &= \frac{1}{\sqrt{2\pi}}\frac{1}{(2\pi\sigma^2)^{1/4}}\int_{-\infty}^{\infty}\exp\left(-\left(y^2+ik_0x+\sigma^2x^2\right)\right)2\sigma dy\\ &= \frac{1}{\sqrt{2\pi}}\frac{2\sigma}{(2\pi\sigma^2)^{1/4}}e^{-ik_0x-\sigma^2x^2}\int_{-\infty}^{\infty}e^{-y^2}dy\\ &= \frac{1}{\sqrt{2}}\frac{2\sigma}{(2\pi\sigma^2)^{1/4}}e^{-ik_0x-\sigma^2x^2}\end{aligned}$$

Therefore,

$$\psi(x) = \left(\frac{2\sigma^2}{\pi}\right)^{1/4} e^{-\sigma^2 x^2} e^{-ik_0 x}$$

which is simply an oscillation with wave number k_0 in a Gaussian envelope.

3.1.3 Time evolution of the free Gaussian wave packet

The Gaussian wave packet is a solution to the stationary state Schrödinger equation. To have a full time-dependent solution we need to multiply each plane-wave mode by the corresponding energy phase, $e^{-\frac{i}{\hbar}Et}$.

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k)\, e^{ikx} e^{-\frac{i}{\hbar}E(k)t} dk$$

where $E(k) = \frac{\hbar^2 k^2}{2m}$. Substituting this, and the normalized Gaussian amplitude $A(k)$

$$\Psi(x,t) = \frac{1}{(8\pi^3\sigma^2)^{1/4}} \int_{-\infty}^{\infty} \exp\left(-\left(\frac{(k-k_0)^2}{4\sigma^2} - ikx + \frac{i\hbar k^2}{2m}t\right)\right) dk$$

To perform the wave vector integral, we complete the square in the modified exponent,

$$\begin{aligned}
\frac{(k-k_0)^2}{4\sigma^2} - ikx + \frac{i\hbar k^2}{2m}t &= \left(\frac{1}{4\sigma^2} + \frac{i\hbar}{2m}t\right)k^2 - \left(\frac{k_0}{2\sigma^2} + ix\right)k + \frac{k_0^2}{4\sigma^2} \\
&= \left[\sqrt{\frac{1}{4\sigma^2} + \frac{i\hbar}{2m}t}k - \frac{1}{2\sqrt{\frac{1}{4\sigma^2} + \frac{i\hbar}{2m}t}}\left(\frac{k_0}{2\sigma^2} + ix\right)\right]^2 - \left(\frac{1}{2\sqrt{\frac{1}{4\sigma^2} + \frac{i\hbar}{2m}t}}\left(\frac{k_0}{2\sigma^2} + ix\right)\right)^2 + \frac{k_0^2}{4\sigma^2} \\
&= y^2 - \frac{\sigma^2}{1 + \frac{2i\hbar\sigma^2}{m}t}\left(\frac{k_0}{2\sigma^2} + ix\right)^2 + \frac{k_0^2}{4\sigma^2} \\
&= y^2 - \frac{1}{1 + \frac{2i\hbar\sigma^2}{m}t}\left(\frac{k_0^2}{4\sigma^2} + ik_0 x - \sigma^2 x^2 - \frac{k_0^2}{4\sigma^2}\left(1 + \frac{2i\hbar\sigma^2}{m}t\right)\right) \\
&= y^2 - \frac{1}{1 + \frac{2i\hbar\sigma^2}{m}t}\left(ik_0 x - \sigma^2 x^2 - \frac{i\hbar k_0^2}{2m}t\right)
\end{aligned}$$

where

$$y = \sqrt{\frac{1}{4\sigma^2} + \frac{i\hbar}{2m}t}k - \frac{1}{2\sqrt{\frac{1}{4\sigma^2} + \frac{i\hbar}{2m}t}}\left(\frac{k_0}{2\sigma^2} + ix\right)$$

Let $E_0 \equiv \frac{\hbar^2 k_0^2}{2m}$ and $p_0 = \hbar k_0$ and define the time-dependent width

$$\Delta(t) \equiv \frac{1}{\sigma}\sqrt{1 + \frac{2i\hbar\sigma^2}{m}t}$$

Then

$$\begin{aligned}
\Psi(x,t) &= \frac{1}{(8\pi^3\sigma^2)^{1/4}} \exp\frac{1}{1 + \frac{2i\hbar\sigma^2}{m}t}\left(ik_0 x - \sigma^2 x^2 - \frac{i\hbar k_0^2}{2m}t\right) \int_{-\infty}^{\infty} e^{-y^2} \frac{dy}{\sqrt{\frac{1}{4\sigma^2} + \frac{i\hbar}{2m}t}} \\
&= \frac{\sqrt{2}\sigma}{(2\pi)^{1/4}} \frac{1}{\sqrt{1 + \frac{2\sigma^2 i\hbar t}{m}}} \exp\frac{1}{1 + \frac{2i\hbar\sigma^2}{m}t}\left(ik_0\left(x - \frac{\hbar k_0}{2m}t\right) - \sigma^2 x^2\right) \\
&= \left(\frac{2}{\pi\sigma^2}\right)^{1/4} \frac{1}{\Delta(t)} e^{-\frac{x^2}{\Delta(t)^2}} \exp\exp\left(\frac{i}{\hbar}\frac{p_0 x - E_0 t}{\sigma^2\Delta^2}\right)
\end{aligned}$$

To see how the position evolves, we must look at the probability density. A great deal of the time dependence is hidden in the width, $\Delta(t)$.

3.1.4 Time evolution of the probability density

Compute the probability density,

$$\Psi^*\Psi = \frac{1}{\Delta^*\Delta}\left(\frac{2}{\pi\sigma^2}\right)^{1/2} e^{-\frac{x^2}{\Delta^2}} e^{-\frac{x^2}{\Delta^{*2}}} \exp\left(\frac{i}{\hbar}\frac{p_0 x - E_0 t}{\sigma^2\Delta^2}\right)\exp\left(-\frac{i}{\hbar}\frac{p_0 x - E_0 t}{\sigma^2\Delta^{*2}}\right)$$

Then

$$\begin{aligned}\Delta(t) &\equiv \frac{1}{\sigma}\sqrt{1+\frac{2i\hbar\sigma^2}{m}t}\\ \Delta^*\Delta &\equiv \frac{1}{\sigma^2}\sqrt{1+\frac{4\hbar^2\sigma^4}{m^2}t^2}\end{aligned}$$

For the exponentials, we have the phase,

$$\begin{aligned}-\frac{x^2}{\Delta^2}-\frac{x^2}{\Delta^{*2}}+\frac{i}{\hbar\sigma^2}(p_0x-E_0t)\left(\frac{1}{\Delta^2}-\frac{1}{\Delta^{*2}}\right) &= -x^2\frac{1}{\Delta^2\Delta^{*2}}\left(\Delta^{*2}+\Delta^2\right)+\frac{i}{\hbar\sigma^2}(p_0x-E_0t)\frac{1}{\Delta^2\Delta^{*2}}\left(\Delta^{*2}-\Delta^2\right)\\ &= \frac{1}{\Delta^2\Delta^{*2}}\left(-x^2\left(\Delta^{*2}+\Delta^2\right)+\frac{i}{\hbar\sigma^2}(p_0x-E_0t)\left(\Delta^{*2}-\Delta^2\right)\right)\\ &= \frac{1}{\Delta^2\Delta^{*2}}\frac{1}{\sigma^2}\left(-x^2(2)+\frac{i}{\hbar\sigma^2}(p_0x-E_0t)\left(-\frac{4i\hbar\sigma^2}{m}t\right)\right)\\ &= \frac{1}{\Delta^2\Delta^{*2}}\frac{2}{\sigma^2}\left(-x^2+\frac{2p_0tx}{m}-\frac{p_0^2}{m^2}t^2\right)\\ &= -\frac{1}{\Delta^2\Delta^{*2}}\frac{2}{\sigma^2}\left(x-\frac{p_0}{m}t\right)^2\end{aligned}$$

Therefore, the probability density evolves as a Gaussian,

$$\Psi^*\Psi = \frac{1}{\sqrt{1+\frac{4\hbar^2\sigma^4}{m^2}t^2}}\left(\frac{2\sigma^2}{\pi}\right)^{1/2}\exp\left[-\frac{2\sigma^2\left(x-\frac{p_0}{m}t\right)^2}{1+\frac{4\hbar^2\sigma^4}{m^2}t^2}\right]$$

The amplitude decreases in time while the width of the Gaussian increases. Meanwhile, the center of the Gaussian moves to the right with velocity $v=\frac{p_0}{m}$.