This paper deals with the probability density for a free particle.

Hope I can help you with learning quantum mechanics.

Note: This is an experimental text and may contain errors.

Contents

Probability density in 1D

The wave function for a free particle:

$$\psi(x,t)$$

The probability P of finding a particle anywhere in space must be one:

$$P(t) = \int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = 1$$

Note: $P(t)$ still is a function of time. But if the particle is stable und would not disappear, the integral must be one for all times. With this assumption $P(t) = 1$ for all times, a constant.

This needs the properties:

$$\lim_{x\to\pm\infty} \psi(x,t) = 0$$

$$\lim_{x\to\pm\infty} \frac{\partial}{\partial x}\psi(x,t) = c < \infty$$

Note: from $\lim_{x\to\pm\infty} \psi(x,t) = 0$ we can deduct that c must be zero.

Probability density

We interpret $|\psi(x,t)|^2$ as a probability distribution $\rho(x,t)$:

$$\rho(x,t) = |\psi(x,t)|^2 = \psi^*(x,t)\psi(x,t)$$

The probability then is the integral:

$$P(t) = \int \rho(x,t) dx$$

The probability over the whole space at any time, especially at time t_0:

$$P(t_0) = 1$$

This holds regardless of what we do with the particle, if we do not destroy it.

If $P(t) = const$ then $\frac{dP}{dt} = 0$.

$$\frac{dP}{dt} = \int \frac{\partial}{\partial t}\rho(x,t)dx = \int \frac{\partial}{\partial t}\big(\psi^*(x,t)\psi(x,t)\big)dx =$$

$$\int \left(\frac{\partial}{\partial t}\psi^*(x,t)\right)\psi(x,t) + \psi^*(x,t)\left(\frac{\partial}{\partial t}\psi(x,t)\right)dx$$

From the Schroedinger equation we use the time dependency of the wave function:

$$\frac{\partial\psi(x,t)}{\partial t} = -\frac{i}{\hbar}\hat{H}\psi(x,t)$$

$$\frac{\partial\psi^*(x,t)}{\partial t} = \frac{i}{\hbar}\big(\hat{H}\psi\big)^*$$

We insert this into the probability distribution:

$$\frac{dP}{dt} = \frac{i}{\hbar}\int \Big(\hat{H}\psi(x,t)\Big)^* \psi(x,t) - \psi^*(x,t)\hat{H}\psi(x,t)dx$$

The particle is stable; it will not vanish in time:

$$\frac{dP}{dt} = 0$$

We get:

$$\int \left(\hat{H}\psi(x,t)\right)^* \psi(x,t) - \psi^*(x,t)\hat{H}\psi(x,t)dx = 0$$

$$\int \hat{H}^*\psi^*(x,t)\psi(x,t)dx = \int \psi^*(x,t)\hat{H}\psi(x,t)dx$$

As we work with operators this is true if the Hamiltonian is Hermitian:

$$\hat{H} = \hat{H}^\dagger$$

We know that the Hamiltonian is Hermitian:

$$H^* = H = -\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial x}\right)^2 + V(x)$$

We get:

$$\frac{dP}{dt} = \int \frac{\partial}{\partial t}\rho(x,t)dx = \frac{i}{\hbar}\int \left(\hat{H}\psi(x,t)\right)^* \psi(x,t) - \psi^*(x,t)\hat{H}\psi(x,t)dx$$

We calculate the integral:

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

$$-\frac{\hbar^2}{2m}\left(\left(\frac{\partial}{\partial x}\right)^2 \psi^*(x,t)\right)\psi(x,t) + V(x)\psi^*(x,t)\psi(x,t) + \psi^*(x,t)\frac{\hbar^2}{2m}\left(\left(\frac{\partial}{\partial x}\right)^2 \psi(x,t)\right) - \psi^*(x,t)V(x)\psi(x,t) =;$$

Real operators commute. The potential $V(x)$ is real, so $V(x)\psi^*(x,t)\psi(x,t)$ and $-\psi^*(x,t)V(x)\psi(x,t)$ cancel out.

We get:

$$-\frac{\hbar^2}{2m}\left(\left(\frac{\partial}{\partial x}\right)^2 \psi^*(x,t)\right)\psi(x,t) + \psi^*(x,t)\frac{\hbar^2}{2m}\left(\left(\frac{\partial}{\partial x}\right)^2 \psi(x,t)\right)$$

We multiply the missing factor $\frac{i}{\hbar}$ we left out in the calculation and get:

$$\frac{\partial}{\partial t}\rho(x,t) = -\frac{i\hbar}{2m}\left(\left(\left(\frac{\partial}{\partial x}\right)^2 \psi^*(x,t)\right)\psi(x,t) - \psi^*(x,t)\left(\left(\frac{\partial}{\partial x}\right)^2 \psi(x,t)\right)\right)$$

We calculate the probability P that a particle is between position x_1 and x_2:

$$P(x_1 < x < x_2, t) = \int_{x_1}^{x_2} \rho(x,t)dx$$

We rewrite x_1 and x_2 by $x - \varepsilon$ and $x + \varepsilon$ use the infinitesimal procedure $\varepsilon \to 0$:

$$x_1 = x - \varepsilon \qquad x_2 = x + \varepsilon$$

In this case we get the value of the integral:

$$P(x,t) = \rho(x,t) \cdot 2\varepsilon$$

provided that the function $\rho(x,t)$ behaves steadily enough (no definition gaps, no uncontrolled oscillations etc.)

Now we define a probability density flowing through positions $x - \varepsilon$ and $x + \varepsilon$:

$$\frac{dP(x,t)}{dt} \coloneqq j(x-\varepsilon) - j(x+\varepsilon)$$

The reason for this: The particle is "undestroyable", so is its probability. Even "parts" of the probability, the probability density is "undestroyable". If the probability changes in regions on the x-axis this can only be the case if some of the probability "flows out" or "flows in" into that region. Probability density comes into effect.

$j(x-\varepsilon)$ is the density at position $(x-\varepsilon)$, $j(x+\varepsilon)$ is the density at position $(x+\varepsilon)$.

We convert:

$$\frac{dP(x,t)}{dt} = j(x-\varepsilon) - j(x+\varepsilon) \to$$

We use $P(x,t) = \rho(x,t) \cdot 2\varepsilon$

$$\frac{d}{dt}(\rho(x,t) \cdot 2\varepsilon) = j(x-\varepsilon) - j(x+\varepsilon)$$

$$\frac{d}{dt}\rho(x,t) = -\frac{j(x+\varepsilon) - j(x-\varepsilon)}{2\varepsilon}$$

We remember that this is the definition of the derivative:

$$\frac{j(x+\varepsilon) - j(x-\varepsilon)}{2\varepsilon} = \frac{d}{dx}j(x,t)$$

We have the standard continuity equation, valid for any kind of fluid (and the probability fluid too):

$$\frac{d}{dt}\rho(x,t) = -\frac{d}{dx}j(x,t)$$

This means: The change of the probability distribution in time is given by the probability density in space. If there is a change in the probability of finding a particle in the same space interval, then there must be a probability density in time. On the other hand, if there is no probability density or the probability flow "in" on the left boundary is the same as the probability flow "out" on the right boundary, then there is no change in probability density (Gauss's law).

If a state is an energy eigenstate, then it is stationary:

$$\frac{d}{dt}\rho(x,t) = 0 \rightarrow \rho(x,t) = \rho(x,0)$$

$$\frac{d}{dt}j(x,t) = 0 \rightarrow j(x,t) = j(x,0)$$

ρ and j depend on x only.

For energy eigenstates we can conclude:

$$if\ \frac{d}{dx}j(x,t) = 0\ \ then\ \ j = const$$

Developing the probability density

We express the probability distribution by wave functions:

$$\rho(x,t) = \psi^*(x,t)\psi(x,t)$$

We use the standard continuity equation:

$$\frac{d}{dx}j(x,t) = -\frac{d}{dt}\rho(x,t)$$

We insert the probability distribution:

$$\frac{d}{dx}j(x,t) = -\frac{d}{dt}\big(\psi^*(x,t)\psi(x,t)\big) =$$

$$-\left(\frac{d}{dt}\psi^*(x,t)\right)\psi(x,t) - \psi^*(x,t)\left(\frac{d}{dt}\psi(x,t)\right)$$

We get:

$$\frac{d}{dx}j(x,t) = -\left(\frac{d}{dt}\psi^*(x,t)\right)\psi(x,t) - \psi^*(x,t)\left(\frac{d}{dt}\psi(x,t)\right)$$

Note: for convenience, in the following we omit the bracket (x,t) and write ψ instead of $\psi(x,t)$, ψ^* instead of $\psi^*(x,t)$, j instead of $j(x,t)$.

We use the Hamiltonian:

$$H^* = H = -\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial x}\right)^2 + V(x)$$

Note: H is Hermitian.

Note: The Hamiltonian is not an explicit function of time.

We use the Schroedinger equation for a single nonrelativistic particle in one dimension:

$$\frac{d\psi}{dt} = -\frac{i}{\hbar}H\psi$$

$$\left(\frac{d\psi}{dt}\right)^* = \left(-\frac{i}{\hbar}H\psi\right)^* = \frac{i}{\hbar}H^*\psi^* = \frac{i}{\hbar}H\psi^*$$

Note: $H^* = H$

We calculate:

$$-\left(\frac{d}{dt}\psi^*\right)\psi-\psi^*\left(\frac{d}{dt}\psi\right)=-\left(\frac{i}{\hbar}H\psi^*\right)\psi-\psi^*\left(-\frac{i}{\hbar}H\psi\right)=$$

$$-\left(\frac{i}{\hbar}H\psi^*\right)\psi+\psi^*\left(\frac{i}{\hbar}H\psi\right)=$$

$$\frac{i}{\hbar}\big(-(H\psi^*)\psi+\psi^*(H\psi)\big)=$$

$$\frac{i}{\hbar}\left(-\left(\left(-\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial x}\right)^2+V(x)\right)\psi^*\right)\psi+\psi^*\left(\left(-\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial x}\right)^2+V(x)\right)\psi\right)\right)=$$

$$\frac{i}{\hbar}\left(\left(\frac{\hbar^2}{2m}\left(\frac{\partial\psi^*}{\partial x}\right)^2-V(x)\psi^*\right)\psi+\psi^*\left(-\frac{\hbar^2}{2m}\left(\frac{\partial\psi}{\partial x}\right)^2+V(x)\psi\right)\right)=$$

$$\frac{i}{\hbar}\left(\frac{\hbar^2}{2m}\left(\frac{\partial\psi^*}{\partial x}\right)^2\psi-V(x)\psi^*\psi-\psi^*\frac{\hbar^2}{2m}\left(\frac{\partial\psi}{\partial x}\right)^2+\psi^*V(x)\psi\right)=$$

Note: $V(x)$ is real and commutes with ψ^*.

$$\frac{i}{\hbar}\left(\frac{\hbar^2}{2m}\left(\frac{\partial\psi^*}{\partial x}\right)^2\psi-\psi^*\frac{\hbar^2}{2m}\left(\frac{\partial\psi}{\partial x}\right)^2\right)=$$

$$\frac{i\hbar}{2m}\left(\left(\frac{\partial\psi^*}{\partial x}\right)^2\psi-\psi^*\left(\frac{\partial\psi}{\partial x}\right)^2\right)$$

What we have so far is:

$$\frac{d}{dx}j=\frac{i\hbar}{2m}\left(\left(\frac{\partial\psi^*}{\partial x}\right)^2\psi-\psi^*\left(\frac{\partial\psi}{\partial x}\right)^2\right)$$

It would be nice if we could have a $\frac{d}{dx}$ too on the right side. We get this by remembering:

$$\left(\frac{\partial\psi^*}{\partial x}\right)^2\psi-\psi^*\left(\frac{\partial\psi}{\partial x}\right)^2=\frac{d}{dx}\left(\left(\frac{\partial\psi^*}{\partial x}\right)\psi-\psi^*\left(\frac{\partial\psi}{\partial x}\right)\right)$$

We write:

$$\frac{d}{dx}j=\frac{i\hbar}{2m}\frac{d}{dx}\left(\left(\frac{\partial\psi^*}{\partial x}\right)\psi-\psi^*\left(\frac{\partial\psi}{\partial x}\right)\right)$$

We get the probability density j:

$$j=\frac{i\hbar}{2m}\left(\left(\frac{\partial\psi^*}{\partial x}\right)\psi-\psi^*\left(\frac{\partial\psi}{\partial x}\right)\right)$$

Note: This is valid up to a constant.

We use the identity for complex numbers:

$$z-z^*=2\cdot i\cdot Im(z)$$

We get the probability density:

$$j = \frac{\hbar}{m} \cdot Im\left(\psi^* \left(\frac{\partial\psi}{\partial x}\right)\right)$$

Probability density in 3D

The Schroedinger equation in three dimensions:

$$\frac{\partial\psi}{\partial t} = -\frac{i}{\hbar}H\psi = -\frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})\right)\psi = \frac{i\hbar}{2m}\nabla^2\psi - \frac{i}{\hbar}V(\vec{x})\psi$$

The complex conjugate:

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

The probability distribution:

$$\rho(\vec{x},t) = |\psi(\vec{x},t)|^2 = \psi^*(\vec{x},t)\psi(\vec{x},t)$$

The time derivative of the probability distribution:

$$\frac{\partial}{\partial t}\rho(\vec{x},t) = \left(\frac{\partial}{\partial t}\psi^*(\vec{x},t)\right)\psi(\vec{x},t) + \psi^*(\vec{x},t)\left(\frac{\partial}{\partial t}\psi(\vec{x},t)\right) =$$

$$\left(-\frac{i\hbar}{2m}\nabla^2\psi^* + \frac{i}{\hbar}V(\vec{x})\psi^*\right)\psi(\vec{x},t) + \psi^*(\vec{x},t)\left(\frac{i\hbar}{2m}\nabla^2\psi - \frac{i}{\hbar}V(\vec{x})\psi\right) =$$

$$-\frac{i\hbar}{2m}(\nabla^2\psi^*)\psi + \frac{i}{\hbar}V(\vec{x})\psi^*\psi + \psi^*\frac{i\hbar}{2m}\nabla^2\psi - \psi^*\frac{i}{\hbar}V(\vec{x})\psi =;$$

We use that $V(\vec{x})$ commutes with ψ and ψ^*:

$$-\frac{i\hbar}{2m}(\nabla^2\psi^*)\psi + \psi^*\frac{i\hbar}{2m}\nabla^2\psi =$$

$$-\frac{i\hbar}{2m}\big((\nabla^2\psi^*)\psi - \psi^*(\nabla^2\psi)\big)$$

We use:

$$(\nabla^2\psi^*)\psi - \psi^*(\nabla^2\psi) = \nabla \cdot \big((\nabla\psi^*)\psi - \psi^*(\nabla\psi)\big)$$

We get:

$$\frac{\partial}{\partial t}\rho(\vec{x},t) = -\nabla \cdot \frac{i\hbar}{2m}\big((\nabla\psi^*)\psi - \psi^*(\nabla\psi)\big)$$

We use the identity for complex numbers:

$$z - z^* = 2 \cdot i \cdot Im(z)$$

We get:

$$\frac{\partial}{\partial t}\rho(\vec{x},t) = -\nabla\left(\frac{i\hbar}{2m} \cdot 2 \cdot i \cdot Im\big(\psi^*(\nabla\psi)\big)\right) = \nabla \cdot \left(\frac{\hbar}{m} \cdot Im\big(\psi^*(\nabla\psi)\big)\right)$$

The standard continuity equation:

$$\frac{\partial}{\partial t}\rho(\vec{x},t) = -\nabla \cdot j(\vec{x},t)$$

We insert the time derivative of the probability distribution:

$$\nabla \cdot \left(\frac{\hbar}{m} \cdot Im\big(\psi^*(\nabla\psi)\big)\right) = -\nabla j(\vec{x},t)$$

We get the probability density:

$$j(\vec{x},t) = \left(\frac{\hbar}{m} \cdot Im\big(\psi^*(\nabla\psi)\big)\right)$$

Applications 1D

App_1:

$$\psi(x,0) = Ae^{\gamma x}, \qquad A \in \mathbb{C}, \gamma \in \mathbb{R}$$

We have:

$$j(\vec{x},0) = \frac{\hbar}{m} \cdot Im\left(\psi^*\left(\frac{\partial}{\partial x}\psi\right)\right)$$

$$\psi^*(x,0) = A^* e^{\gamma x}$$

$$\frac{\partial}{\partial x}\psi(x) = \gamma A e^{\gamma x}$$

$$\psi^*\left(\frac{\partial}{\partial x}\psi\right) = A^* e^{\gamma x}\gamma A e^{\gamma x} = \gamma |A|^2 e^{2\gamma x} \in \mathbb{R} \Longrightarrow j(\vec{x},0) = \frac{\hbar}{m} \cdot Im\left(\psi^*\left(\frac{\partial}{\partial x}\psi\right)\right) = 0$$

Note: $\psi^*\left(\frac{\partial}{\partial x}\psi\right)$ is a real quantity

App_2:

$$\psi(x,0) = N(x)e^{i\frac{S(x)}{\hbar}}, \qquad N(x), S(x) \in \mathbb{R}$$

We have:

$$j(\vec{x},0) = \frac{\hbar}{m} \cdot Im\left(\psi^*\left(\frac{\partial}{\partial x}\psi\right)\right)$$

$$\psi^*(x,0) = N(x)e^{-i\frac{S(x)}{\hbar}}$$

$$\frac{\partial}{\partial x}\psi(x) = \left(\frac{\partial}{\partial x}N(x)\right)e^{i\frac{S(x)}{\hbar}} + N(x)\frac{i}{\hbar}e^{i\frac{S(x)}{\hbar}}\frac{\partial}{\partial x}S(x)$$

$$\psi^*\left(\frac{\partial}{\partial x}\psi\right) = N(x)e^{-i\frac{S(x)}{\hbar}}\left(\left(\frac{\partial}{\partial x}N(x)\right)e^{i\frac{S(x)}{\hbar}} + N(x)\frac{i}{\hbar}e^{i\frac{S(x)}{\hbar}}\frac{\partial}{\partial x}S(x)\right) =$$

$$N(x)\left(\frac{\partial}{\partial x}N(x)\right)+\big(N(x)\big)^2\frac{i}{\hbar}\frac{\partial}{\partial x}S(x)$$

We need the imaginary part only:

$$\frac{\big(N(x)\big)^2\frac{\partial}{\partial x}S(x)}{\hbar}$$

Result:

$$j(\vec{x},0)=\frac{1}{m}\cdot\big(N(x)\big)^2\frac{\partial}{\partial x}S(x)$$

App_3:

$$\psi(x,0)=Ae^{ikx}+Be^{-ikx},\qquad A,B\in\mathbb{C},k\in\mathbb{R}$$

We have:

$$j(\vec{x},0)=\frac{\hbar}{m}\cdot Im\left(\psi^*\left(\frac{\partial}{\partial x}\psi\right)\right)$$

$$\psi^*(x,0)=A^*e^{-ikx}+B^*e^{ikx}$$

$$\frac{\partial}{\partial x}\psi(x)=ikAe^{ikx}-ikBe^{-ikx}$$

$$\psi^*\left(\frac{\partial}{\partial x}\psi\right)=\big(A^*e^{-ikx}+B^*e^{ikx}\big)\big(ikAe^{ikx}-ikBe^{-ikx}\big)=$$

$$ik|A|^2-ikA^*Be^{-2ikx}+ikB^*Ae^{2ikx}-ik|B|^2=;$$

We look at:

$$\big(ikA^*Be^{-2ikx}\big)^*=-ikAB^*e^{2ikx}\Longrightarrow$$

$$ikB^*Ae^{2ikx}-ikA^*Be^{-2ikx}=2Im\big(ikAB^*e^{2ikx}\big)$$

$$2Im\big(ikAB^*e^{2ikx}\big)=2Re\big(kAB^*e^{2ikx}\big)$$

We get:

$$ik(|A|^2-|B|^2)+2Re\big(kAB^*e^{2ikx}\big)$$

We need the imaginary part only:

$$k(|A|^2-|B|^2)$$

Result:

$$j(\vec{x},0)=\frac{\hbar}{m}k(|A|^2-|B|^2)$$

App_4:

$$\psi(x,0) = Ae^{i(kx-\omega t)}, \qquad A \in \mathbb{C}, k, \omega \in \mathbb{R}$$

We have:

$$j(\vec{x},0) = \frac{\hbar}{m} \cdot Im\left(\psi^*\left(\frac{\partial}{\partial x}\psi\right)\right)$$

$$\psi^*(x,0) = A^* e^{-i(kx-\omega t)}$$

$$\frac{\partial}{\partial x}\psi(x) = ikAe^{i(kx-\omega t)}$$

$$\psi^*\left(\frac{\partial}{\partial x}\psi\right) = A^* e^{-i(kx-\omega t)} \cdot ikAe^{i(kx-\omega t)} =$$

$$ik|A|^2$$

We need the imaginary part only:

$$k|A|^2$$

Result:

$$j(\vec{x},0) = \frac{\hbar}{m} k|A|^2$$

Note: as $p = mv$ and $p = \hbar k$ we can write this as $v|A|^2$.