This paper deals with the probability current density, a quantity used with the Ehrenfest-Theorem. We will work with a one-dimensional access.

Related information you find at:

https://web.pa.msu.edu/people/mmoore/Lect15_ProbCurrent1.pdf

https://web.pa.msu.edu/people/mmoore/Lect16_Scattering1D.pdf

Hope I can help you with learning quantum mechanics.

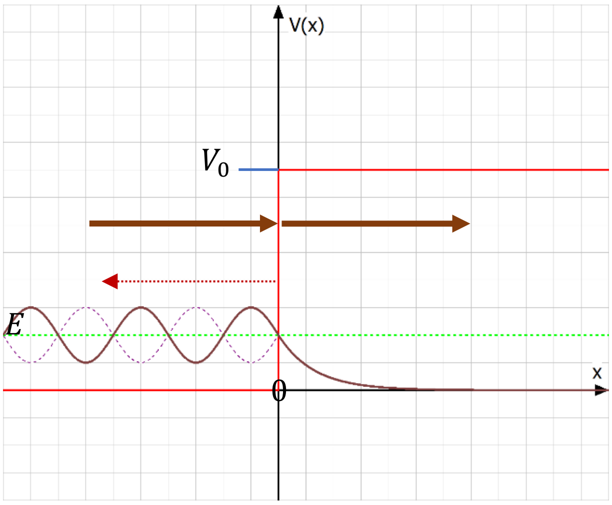
Contents

The 1D barrier

Conservation of the probability current density flow at the boundary of the one-dimensional barrier problem for a plane wave.

For convenience we have the barrier at $x = 0$, the energy $E < V_0$.

The wave function on the left side becomes reflected, the wave function on the right side of the barrier will show an exponential decay.



We use separate wave functions for left and right region:

$$\psi_l(x) = e^{ik_lx} + re^{-ik_lx}\ for\ x \leq 0$$

$$\psi_r(x) = te^{ik_rx}\ \ for\ x \geq 0$$

Note: coefficients r and t refer to “reflection” and “transmission”.

Note: the wave function left is a superposition of incoming and reflected wave.

We will need the derivatives:

$$\psi'_l(x) = ik_le^{ik_lx} - ik_lre^{-ik_lx}\ for\ x \leq 0$$

$$\psi'_r(x) = ik_rte^{ik_rx}\ \ for\ x \geq 0$$

The functions and their derivatives must fit at border $x = 0$:

$$\psi_l(0) = \psi_r(0)$$

$$\psi'_l(0) = \psi'_r(0)$$

We get the match of functions left and right:

$$\psi_l(0) = \psi_r(0) \rightarrow$$

$$e^{ik_l0} + re^{-ik_l0} = te^{ik_r0}$$

$$1 + r = t$$

We get the match of derivatives left and right:

$$\psi'_l(0) = \psi'_r(0) \rightarrow$$

$$ik_le^{ik_l0} - ik_lre^{-ik_l0} = ik_rte^{ik_r0}$$

$$ik_l - ik_l r = ik_r t$$

$$ik_l(1 - r) = ik_r t$$

$$\frac{k_l}{k_r}(1 - r) = t$$

We resolve the system of equations for r and t:

$$1 + r = \frac{k_l}{k_r}(1 - r)$$

$$k_r + rk_r = k_l - rk_l$$

$$rk_r + rk_l = k_l - k_r$$

Result for r:

$$r = \frac{k_l - k_r}{k_r + k_l}$$

$$1 + \frac{k_l - k_r}{k_r + k_l} = t$$

$$\frac{k_l - k_r + k_r + k_l}{k_r + k_l} = t$$

Result for t:

$$\frac{2k_l}{k_r + k_l} = t$$

Case $E < V_0$

We remember: the stationary solution of the Schrödinger equation for a free particle:

$$E = \frac{\hbar^2 k^2}{2m}$$

For the wave function on the left we use the wave number k:

$$k_l = \frac{\sqrt{2mE}}{\hbar} := k$$

For the wave function on the right (in the forbidden area) we need a real exponential and write it somewhat complicated as:

$$k_r = \frac{\sqrt{-2m(V_0 - E)}}{\hbar} = i\frac{\sqrt{2m(V_0 - E)}}{\hbar} := i\gamma$$

Note: i is necessary to have a real exponent for ψ_r if $E < V_0$.

We express r and t in the new constants k and $i\gamma$:

$$r = \frac{k - i\gamma}{k + i\gamma}$$

$$t = \frac{2k}{k + i\gamma}$$

We note:

$$|r|^2 = \frac{(k - i\gamma)(k + i\gamma)}{(k + i\gamma)(k - i\gamma)} = 1$$

$$|t|^2 = \frac{4k^2}{k^2 + \gamma^2}$$

Note: $|r|^2 + |t|^2 \neq 1$, $|r|^2$ and $|t|^2$ cannot be reflection and transmission probability.

Result: The wave is reflected; a small amount $(t^2 < 4 \to t < 2)$ enters the barrier.

Case $E = V_0$.

We have:

$$k_l = \frac{\sqrt{2mE}}{\hbar} := k$$

$$k_r = \frac{\sqrt{-2m(V_0 - V_0)}}{\hbar} = 0$$

We express r and t in the new constants k and $i\gamma$:

$$r = \frac{k - 0}{k + 0} = 1$$

$$t = \frac{2k}{k + 0} = 2$$

Result: The wave is reflected; the part entering the barrier is maximal.

Case $E > V_0$.

We have:

$$E = V_0 + \delta$$

$$k_l = \frac{\sqrt{2mE}}{\hbar} := k$$

$$k_r = \frac{\sqrt{-2m\big(V_0 - (V_0 + \delta)\big)}}{\hbar} =$$

$$\frac{\sqrt{2m\delta}}{\hbar} := \Delta$$

Note: k_r is real, $k > 0$.

We express r and t in the new constants k and $i\gamma$:

$$r = \frac{k - \Delta}{k + \Delta} < 1$$

$$t = \frac{2k}{k + \Delta} < 2$$

Note: although $E > V_0$, a part of the wave is being reflected or in other words – “you can stumble over a small step …”

Case $E \gg V_0$.

We have:

$$k_l = \frac{\sqrt{2mE}}{\hbar} := k$$

$$k_r \approx \frac{\sqrt{2mE}}{\hbar} = k$$

We express r and t in the new constants k and $i\gamma$:

$$r = \frac{k-k}{k+k} = 0$$

$$t = \frac{2k}{k+k} = 1$$

The wave shows no reflection. The part “entering the barrier” is more or less the wave function itself.

Probability current

We will use the example of the step barrier to develop the probability current.

Probability density

We start with the probability density:

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

The probability P a particle found between position x_1 and x_2:

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

If we use the infinitesimal procedure and work with ε, we get the probability P a particle found between position $x - \varepsilon$ and $x + \varepsilon$:

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

We define a probability current flowing through positions $x - \varepsilon$ and $x + \varepsilon$:

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

Positive current is defined flowing from left to right, negative current flowing from right to left.

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

We convert:

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

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

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

Note:

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

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

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

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 current

We express the probability density by wave functions:

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

We use the standard continuity equation:

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

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

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

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:

$$\frac{\partial\psi}{\partial t}=-\frac{i}{\hbar}H\psi$$

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

$$\frac{\partial\psi^*}{\partial t}=\frac{i}{\hbar}H^*\psi^*=\frac{i}{\hbar}H\psi^*$$

We calculate:

$$-\left(\frac{d}{dt}\psi^*\right)\psi-\psi^*\left(\frac{d}{dt}\psi\right)\rightarrow$$

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

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

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

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

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

Note: $V(x)$ commutes with ψ^*.

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

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

What we have so far is:

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

Note: for real functions, $\frac{d}{dx}j=0$.

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 current 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.

With the full notation we have the result:

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

Application plane wave

The wave function for a plane wave:

$$\psi(x) = a \cdot e^{ikx}$$

Note: a might be a complex number.

Note: $\psi(x)$ is a function of x only.

We will need:

$$\frac{\partial\psi}{\partial x}(x) = ika \cdot e^{ikx}$$

$$\psi^*(x) = a^* \cdot e^{-ikx}$$

$$\frac{\partial\psi^*(x)}{\partial x} = -ika^* \cdot e^{-ikx}$$

The corresponding probability current:

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

We calculate:

$$j(x) = \frac{i\hbar}{2m}\left(-ika^* \cdot e^{-ikx} a \cdot e^{ikx} - a^* \cdot e^{-ikx} ika \cdot e^{ikx}\right) =$$

$$\frac{\hbar k|a|^2}{2m}\left(e^{-ikx}e^{ikx} + e^{-ikx}e^{ikx}\right) =$$

$$\frac{\hbar k}{m} \cdot |a|^2$$

We identify: $\frac{\hbar k}{m} := v_0$ is a velocity, $|a|^2 := \rho_0$ a density.

We rewrite this:

$$j(x) = \rho_0 \cdot v_0$$

Note: the probability current is the probability density times a velocity.

Note: in more than one dimension $\vec{j}(x)$ and $\vec{v}_0$ are vectors.

Application superposition of two plane waves

The wave function for a superposition of two plane waves:

$$\psi(x) = a \cdot e^{ik_1 x} + b \cdot e^{ik_2 x}$$

Note: a_1 and a_2 might be complex numbers.

Note: $\psi(x)$ is a function of x only, no time dependency.

We will need:

$$\frac{d}{dx}\psi(x) = ik_1a \cdot e^{ik_1x} + ik_2b \cdot e^{ik_2x}$$

$$\psi^*(x) = a^* \cdot e^{-ik_1x} + b^* \cdot e^{-ik_2x}$$

$$\frac{d}{dx}\psi^*(x) = -ik_1a^* \cdot e^{-ik_1x} - ik_2b^* \cdot e^{-ik_2x}$$

The corresponding probability current:

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

We get:

$$j(x) = \frac{i\hbar}{2m}\Big(\left(-ik_1a^* \cdot e^{-ik_1x} - ik_2b^* \cdot e^{-ik_2x}\right)\left(a \cdot e^{ik_1x} + b \cdot e^{ik_2x}\right) - \left(a^* \cdot e^{-ik_1x} + b^* \cdot e^{-ik_2x}\right)\left(ik_1a \cdot e^{ik_1x} + ik_2b \cdot e^{ik_2x}\right)\Big) =$$

$$\frac{\hbar}{2m}\Big(\left(k_1a^* \cdot e^{-ik_1x} + k_2b^* \cdot e^{-ik_2x}\right)\left(a \cdot e^{ik_1x} + b \cdot e^{ik_2x}\right) + \left(a^* \cdot e^{-ik_1x} + b^* \cdot e^{-ik_2x}\right)\left(k_1a \cdot e^{ik_1x} + k_2b \cdot e^{ik_2x}\right)\Big) =$$

$$\frac{\hbar}{2m}\Big(k_1a^*a + k_1a^*b \cdot e^{-ik_1x}e^{ik_2x} + k_2b^*a \cdot e^{-ik_2x}e^{ik_1x} + k_2b^*b + k_1a^*a + k_2a^*b \cdot e^{ik_2x}e^{-ik_1x} + k_1ab^* \cdot e^{ik_1x}e^{-ik_2x} + k_2b^*b\Big) =$$

$$\frac{\hbar}{2m}\Big(2k_1a^*a + 2k_2b^*b + k_1a^*b \cdot e^{-ik_1x}e^{ik_2x} + k_2b^*a \cdot e^{-ik_2x}e^{ik_1x} + k_2a^*b \cdot e^{ik_2x}e^{-ik_1x} + k_1ab^* \cdot e^{ik_1x}e^{-ik_2x}\Big) =$$

$$\frac{\hbar k_1}{m}|a|^2 + \frac{\hbar k_2}{m}|b|^2 + \frac{\hbar}{2m}\Big((k_1a^*b + k_2a^*b) \cdot e^{-ik_1x}e^{ik_2x} + (k_2b^*a + k_1ab^*) \cdot e^{-ik_2x}e^{ik_1x}\Big) =$$

$$\frac{\hbar k_1}{m}|a|^2 + \frac{\hbar k_2}{m}|b|^2 + \frac{\hbar}{2m}\left(a^*b(k_1 + k_2) \cdot e^{-ik_1x}e^{ik_2x} + b^*a(k_2 + k_1) \cdot e^{-ik_2x}e^{ik_1x}\right) =$$

$$\frac{\hbar k_1}{m}|a|^2 + \frac{\hbar k_2}{m}|b|^2 + \frac{\hbar}{2m}(k_1 + k_2)\left(a^*b \cdot e^{-ik_1x}e^{ik_2x} + ab^* \cdot e^{-ik_2x}e^{ik_1x}\right) =$$

$$\frac{\hbar k_1}{m}|a|^2 + \frac{\hbar k_2}{m}|b|^2 + \frac{\hbar}{2m}(k_1 + k_2)\left(a^*b \cdot e^{-i(k_1-k_2)x} + ab^* \cdot e^{i(k_1-k_2)x}\right)$$

The expression $\left(a^*b \cdot e^{-i(k_1-k_2)x} + ab^* \cdot e^{i(k_1-k_2)x}\right)$ is of kind $z + z^*$, giving back $2 \cdot Re(z)$:

$$a^*b \cdot e^{-ik_1x}e^{ik_2x} + ab^* \cdot e^{ik_1x}e^{-ik_2x} = 2 \cdot Re\left(abe^{i(k_1-k_2)x}\right)$$

We get:

$$j(x) = \frac{\hbar}{m}\left(k_1|a|^2 + k_2|b|^2 + (k_1 + k_2)Re\left(abe^{i(k_1-k_2)x}\right)\right)$$

Note: $(k_1 + k_2)Re\left(abe^{i(k_1-k_2)x}\right)$ is called the interference term.

Remarks

Remark 1)

The interference term $(k_1 + k_2)Re\left(abe^{i(k_1-k_2)x}\right)$ vanishes if $k_1 = -k_2$.

Remark 2)

For energy eigenstates $k_1 = -k_2$ we have $(k_1 - k_2)Re\left(abe^{i(k_1-k_2)x}\right) = 0$, the currents are additive.

Remark 3)

If we have a superposition of a plane wave with itself, $a = b$ and $k_1 = k_2 \coloneqq k$:

$$\psi(x) = ae^{ikx} + ae^{ikx} = 2ae^{ikx}$$

We get the probability current:

$$j(x) = \frac{\hbar}{m}\left(2k|a|^2 + 2kRe(a^2)\right) =$$

$$j(x) = \frac{2k\hbar}{m}\left(|a|^2 + Re(a^2)\right)$$

We examine this expression further and replace:

$$a \coloneqq x + iy$$

The we get:

$$|a|^2 = (x+iy)(x-iy) = x^2 + y^2$$

$$a^2 = (x+iy)(x+iy) = x^2 + i2xy - y^2$$

$$Re(a^2) = x^2 - y^2$$

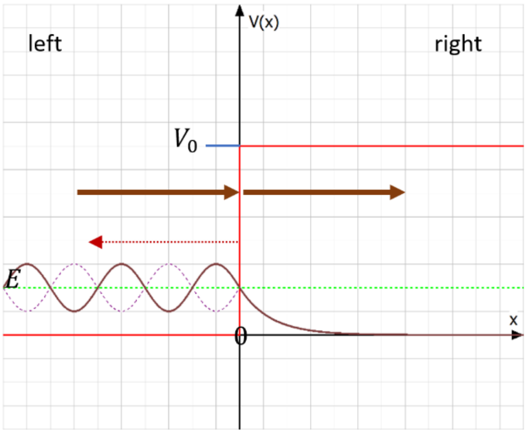
$$|a|^2 + Re(a^2) = 2x^2 = 2Re(a)^2$$

The probability current becomes:

$$j(x) = \frac{2k\hbar}{m}\left(2Re(a)^2\right) = \frac{4k\hbar}{m}Re(a)^2$$

Transmission and reflection probability

We remember:



We use separate wave functions for left and right region:

$$\psi_l(x) = e^{ik_l x} + re^{-ik_l x} \; for \; x \le 0$$

We rewrite:

$$\psi_l(x) = e^{ik_l x} + re^{i(-k_l)x} \; for \; x \le 0$$

$$\psi_r(x) = te^{ik_r x} \;\; for \; x \ge 0$$

Note: $\psi_l(x)$ and $\psi_r(x)$ are functions of x only.

$$\frac{k_l - k_r}{k_r + k_l} = r$$

$$\frac{2k_l}{k_r + k_l} = t$$

We remember remark 1) above, the interference term vanishes because of k_l and $-k_l$. We get the probability current for the left wave:

$$j_l(x) = \frac{\hbar}{m}(k_l - k_l|r|^2) = \frac{\hbar k_l}{m}(1 - |r|^2)$$

The probability current for the right wave:

$$j_r(x) = \frac{\hbar k_r}{m} \cdot |t|^2$$

We use $j_l(x) = j_r(x)$ at the boundary:

$$\frac{\hbar k_l}{m}(1 - |r|^2) = \frac{\hbar k_r}{m} \cdot |t|^2$$

We transform:

$$1 - |r|^2 = \frac{m\hbar k_r}{\hbar k_l m} \cdot |t|^2 = \frac{k_r}{k_l} \cdot |t|^2$$

$$1 = \frac{k_r}{k_l} \cdot |t|^2 + |r|^2$$

Note: $\frac{k_r}{k_l}$ is the ratio of velocities.

We derive the transmission probability T and the reflection probability R:

$$T := \frac{k_r}{k_l} \cdot |t|^2$$

$$R := |r|^2$$

We expand $|r|^2$ and $|t|^2$:

$$T = \frac{k_r}{k_l} \cdot \frac{4{k_l}^2}{(k_r + k_l)^2} =$$

$$\frac{4k_l k_r}{(k_r + k_l)^2}$$

$$R = \left(\frac{k_l - k_r}{k_r + k_l}\right)^2 = \frac{(k_l - k_r)^2}{(k_r + k_l)^2}$$

We build the sum:

$$T + R = \frac{4k_l k_r}{(k_r + k_l)^2} + \frac{(k_l - k_r)^2}{(k_r + k_l)^2} =$$

$$\frac{4k_l k_r + (k_l - k_r)^2}{(k_r + k_l)^2} = 1$$

The sum of transmission probability T and reflection probability P equals 1, as it should be.

Remarks

- The probability current allows to compute probabilities in scattering problems like e. g. the step problem
- The probability for a particle to split int the ongoing wave and the reflected wave is the ratio of the ongoing current to the reflected current
- In 1D scattering and fixed energy, we have no interference term in the current density. We can treat the left and right travelling components of the current independent
- For a plane wave, the current is the amplitude squared times the velocity