WAVE MECHANICS IN ONE DIMENSION

Solving the Schrödinger Equation

Consider a particle moving in one space dimension through the potential $V(x)$, so its Hamiltonian is

$$\hat{H} \;=\; \frac{\hat{p}^2}{2M} \;+\; V(\hat{x}). \tag{1}$$

In the wave-function formalism, the Schrödinger equation $\hat{H}\,|\psi\rangle = E\,|\psi\rangle$ for a stationary state $|\psi\rangle$ becomes

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

or equivalently

$$\psi''(x) \;=\; \frac{2M}{\hbar^2}\big(V(x)-E\big)\times\psi(x). \tag{3}$$

This is a linear second-order differential equation, so for any energy E it has 2 independent solutions. But any such solution could be physical or unphysical, depending on its asymptotic behavior at $x\to\pm\infty$.

To clarify this point, consider the behavior of the 2 solutions of (3) at $x\to+\infty$ depending on $V(+\infty)\stackrel{\text{def}}{=}\lim_{x\to+\infty}V(x)$:

- $V(+\infty)>E$.

  First, consider a finite $V(+\infty)$ which happens to be larger than the energy E. In this case, eq. (3) for $x\to+\infty$ becomes

  $$\psi''(x) \;=\; +\kappa^2\psi(x) \quad\text{for}\quad \kappa \;=\; \frac{1}{\hbar}\sqrt{2M(V(+\infty)-E)}, \tag{4}$$

  so its two solutions behave as

  $$\psi_1(x) \;=\; \text{const}\times e^{-\kappa x} \quad\text{and}\quad \psi_2(x) \;=\; \text{const}\times e^{+\kappa x}. \tag{5}$$

  But physically, only the $\psi_1\propto e^{-\kappa x}$ is a good, normalizable solution with $\langle\psi|\psi\rangle = \int|\psi|^2dx<\infty$. OOH, the $\psi_2\propto e^{+\kappa x}$ solution is not only un-normalizable, but it does not even obtain as a sensible limit of normalizable wavefunctions, so it is completely unphysical.

Likewise, for $V(+\infty) = +\infty$ (which is of course larger than E), the two solutions of the Schrödinger equation have form

$$\psi_1(x) \ \approx\ \text{const} \times e^{-S(x)} \quad \text{and} \quad \psi_2(x) \ \approx\ \text{const} \times e^{+S(x)} \tag{6}$$

where

$$S(x) \ \approx \int \frac{\sqrt{2M(V(x) - E)}}{\hbar}\, dx, \tag{7}$$

which grows with x in a faster-than-linear fashion. Again, the $\psi_1(x)$ is a good, normalizable solution while the $\psi_2(x)$ solution is unphysical.

⋆ In general, any solution which grows with $x \to +\infty$ as $e^{+\kappa x}$ or even faster is completely unphysical.

- $V(+\infty) < E$.

  For finite $V(+\infty)$ which happens to be smaller than the energy E, eq. (3) for $x \to +\infty$ becomes

$$\psi''(x) \ =\ -k^2 \psi(x) \quad \text{for} \quad k \ =\ \frac{1}{\hbar}\sqrt{2M(E - V(+\infty))}, \tag{8}$$

  so its two solutions behave as

$$\psi_1(x) \ =\ \text{const} \times e^{+ikx} \quad \text{and} \quad \psi_2(x) \ =\ \text{const} \times e^{-ikx}. \tag{9}$$

  This time both solutions are un-normalizable but physical, as they obtain from sensible limits of normalizable wavefunctions.

  Likewise, for $V(+\infty) = -\infty$ (which is of course smaller that E), we have two rapidly oscillating solutions, and both solutions look physical as they obtain from sensible limits of normalizable wavefunctions. However, the whole Hamiltonian with $V(\pm\infty) = -\infty$ is a but unphysical, as we shall see in a moment.

Clearly, the same dependence of the wave function asymptotics at $x \to +\infty$ on the sign of $V(+\infty) - E$ also applies to at the other end $x \to -\infty$ of the one-dimensional space. So when we take both ends into account we get one of the following situations:

1. At both ends $x \to \pm\infty$ the potential is higher than the energy, $V(+\infty), V(-\infty) > E$. In this case, each end selects a unique linear combination of the two Schrödinger equation's solutions which happens to asymptotically shrink rather than blow up at that end. However, for a general value of the energy E, the linear combination which shrinks for $x \to -\infty$ differs from the linear combination which shrinks for $x \to +\infty$, and there is no combination that behaves physically at both ends $x \to \pm\infty$.

   However, for some *discrete* values of the energy, the same linear combination of the two solutions happens to shrink for both $x \to -\infty$ and $x \to +\infty$, so it behaves physically at both ends. Thus, in this energy range, the Hamiltonian's spectrum is discrete and non-degenerate (a unique eigenstate for each eigenvalue). Also, the eigenstates for these discrete energies are normalizable,

$$\langle\psi|\psi\rangle \;=\; \int\limits_{-\infty}^{+\infty} |\psi(x)|^2\,dx \;<\; \infty. \tag{10}$$

2. The potentials at the two ends are different, and the energy lies between them, $V(-\infty) < E < V(+\infty)$ or $V(-\infty) > E > V(+\infty)$.
   In this case, the end with the potential higher than the energy selects the unique linear combination of the two solutions (which shrinks rather than blows up at that end). At the other end, the same combination oscillates rather than shrinks or blows up (because both solutions oscillate rather than shrink or blow up at that end), so it's physical albeit un-normalizable.

   Consequently, in this energy range, the Hamiltonian's spectrum is continuous and non-degenerate. Also, the eigenstates for such continuous-spectrum energies are un-normalizable, $\langle\psi|\psi\rangle = \infty$.

3. At both ends $x \to \pm\infty$ the potential is lower than the energy, $V(+\infty), V(-\infty) < E$. In this case, any linear combinations of the two solutions oscillates at both ends, which makes its physical albeit unnormalizable.

   Thus, in this energy range, the Hamiltonian's spectrum is continuous and doubly-degenerate (two independent eigenstates for each eigenvalue), and all the eigenstates are un-normalizable.

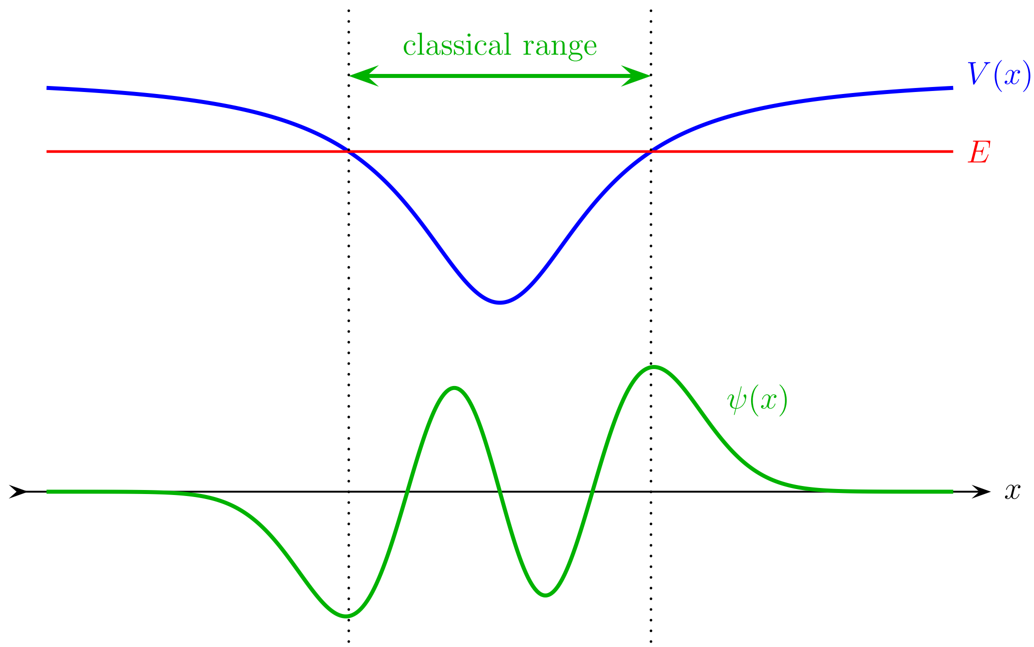
Note that if the potential asymptotes to $-\infty$ at either end — or both ends — then the continuous spectrum of the Hamiltonian stretches all the way to $E = -\infty$. For a particle that's utterly isolated from the rest of the Universe, this may seem OK. But any kind of an interaction — however weak — between such a particle and anything else would make it seek a lower energy level, and without a bottom to its energy spectrum, it would keep losing energy forever. In the classical limit, this corresponds to the particle falling of an infinite potential hill and accelerating while it runs away to $x = \pm\infty$, while the energy loss corresponds to a small friction force.

In any case, the classical potential hill with $V \to -\infty$ for $x \to \pm\infty$ is quite unphysical, and its quantum analogues — Hamiltonians with energy spectra without finite lower limits — are similarly unphysical. So from now on in this class, we shall assume that at each end $x \to \pm\infty$ either has a finite limit or asymptotes to $+\infty$ (as in the harmonic oscillator) but never to $-\infty$.

Bound and Unbound States

Physically, the the eigenstates for the discrete energy eigenvalues correspond to the bound motion of the particle while the eigenstates for the continuous energy eigenvalues correspond to the un-bound motion.

Indeed, consider the wave-function $\psi(x)$ for a discrete energy eigenvalue $E < V(\pm\infty)$. This is a normalizable wave-function which decreases exponentially (or faster) for both $x \to +\infty$ and $x \to -\infty$, so the probability of finding the particle outside of some finite range $x_1 < x < x_2$ is very small, and shrinks as we extend the range. In the classical limit, this corresponds to the particle bouncing back and force between x_1 and x_2 but never exiting this range, thus bound motion:



Since the bound state has a normalizable wave-function, it has a well-defined expectation value of the position $\langle x\rangle = \langle\psi|\,\hat{x}\,|\psi\rangle$. However, since $|\psi\rangle$ is a stationary state, the classical meaning of this expectation value is the time-averaged value of the position over the period of motion rather than the actual position at any particular time. Also, by the Ehrenfest equation,

$$\langle\psi|\,\hat{p}\,|\psi\rangle \;=\; m\frac{d}{dt}\,\langle\psi|\,\hat{x}\,|\psi\rangle \;=\; 0 \quad \langle\!\langle\,\text{in a stationary state}\,\rangle\!\rangle. \tag{11}$$

Now consider the un-normalizable wave function for $E \in$ continuous spectrum. In the non-degenerate case of $V(-\infty) < E < V(+\infty)$ (or vice verse), the wave function which shrinks at the high end of V but oscillates at the low end, describes the un-bound motion: the particle flies in from the low end, slows down, turns around near the classical turning point where $V(x) = E$, and flies back to the low end. In the degenerate case of $V(\pm\infty) < E$, we have a more general kind of un-bound motion: the particle can fly in from either end and continue moving in the same direction until it flies out to the other end, or it may turn around and fly back to the same end it came from.

In any case, all the continuous-spectrum eigenstates correspond to un-bound motion, and all such states are unnormalizable,

$$\langle\psi|\psi\rangle \;=\; \int\limits_{-\infty}^{+\infty} |\psi(x)|^2\,dx \;=\; \infty, \tag{12}$$

which makes for *ill-defined expectation values of the position*

$$\langle x\rangle \;=\; \frac{\langle\psi|\,\hat{x}\,|\psi\rangle}{\langle\psi|\psi\rangle} \;=\; \frac{\int dx\,|\psi(x)|^2\times x}{\int dx\,|\psi(x)|^2} \;=\; ???. \tag{13}$$

Consequently, despite the Ehrenfest equation (11), and un-bound state may have a non-zero expectation value of the momentum, $\langle p\rangle \neq 0$.

Wave Packets for the Unbound Motion

Consider the asymptotic behavior of the un-bound state's wave function $\psi(x)$ for $x \to +\infty$ **or** $x \to -\infty$ where $V(x) \approx \text{const} < E$. In this region,

$$\psi(x) \;\approx\; A\times e^{+ikx} \;+\; B\times e^{-ikx} \tag{14}$$

for some constants A and B and $\hbar k = \sqrt{2M(E - V(\infty))}$. To understand the motion described by this wave function, we need to step away from the exactly stationary states and consider the wave packets with a small but finite energy uncertainty $\epsilon \ll E$. Thus, consider the wave functions of the form

$$\psi_{\rm wp}(x) \;=\; \int dE\,F(E)\times\psi_E(x), \tag{15}$$

where $\psi_E(x)$ is the wave-function of the stationary state of energy E while $F(E)$ is some function of the energy which has a narrow peak near $E = E_0$, for example a Gaussian peak

$$F(E) \;=\; \frac{1}{\sqrt{2\pi}\,\epsilon}\exp\bigl(-(E-E_0)^2/2\epsilon^2\bigr), \qquad \epsilon \ll E - V(\infty). \tag{16}$$

Most generally, the stationary state's wavefunction at $x \to \infty$ is

$$\psi_E(x,t) \;=\; A(E)\times e^{+ikx-i\omega t} \;+\; B(E)\times e^{-ikx-i\omega t}, \qquad \omega \;=\; \frac{E}{\hbar}, \quad k \;=\; \frac{\sqrt{2M(E-V(\infty))}}{\hbar}, \tag{17}$$

but for $\epsilon \ll E - V(\infty)$ the wave packet (15) is dominated by the energies very close to the

E_0, so we can make the following approximations:

$$k(E) \;\approx\; k_0 \;+\; \frac{E-E_0}{\hbar u} \tag{18}$$

where $u = \hbar k/M$ is the particle's speed, and also

$$\begin{aligned} A(E) \;&\approx\; A(E_0),\ \text{which we shall call simply } A,\\ B(E) \;&\approx\; B(E_0),\ \text{which we shall call simply } B. \end{aligned} \tag{19}$$

Consequently, the wave-packet's time-dependent wave-function becomes

$$\begin{aligned} \psi_{\mathrm{wp}}(x,t) \;&=\; \int\frac{dE}{\sqrt{2\pi}\epsilon}\left(Ae^{+ikx}+Be^{-ikx}\right)\times e^{-iEt/\hbar}\times e^{-(E-E_0^2)/2\epsilon^2}\\ &=\; Ae^{+ik_0x}e^{-i\omega_0 t}\times\int\frac{dE}{\sqrt{2\pi}\epsilon}\,\exp\left(+ix\frac{E-E_0}{\hbar u}\;-\;it\frac{E-E_0}{\hbar}\;-\;\frac{(E-E_0)^2}{2\epsilon^2}\right)\\ &\quad+\,Be^{-ik_0x}e^{-i\omega_0}\times\int\frac{dE}{\sqrt{2\pi}\epsilon}\,\exp\left(-ix\frac{E-E_0}{\hbar u}\;-\;it\frac{E-E_0}{\hbar}\;-\;\frac{(E-E_0)^2}{2\epsilon^2}\right), \end{aligned} \tag{20}$$

where the net exponents in the two integrands amount to

$$\begin{aligned} \mathcal{E} \;&=\; \pm ix\frac{E-E_0}{\hbar u}\;-\;it\frac{E-E_0}{\hbar}\;-\;\frac{(E-E_0)^2}{2\epsilon^2}\\ &=\; -\frac{(E-E_0)^2}{2\epsilon^2}\;-\;i\left(t\mp\frac{x}{u}\right)\times\frac{E-E_0}{\hbar}\\ &=\; -\frac{1}{2\epsilon^2}\left(E\;-\;E_0\;+\;\frac{i\epsilon^2}{\hbar}\left(t\mp\frac{x}{u}\right)\right)^2\;-\;\frac{\epsilon^2}{2\hbar^2}\left(t\mp\frac{x}{u}\right)^2, \end{aligned} \tag{21}$$

hence

$$\begin{aligned} \int\frac{dE}{\sqrt{2\pi}\epsilon}\,\exp(\mathcal{E}) \;&=\; \exp\left(-\frac{\epsilon^2}{2\hbar^2}\left(t\mp\frac{x}{u}\right)^2\right)\times\int\frac{dE}{\sqrt{2\pi}\epsilon}\,\exp\left(-\frac{1}{2\epsilon^2}(E+\mathrm{const})^2\right)\\ &=\; \exp\left(-\frac{\epsilon^2}{2\hbar^2}\left(t\mp\frac{x}{u}\right)^2\right)\times 1\\ &=\; \exp\left(-\frac{(x\mp ut)^2}{2(u\hbar/\epsilon)^2}\right). \end{aligned} \tag{22}$$

Altogether, this gives us

$$\begin{aligned}\psi_{\rm wp}(x,t) \;&=\; A\times e^{+ik_0x-i\omega_0t}\times\exp\left(-\frac{(x-ut)^2}{2(u\hbar/\epsilon)^2}\right)\\ &+\; B\times e^{-ik_0x-i\omega_0t}\times\exp\left(-\frac{(x+ut)^2}{2(u\hbar/\epsilon)^2}\right).\end{aligned}\tag{23}$$

which is a superposition of two Gaussian wave packets:

- First wave packet of amplitude A is centered at $x=+ut$, so it travels right at velocity $v=+u$;
- Second wave packet of amplitude B is centered at $x=-ut$, so it travels left at velocity $v=-u$.

Now let's focus on the motion unbound in both directions — thus, the doubly-degenerate spectrum of E, — and consider the asymptotic behavior of a general stationary wave-function $\psi_E(x)$ at both ends $x\to\mp\infty$. In general, we have

$$\text{for } x\to-\infty: \quad \psi_E(x) \;=\; A_1\times e^{+ik_1x} \;+\; B_1\times e^{-ik_1x},\tag{24}$$

$$\text{for } x\to+\infty: \quad \psi_E(x) \;=\; A_2\times e^{+ik_2x} \;+\; B_2\times e^{-ik_2x},\tag{25}$$

where

$$k_1 \;=\; \frac{\sqrt{2M(E-V(-\infty))}}{\hbar}, \qquad k_2 \;=\; \frac{\sqrt{2M(E-V(+\infty))}}{\hbar},\tag{26}$$

and there are 2 linear relations between the 4 coefficients A_1, B_1, A_2, B_2. Consequently, when we replace the exactly stationary states with the wave packets (23), we end up with

$$\begin{aligned}\text{for } x\to-\infty: \quad \psi_{\rm wp}(x,t) \;&=\; A_1\times\exp(+ik_1x-i\omega t)\times\exp\left(-\frac{(x-u_1t)^2}{2(u_1\hbar/\epsilon)^2}\right)\\ &+\; B_1\times\exp(-ik_1x-i\omega t)\times\exp\left(-\frac{(x+u_1t)^2}{2(u_1\hbar/\epsilon)^2}\right),\end{aligned}\tag{27}$$

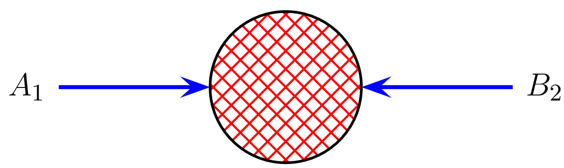
$$\begin{aligned}\text{for } x\to+\infty: \quad \psi_{\rm wp}(x,t) \;&=\; A_2\times\exp(+ik_2x-i\omega t)\times\exp\left(-\frac{(x-u_2t)^2}{2(u_2\hbar/\epsilon)^2}\right)\\ &+\; B_2\times\exp(-ik_2x-i\omega t)\times\exp\left(-\frac{(x+u_2t)^2}{2(u_2\hbar/\epsilon)^2}\right).\end{aligned}\tag{28}$$

Altogether, this seems like 2 wave packets in each asymptotic region, but but actually each such wave packet shows up in the appropriate asymptotic region only for the very early or very late time. Specifically:

$$\begin{array}{l}
\text{the wave packet centered at } x=+u_1t \text{ is the } x\to-\infty \text{ region } \textbf{only} \text{ for } t\to-\infty\ ,\\
\text{the wave packet centered at } x=-u_1t \text{ is the } x\to-\infty \text{ region } \textbf{only} \text{ for } t\to+\infty\ ,\\
\text{the wave packet centered at } x=+u_2t \text{ is the } x\to+\infty \text{ region } \textbf{only} \text{ for } t\to+\infty\ ,\\
\text{the wave packet centered at } x=-u_2t \text{ is the } x\to+\infty \text{ region } \textbf{only} \text{ for } t\to-\infty\ .
\end{array} \tag{29}$$

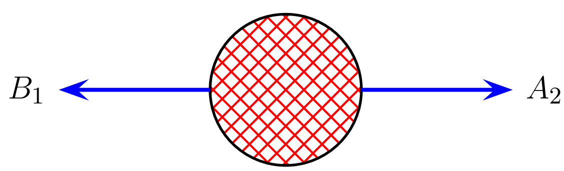
Reorganizing this info by t rather than by x, we have:

- At the very early times $t\to-\infty$, we have two incoming wave packets: a packet of amplitude A_1 at the left end and moving right at velocity $+u_1$, and a packet of amplitude B_2 at the right and moving left at velocity $-u_2$:



(30)

- At the very late times $t\to+\infty$, we have two outgoing wave packets: a packet of amplitude B_1 at the left end and moving further left at velocity $-u_1$, and a packet of amplitude A_2 at the right end and moving further right at velocity $+u_2$:



(31)

Physically, a particle initially coming from the left side can either be reflected back to the left or continue moving to the right. Likewise, a particle initially coming from the right can either be reflected back to the right or continue moving to the left. And a generic solution to the Schrödinger equation allows for an arbitrary superposition of these two scenarios, although in most setups the initial particles come from one side only, usually from the left.

In such a set up,

$$\begin{aligned}
A_1 &= \text{amplitude of the incident wave packet,} \\
B_1 &= \text{amplitude of the reflected wave packet,} \\
A_2 &= \text{amplitude of the transmitted wave packet,} \\
B_2 &= 0.
\end{aligned} \tag{32}$$

Consequently, an incident particle coming from the left is reflected back to the left with probability

$$R = \frac{\langle \text{refl}|\text{refl}\rangle}{\langle \text{inc}|\text{inc}\rangle} = \frac{|B_1|^2}{|A_1|^2} \tag{33}$$

or is transmitted to the right with probability

$$T = \frac{\langle \text{trans}|\text{trans}\rangle}{\langle \text{inc}|\text{inc}\rangle} = \frac{k_2}{k_1} \times \frac{|A_2|^2}{|A_1|^2}\,, \tag{34}$$

where the k_2/k_1 factor comes from the different widths of the incident and the transmitted wave packets. Indeed, for a wave packet of the form

$$\psi(x,t) = C \times \exp(\pm ikx - i\omega t) \times \exp\left(-\frac{(x \mp ut)^2}{2(u\hbar/\epsilon)^2}\right) \tag{35}$$

we have

$$\langle \text{wp}|\text{wp}\rangle = \int dx\,|\psi|^2 = |C|^2 \times \int dx\,\exp\left(-\frac{(x \mp ut)^2}{(u\hbar/\epsilon)^2}\right) = |C|^2 \times \sqrt{\pi}\frac{u\hbar}{\epsilon} = \frac{\sqrt{\pi}\hbar^2}{M} \times k \times |C|^2, \tag{36}$$

hence

$$\frac{\langle \text{trans}|\text{trans}\rangle}{\langle \text{inc}|\text{inc}\rangle} = \frac{k_2|A_2|^2}{k_1|A_1|^2}\,. \tag{37}$$

At this point, we have learned how to interpret the wave-packet solutions in terms of the reflection and transmission probabilities, AKA reflection and transmission coefficients. But the amplitudes $A_1, \ldots$ ultimately come from the stationary-state solutions $\psi_E(x)$, so let's learn how to calculate them. The basic algorithm is as follows:

1. Write a general solution $\psi_E(x)$ of the Schrödinger equation for $E > V(-\infty), V(+\infty)$ and spell them out at all x.

2. Take the $x \to \pm\infty$ limit of this general solution: It should have form

$$\begin{aligned} \text{for } x \to -\infty: \quad \psi_E(x) &= A_1 \times e^{+ik_1x} + B_1 \times e^{-ik_1x}, \\ \text{for } x \to +\infty: \quad \psi_E(x) &= A_2 \times e^{+ik_2x} + B_2 \times e^{-ik_2x}, \end{aligned} \tag{38}$$

   where the 4 coefficients A_1, B_1, A_2, B_2 are related by two linear equations. Spell out these linear equations.

3. Add another linear equation $B_2 = 0$ since the incident particles come only from the left side. Then solve all these linear equations for the ratios A_2/A_1 and B_1/A_1.

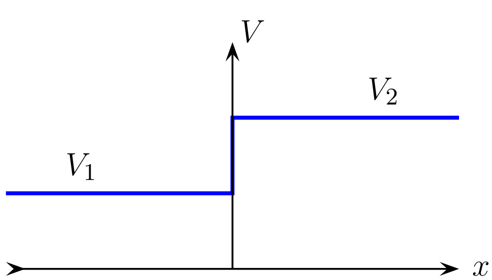
4. Given these ratios, the reflection and the transmission probabilities are

$$R = \frac{|B_1|^2}{|A_1|^2}, \qquad T = \frac{k_2}{k_1} \times \frac{|A_2|^2}{|A_1|^2}. \tag{39}$$

   Make sure these 2 probabilities add up to $R + T = 1$; if they do not, you have made a mistake.

Example: Potential Step

For a simple example of calculating the transmission and the reflection probabilities, consider the step potential



$$V(x) = \begin{cases} V_1 & \text{for } x < 0, \\ V_2 & \text{for } x > 0. \end{cases} \tag{40}$$

For $E > V_2 > V_1$, the exact solution $\psi_E(x)$ of the Schrödinger equation has general form

$$\begin{aligned} \forall x < 0: \quad \psi_E(x) &= A_1 \times e^{+ik_1x} + B_1 \times e^{-ik_1x}, \\ \forall x > 0: \quad \psi_E(x) &= A_2 \times e^{+ik_2x} + B_2 \times e^{-ik_2x}, \end{aligned} \tag{41}$$

for

$$k_{1,2} \;=\; \frac{1}{\hbar}\sqrt{2M(E-V_{1,2})}\,. \tag{42}$$

For the step potential, the relations between the coefficients A_1, B_1 for $x<0$ and A_2, B_2 for $x>0$ follow continuity rules for the wave functions:

- Rule 1: regardless of any discontinuities — or even singularities — of the potential $V(x)$, the wave-function $\psi(x)$ is *always* a continuous function of x at all x.
- Rule 2: at all points where the potential $V(x)$ is finite — even if it's discontinuous, — the first derivative $\psi'(x)$ of the wave-function remains continuous.

Proof of the continuity rules:
First, any (normalizable) state with a finite expectation value of the kinetic energy must have a continuous wave-function $\psi(x)$. Indeed,

$$\langle\psi|\,\hat{H}_{\rm kin}\,|\psi\rangle \;=\; \int\!dx\,\psi^*(x)\times\frac{-\hbar^2}{2M}\psi''(x) \;=\; +\frac{\hbar^2}{2M}\int\!dx\,|\psi'(x)|^2, \tag{43}$$

so to keep this (expectation value of) the kinetic energy finite, the derivative $\psi'(x)$ may not have any singularities worse than $\sqrt{\delta(x-x_0)}$. In particular, it may not have $\delta(x-x_0)$ singularities which would obtain from any discontinuity of the wave-function $\psi(x)$ itself.

If the state $|\psi\rangle$ is un-normalizable due to the behavior of its wave-function at $x\to\pm\infty$ rather than any singularities at finite x, we should regulate the wave function's behavior at infinity — for example, by multiplying it by a $\exp(-\alpha x^2)$ factor with a small α — in a way that does not affect its continuity or discontinuity at finite x. Again, a finite expectation value of the kinetic energy requires a continuous wave-function.

Note that this argument does not care about the potential $V(x)$, and it does not care if the state $|\psi\rangle$ is a stationary state or not, all it care is the finite expectation value of the kinetic energy. But any stationary state with a finite net energy must have a finite $\langle H_{\rm kin}\rangle$, so all such states have continuous wave-functions $\psi(x)$, regardless of any discontinuities of the potential $V(x)$. This completes the proof of the continuity rule#1.

The second continuity rule applies only to the stationary states, so let the wave-function $\psi(x)$ obey the Schrödinger equation

$$\psi''(x) \;=\; \frac{2M}{\hbar^2}\,\bigl(V(x)-E\bigr)\times\psi(x). \tag{44}$$

On the RHS here, the $\psi(x)$ factor is finite at all x, so as long as the potential $V(x)$ is finite, the second derivative on the LHS must also be finite. Note: if $V(x)$ is finite but discontinuous at some point, then $\psi''(x)$ would also be discontinuous at that point, but as long as the potential does not jump all the way to infinity, the second derivative would have only a finite discontinuity. Consequently, the first derivative $\psi'(x)$ must be differentiable — and hence continuous — at all x. *Quod erat demonstrandum.*

Now let's apply the continuity rules to the step potential. For the wave function (41), the limits of the wave function and its derivative for $x\to 0$ from the left and from the right are as follows:

$$\begin{array}{llll}
\text{for } x\to -0: & \psi \;\to\; A_1 \,+\, B_1, & \qquad \psi' \;\to\; ik_1A_1 \,-\, ik_1B_1, \\
\text{for } x\to +0: & \psi \;\to\; A_2 \,+\, B_2, & \qquad \psi' \;\to\; ik_2A_2 \,-\, ik_2B_2,
\end{array} \tag{45}$$

hence the the continuity rules at $x=0$ impose 2 linear relations between the coefficients A_1, B_1, A_2, B_2, namely

$$\begin{aligned}
A_1 \,+\, B_1 \;&=\; A_2 \,+\, B_2\,, \\
ik(A_1-B_1) \;&=\; ik_2(A_2-B_2).
\end{aligned} \tag{46}$$

Adding another linear equation $B_2=0$ — the incident wave comes from the left — we get

$$\begin{aligned}
A_1 \,+\, B_1 \;&=\; A_2\,, \\
A_1 \,-\, B_1 \;&=\; \frac{k_2}{k_1}\times A_2\,,
\end{aligned} \tag{47}$$

hence adding and subtracting these 2 equations gives us

$$2A_1 \;=\; \left(1+\frac{k_2}{k_1}\right)A_2\,, \qquad 2B_1 \;=\; \left(1-\frac{k_2}{k_1}\right)A_2\,, \tag{48}$$

and therefore

$$\frac{A_2}{A_1} = \frac{2k_1}{k_1+k_2}\,, \qquad \frac{B_1}{A_1} = \frac{k_1-k_2}{k_1+k_2}\,. \tag{49}$$

Finally, the reflection coefficient obtains as

$$R = \left|\frac{B_1}{A_1}\right|^2 = \frac{(k_1-k_2)^2}{(k_1+k_2)^2}\,, \tag{50}$$

while the transmission coefficient obtains as

$$T = \frac{k_2}{k_1}\times\left|\frac{A_2}{A_1}\right|^2 = \frac{4k_1k_2}{(k_1+k_2)^2}\,. \tag{51}$$

By inspection,

$$R + T = \frac{(k_1-k_2)^2 + 4k_1k_2(k_1+k_2)^2}{(k_1+k_2)^2} = 1, \tag{52}$$

so the net probability of reflection or transmission is indeed 1.

Total reflection

Finally, let's consider the non-degenerate continuous spectrum of unbound states with $V<E$ at one end but $V>E$ at the other end. For the sake of definiteness, let $V(-\infty)<E<V(+\infty)$. In this case, a general solution of the Schrödinger equation behaves at $x\to\pm\infty$ as

$$\begin{aligned}\text{for } x\to-\infty: \quad \psi_E(x) &= A_1\times e^{+ik_1x} + B_1\times e^{-ik_1x},\\ \text{for } x\to+\infty: \quad \psi_E(x) &= A_2\times e^{-\kappa x} + B_2\times e^{+\kappa_2 x},\end{aligned} \tag{53}$$

where

$$\hbar k_1 = \sqrt{2M(E-V(-\infty))}, \qquad \hbar\kappa_2 = \sqrt{2M(V(+\infty)-E)}, \tag{54}$$

and again there are two linear relations between the coefficients A_1, B_1, A_2, B_2. But this time, only the solutions with $B_2=0$ are physical. Also, the A_2 amplitude belongs to the *evanescent wave* which decays for $x\to+\infty$ rather than to the transmitted wave. Consequently, an incident particle coming from the left must be reflected back to the left with probability = 1, so we should have

$$R = \left|\frac{B_1}{A_1}\right|^2 = 1. \tag{55}$$

As a simple example, let's go back to the step potential but now for energies $V_1 < E < V_2$. This time, the exact solution $\psi_E(x)$ of the Schrödinger equation has general form

$$\begin{aligned} \forall x < 0: \quad \psi_E(x) &= A_1 \times e^{+ik_1 x} + B_1 \times e^{-ik_1 x}, \\ \forall x > 0: \quad \psi_E(x) &= A_2 \times e^{-\kappa_2 x} + B_2 \times e^{+\kappa_2 x}, \end{aligned} \tag{56}$$

for

$$\hbar k_1 = \sqrt{2M(E - V_1)}, \qquad \hbar\kappa_2 = \sqrt{2M(V_2 - E)}. \tag{57}$$

Clearly, this solution is the analytic continuation of the solution (41) from $E > V_2$ to $E < V_2$ by means of turning a real k_2 into imaginary $i\kappa_2$. Moreover, the continuity rules at $x = 0$ obtain by via the same analytic continuation to

$$\begin{aligned} A_1 + B_1 &= A_2 + B_2, \\ ik_1 A_1 - ik_1 B_1 &= -\kappa_2 A_2 + \kappa_2 B_2, \end{aligned} \tag{58}$$

and the third linear constraint $B_2 = 0$ also has the same form. Consequently, the solutions to these linear equations also obtain by simply plugging $i\kappa_2$ for the k_2, thus

$$\frac{A_2}{A_1} = \frac{2k_1}{k_1 + i\kappa_2}, \qquad \frac{B_1}{A_1} = \frac{k_1 - i\kappa_2}{k_1 + i\kappa_2}. \tag{59}$$

Finally, the reflection probability obtains as

$$R = \left|\frac{k_1 - i\kappa_2}{k_1 + i\kappa_2}\right|^2, \tag{60}$$

which indeed evaluates to 1 for any real k_1 and real κ_2.