7 Schrödinger equation with one-dimensional potentials

7.1 Generalities

We now want to study the quantum mechanics of a single point-particle that classically would be characterised by its position x in a single direction, and corresponding momentum $p_x \equiv p$. From Ehrenfest's theorem, we see that we should expect a "good classical limit" for appropriate quantum states, if the quantum Hamiltonian is obtained from the classical Hamilton function by the replacements $p \to P$ and $x \to X$. Since X and P do not commute, there may be ordering issues if the Hamilton function involves products of x and p. However, in the simplest situations (in the absence of a magnetic field), the classical Hamilton function is just $\mathscr{H} = \frac{p^2}{2m} + V(x)$, so that we have as our starting point

$$H = \frac{P^2}{2m} + V(X) \ . \tag{7.1}$$

From our previous discussion we know that $\langle x| X |\psi\rangle = x\langle x |\psi\rangle = x\psi(x)$ and $\langle x| P |\psi\rangle = -i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\langle x |\psi\rangle = -i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\psi(x)$ and then also

$$\langle x| P^2 |\psi\rangle \equiv \langle x| P\big(P |\psi\rangle\big) = -i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\langle x| P |\psi\rangle = \big(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\big)^2\langle x |\psi\rangle = -\hbar^2\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) \ , \tag{7.2}$$

so that

$$\langle x| H |\psi\rangle = \Big(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\Big)\psi(x) \equiv \widehat{H}\psi(x) \ . \tag{7.3}$$

The Schrödinger equation then is

$$i\frac{\mathrm{d}}{\mathrm{d}t}\psi(t,x) = \widehat{H}\psi(t,x) \equiv \Big(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\Big)\psi(t,x) \ , \tag{7.4}$$

where now $\psi(t,x) = \langle x |\psi(t)\rangle$. We are interested in the eigenvalue problem of $\widehat{H}$:

$$H |\varphi\rangle = E |\varphi\rangle \quad \Leftrightarrow \quad \widehat{H}\varphi(x) = E\varphi(x) \ . \tag{7.5}$$

This is also sometimes called the stationary Schrödinger equation. From our general discussion of the previous section we know that one can have discrete eigenvalues E_n with normalisable (and actually orthonormal) eigenstates $|\varphi_{n,i}\rangle$ or continuous eigenvalues $E(\nu)$ with non-normalisable ("delta-function" normalised) eigenstates $|\varphi_\nu\rangle$. From the spectral theorem ((6.67)) we know that a general *normalised* state is given by a general superposition of the form

$$\psi(t,x) = \sum_{n,i} c_{n,i}(t)\varphi_{n,i}(x) + \int \mathrm{d}\nu\, c_\nu(t)\varphi_\nu(x) \quad , \quad \sum_{n,i} |c_{n,i}(t)|^2 + \int \mathrm{d}\nu\, |c_\nu(t)|^2 = 1 \ . \tag{7.6}$$

Applying the Schrödinger equation to this decomposition and using the fact that the $\varphi_{n,i}$ and φ_ν are eigenstates of H with eigenvalues E_n and $E(\nu)$, we get (denoting as usual $\frac{\mathrm{d}f}{\mathrm{d}t}$ by $\dot{f}$)

$$i\hbar\sum_{n,i}\dot{c}_{n,i}(t)\varphi_{n,i}(x) + i\hbar\int \mathrm{d}\nu\, \dot{c}_\nu(t)\varphi_\nu(x) = \sum_{n,i} E_n c_{n,i}(t)\varphi_{n,i}(x) + \int \mathrm{d}\nu\, E(\nu)c_\nu(t)\varphi_\nu(x) \ . \tag{7.7}$$

The orthogonality of the basis then implies

$$
\begin{aligned}
i\hbar\, \dot c_{n,i}(t) = E_n\, c_{n,i}(t) \quad &\Rightarrow \quad c_{n,i}(t) = c_{n,i}(t_0)\, e^{-iE_n(t-t_0)/\hbar} \ , \\
i\hbar\, \dot c_{\nu}(t) = E(\nu)\, c_{\nu}(t) \quad &\Rightarrow \quad c_{\nu}(t) \ = \ c_{\nu}(t_0)\, e^{-iE(\nu)(t-t_0)/\hbar} \ ,
\end{aligned}
\tag{7.8}
$$

so that

$$
\psi(t,x) = \sum_{n,i} c_{n,i}(t_0)\, e^{-iE_n(t-t_0)/\hbar} \varphi_{n,i}(x) + \int \mathrm{d}\nu\, c_\nu(t_0)\, e^{-iE(\nu)(t-t_0)/\hbar} \varphi_\nu(x) \ . \tag{7.9}
$$

Note that the modulus of the coefficients remains constant in time, so that the norm of $|\psi\rangle$ also remains unchanged.

Whether the spectrum of H only contains discrete eigenvalues E_n or only continuous $E(\nu)$ or both depends on the shape of the potential. We will see different examples below. But we can already give a preliminary general discussion here. First, suppose that, for $x \to \pm\infty$ the potential goes to some constant values $V_\pm$. For simplicity we will assume $V_+ = V_-$. We can then always "shift" the potential and the energy eigenvalues by a common constant. So let us assume that as $|x| \to \infty$ we have $V(x) \to 0$. Then, asymptotically the eigenvalue problem $\widehat{H}\varphi(x) = E\varphi(x)$ becomes (we write φ' instead of $\mathrm{d}\varphi/\mathrm{d}x$)

$$
-\frac{\hbar^2}{2m}\varphi''(x) \sim E\varphi(x) \quad , \quad |x| \to \infty \ . \tag{7.10}
$$

For $E > 0$ we set $k = \sqrt{2mE}/\hbar$, while for $E < 0$ we set $\alpha = \sqrt{-2mE}/\hbar$. Then

$$
\begin{aligned}
\varphi(x) &\sim_{x\to\pm\infty} c_\pm e^{\alpha x} + d_\pm e^{-\alpha x} \quad , \quad \text{if } E < 0 \ , \\
\varphi(x) &\sim_{x\to\pm\infty} \widetilde{c}_\pm e^{ikx} + \widetilde{d}_\pm e^{-ikx} \quad , \quad \text{if } E > 0 \ .
\end{aligned}
\tag{7.11}
$$

• For the case $E > 0$ we have oscillating solutions as $x \to \pm\infty$ for any choice of constants $\widetilde{c}_\pm$ and $\widetilde{d}_\pm$. It follows that $\int_{x_0}^{\infty} |\varphi(x)|^2$ and $\int_{-\infty}^{-x_0} |\varphi(x)|^2$ always diverge in this case and the corresponding solutions $\varphi(x)$ always are non-normalisable for all $E > 0$. We see that for $E > 0$ there is no quantisation of the energies, i.e. this is the continuous spectrum, and the eigenfunctions are indeed non-normalisable.

• On the other hand, for $E < 0$, we may choose $c_+ = d_- = 0$ so that $\varphi(x) \sim_{x\to\infty} d_+ e^{-\alpha x}$ and $\varphi(x) \sim_{x\to-\infty} c_- e^{\alpha x}$. Then φ goes to 0 exponentially for $|x| \to \infty$ and the normalisation integrals converge. However, this is not the end of the story, since φ must be a solution of $-\frac{\hbar^2}{2m}\varphi''(x) = (E - V(x))\varphi(x)$ for all x. Such a second-order differential equation always has two linearly independent solutions, $\varphi_1(x)$ and $\varphi_2(x)$ and we can then choose the linear combination $a\varphi_1(x) + b\varphi_2(x)$ that matches $e^{\alpha x}$ (up to a multiplicative constant) as $x \to -\infty$. This fixes the coefficients a and b up to an overall constant. But, in general, this solution will *not* match $e^{-\alpha x}$ for $x \to \infty$. Since the exact solutions φ_1 and φ_2 depend on the value of E, the choice of the a and b also depends on E. As we change E it may happen that for certain discrete values E_n

of E the $a\varphi_1(x) + b\varphi_2(x)$ does match $e^{-\alpha x}$ for $x \to \infty$. If this is the case, we have a solution that decreases exponentially for both $x \to \pm\infty$ and this then is a normalisable solution $\varphi_n(x)$. This is how the quantisation of the energies is related to the requirement that the solutions of the eigenvalue equation are normalisable.

Let us mention a certain interpretation that will be useful below. We have seen that $\rho(t,x) = |\psi(t,x)|^2$ is the probability density to find the particle at x. We have also seen that the hermiticity of the Hamiltonian implies that the norm $\int \mathrm{d}x\, |\psi(t,x)|^2 = \int \mathrm{d}x\, \rho(t,x)$ is conserved in time. This is similar to the total electric charge being conserved. But for the electric charge we also have a local conservation law that states that the charge within any (small) volume only changes because there is some current flowing into or out of this volume. The local version then is $\dot\rho + \vec\nabla \cdot \vec j = 0$, or in one dimension $\dot\rho + j' = 0$. We can similarly derive a local conservation law for the probability density as follows

$$\begin{aligned} \frac{\partial}{\partial t}\rho &= \frac{\partial}{\partial t}|\psi|^2 = \psi^* \frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t}\psi = \frac{1}{i\hbar}\psi^*\Big(-\frac{\hbar^2}{2m}\psi'' + V(x)\psi\Big) - \frac{1}{i\hbar}\Big(-\frac{\hbar^2}{2m}\psi^{*\prime\prime} + V(x)\psi^*\Big)\psi \\ &= \frac{\hbar}{2im}\big(-\psi^*\psi'' + \psi^{*\prime\prime}\psi\big) = -\frac{\hbar}{2im}\frac{\partial}{\partial x}\big(\psi^*\psi' - \psi^{*\prime}\psi\big)\ . \end{aligned} \tag{7.12}$$

This yields the local conservation law for the probability density ρ and the probability current j as

$$\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0 \quad , \quad \rho = |\psi|^2\ , \quad j = \frac{\hbar}{2im}\big(\psi^*\psi' - \psi^{*\prime}\psi\big) \tag{7.13}$$

This will be useful, in particular, when one deals with non-normalisable states where one may nevertheless want to interpret ρ as a local "particle probability density" and j as a local "particle probability current" decribing the analogue of a classical current of particles with density ρ and velocity v such that $j \sim \rho v$.

7.2 Piecewise constant potentials

In this subsection we study a few simple cases where the potential is piecewise constant and discontinuous at certain points. Then we divide the (physical) space into a finite number of regions where the potential is constant and which we label by the letter A. Then in each region $V(x) = V_A$. Solving $-\frac{\hbar^2}{2m}\varphi''(x) = (E - V_A)\varphi(x)$ in each region A then is trivial. As before,

$$\begin{aligned} &\text{if } E > V_A \text{ we set } k_A = \sqrt{2m(E-V_A)}/\hbar \ \text{ and have solutions } \varphi_\pm^A = e^{\pm i k_A x} \\ &\text{if } E < V_A \text{ we set } \alpha_A = \sqrt{2m(V_A-E)}/\hbar \ \text{ and have solutions } \varphi_\pm^A = e^{\pm \alpha_A x}\ . \end{aligned} \tag{7.14}$$

We still need to match the solutions φ_A and φ_{A+1} at the boundaries between the regions A and $A+1$. Let x_A be the coordinate of this boundary. Clearly, as $V(x)$ is discontinuous, the stationary Schrödinger equation $\varphi''(x) = -2m(E - V(x))\varphi(x)$ implies that φ'' cannot be continuous at x_A.

But integrating from $x_A - \epsilon$ to $x_A + \epsilon$ gives

$$\varphi'(x_A+\epsilon)-\varphi'(x_A-\epsilon) = -\frac{2m}{\hbar^2}\int_{x_A-\epsilon}^{x_A+\epsilon} \mathrm{d}x\,(E-V(x))\varphi(x) = -\frac{2m}{\hbar^2}\epsilon\,(2E-V_{A+1}-V_A)\varphi(x_A)+\mathcal{O}(\epsilon^2)\ , \tag{7.15}$$

Taking $\epsilon \to 0$ shows that φ' is continuous at x_A and then φ is also continuous. Note that this argument is valid as long as $V_{A+1} + V_A$ is finite. If the potential has an infinite discontinuity (because it is assumed infinite in one of the two neighbouring regions) this argument no longer applies and then only φ will be continuous. This is best seen by first taking a large but finite discontinuity and then taking the limit. To summarise :

$$\begin{aligned}&\text{If } V(x) \text{ has a finite discontinuity at } x_A \text{ then } \varphi(x) \text{ and } \varphi'(x) \text{ are continuous at } x_A\text{, but not } \varphi''(x).\\ &\text{If } V(x) \text{ has an infinite discontinuity at } x_A \text{ then } \varphi(x) \text{ is continuous at } x_A \text{ but not } \varphi'(x).\end{aligned} \tag{7.16}$$

7.3 Bound states of the finite potential well

Consider the potential well of depth $-V_0$ defined by

$$V(x) = 0 \quad \text{for} \quad |x| > a \quad , \quad V(x) = V_0 < 0 \quad \text{for} \quad |x| \leq a\ . \tag{7.17}$$

We then have the different regions : $x < -a$ and $-a \leq x \leq a$ and $x > a$. One can consider 3 different possibilities for the energy E : $E < V_0 < 0$ or $V_0 \leq E < 0$ or $E \geq 0$. The last case will be considered in a later subsection. Here we only look at the two cases with $E < 0$. First suppose $V_0 \leq E < 0$. Then we set $k = \sqrt{2m(E-V_0)}/\hbar$ and $\alpha = \sqrt{-2mE}/\hbar$. The solutions then are

$$\begin{aligned}\varphi(x) &= Ae^{\alpha x} \quad , && x < -a\ ,\\ \varphi(x) &= Be^{ikx} + Ce^{-ikx} \quad , && -a \leq x \leq a\ ,\\ \varphi(x) &= De^{-\alpha x} \quad , && x > a\ .\end{aligned} \tag{7.18}$$

We already have imposed that φ must be normalisable by discarding the solution $e^{\alpha x}$ for $x > a$ and $e^{-\alpha x}$ for $x < -a$. The matching conditions (continuity of φ and of φ') at $x = -a$ and $x = a$ are

$$\begin{aligned}Ae^{-\alpha a} &= Be^{-ika} + Ce^{ika}\ ,\\ A\alpha e^{-\alpha a} &= ik(Be^{-ika} - Ce^{ika})\ ,\\ Be^{ika} + Ce^{-ika} &= De^{-\alpha a}\ ,\\ ik(Be^{ika} - Ce^{-ika}) &= -D\alpha e^{-\alpha a}\ .\end{aligned} \tag{7.19}$$

This is a linear homogeneous system of 4 equations for the 4 unknown coefficients A, B, C, D, which we can write as $(A, B, C, D)\, M = 0$ with some 4×4 matrix one can read from the above equations. Generically such a homogenous system only has the trivial solution $A = B = C = D = 0$, unless the matrix M is singular, i.e. $\det M = 0$. The matrix M depends on E (through the α and k), so that this is an equation $\det M(E) = 0$. The solutions E are those values of the energy for which (non-vanishing) normalisable solutions exist.

Rather than computing the determinant, we can try to solve this system in a pedestrian way. One can combine the first 2 equations to yield A in terms of B and the last two equations to yield D in terms of B :

$$A = \frac{2ik}{ik+\alpha} e^{(\alpha - ik)a} B \quad , \quad D = \frac{2ik}{ik-\alpha} e^{(\alpha+ik)a} B \ . \tag{7.20}$$

The remaining equations then give

$$C = \frac{ik-\alpha}{ik+\alpha} e^{-2ika} B \quad \text{and} \quad C = \frac{ik+\alpha}{ik-\alpha} e^{+2ika} B \ . \tag{7.21}$$

Both equations are compatible only if

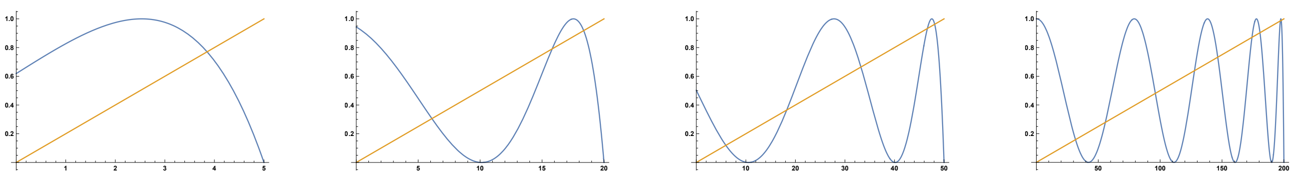
$$\frac{ik-\alpha}{ik+\alpha} e^{-2ika} = \frac{ik+\alpha}{ik-\alpha} e^{+2ika} \quad \Rightarrow \quad \frac{ik-\alpha}{ik+\alpha} e^{-2ika} = \pm 1 \ . \tag{7.22}$$

If the upper sign $(+1)$ is realised this leads to $k \tan ka = \alpha$, and if the lower sign is realised this gives $k \cot ka = -\alpha$:

$$k \tan ka = \alpha \ , \ C = B \quad \text{or} \quad k \cot ka = -\alpha \ , \ C = -B \ . \tag{7.23}$$

For $B = C$ we have $\varphi(x) = 2B \cos kx$ inside the well, while for $B = -C$ we have $\varphi(x) = 2iB \sin kx$. Recall that k and α are functions of the energy E. Thus the conditions (7.23) are (transcendental) equations for E. They admit a finite number of solutions, corresponding to a finite number of allowed (negative) energies E_n, $n = 1, 2, \ldots n_0$ where the total number depends on V_0 and a. The deeper and the larger the well, the more allowed energy levels on gets. One can proceed with a graphical or numerical solution of (7.23).

In either case, one must first identify the relevant dimensionless quantities. We can convert the size a of the well into an energy by letting $E_0 = \frac{\hbar^2}{2ma^2}$. We introduce the dimensionless $\epsilon = \frac{(-E)}{E_0}$ and $w \equiv \frac{(-V_0)}{E_0}$. Then the number of solutions ϵ can only depend on w. We have $\frac{k^2}{\alpha^2} = \frac{V_0}{E} - 1$ and $ka = \sqrt{\frac{E-V_0}{E_0}}$. Then $k \tan ka = \alpha$ implies $\frac{k^2}{\alpha^2} = \frac{1}{\tan^2 ka}$. i.e. $\frac{V_0}{E} = 1 + \frac{1}{\tan^2 ka} = \frac{1}{\sin^2 ka}$, i.e. $\frac{E}{V_0} = \sin^2 \sqrt{\frac{E-V_0}{E_0}}$. In terms of ϵ and w this reads $\frac{\epsilon}{w} = \sin^2 \sqrt{w-\epsilon}$. The figures show the graphs of $\frac{\epsilon}{w}$ and $\sin^2 \sqrt{w-\epsilon}$ for four different values of w, namely $w = 5$, $w = 20$, $w = 50$ and $w = 200$.



Each intersection of the yellow and blue curve corresponds to a solution of the squared equation, but only every other intersection corresponds to the correct sign in the original equation $k \tan ka =$

α, and thus to an allowed value of the energy E_n. One sees indeed that there is a finite number of solutions, and the larger $w = \frac{-V_0}{E_0} = \frac{-2ma^2V_0}{\hbar^2}$ the more allowed values of E there are. It is interesting to note that even for $w \to 0$ there is always one solution $\epsilon = w^2$ corresponding[37] to $E = -\frac{2ma^2V_0^2}{\hbar^2}$. The other case, $k \cot ka = -\alpha$ can be discussed similarly.

Note that the eigenfunctions are either $\sim \sin kx$ or $\sim \cos kx$ which are either odd or even functions. Indeed, we can define a parity operator $\hat{\Pi}$ that acts on functions as $(\hat{\Pi}f)(x) = f(-x)$. Obviously applying $\hat{\Pi}$ twice acts as the identity, $\hat{\Pi}^2 = \mathbf{1}$, and one can easily see that $\hat{\Pi}$ is self-adjoint.

Exercise 7.1 : *Show that the eigenvalues of $\hat{\Pi}$ are ± 1 and that the corresponding eigenfunctions are the even and odd functions in $L^2(\mathbf{R})$. Show that one has th operator relation $\hat{\Pi}\frac{\mathrm{d}}{\mathrm{d}x} = -\frac{\mathrm{d}}{\mathrm{d}x}\hat{\Pi}$ and that $[\hat{H}, \hat{\Pi}] = 0$ if the potential is an even function of x. Conclude that in this case the eigenfunctions of H can be chosen to be either even or odd.*

Finally, we should discuss what happens if $E < V_0 < 0$. Then $2m(E - V_0) < 0$ and instead of k we introduce $\beta = \sqrt{-2m(E - V_0)}/\hbar$ and then the solution for $-a \le x \le a$ is $\varphi(x) = B'e^{\beta x} + C'e^{-\beta x}$. Note that $0 < \beta < \alpha$. Compared to the previous case we have replaced $ik \to \beta$. The condition (7.22) then reads

$$\left(\frac{\alpha - \beta}{\alpha + \beta}\right)^2 = e^{4\beta a} \ . \tag{7.24}$$

Now the left-hand side is less than 1 while the right-hand side is larger than 1 and there is no solution. We conclude that there is no eigenvalue E with $E < V_0$.

7.4 The infinite potential well

One could take the limit of $V_0 \to -\infty$ to get an infinitely deep potential well. However, this does not correspond to the physical situations one encounters. One rather has the situation were the particle is confined to within the region $-a \le x \le a$ by imposing $V(x) = \infty$ for $|x| > 0$. Hence it makes more sense to start with the previous example and shift the energies and potentials by $\widetilde{V}_0 = -V_0 > 0$ so that one has $V(x) = \widetilde{V}_0$ for $|x| > a$ and $V(x) = 0$ for $-a \le x \le a$. In the limit $\widetilde{V}_0 \to \infty$ one then sees that $\alpha \to \infty$ so that $\varphi(x)$ vanishes for $|x| > a$. One also sees that in this limit the derivative φ' no longer is continuous at $x = \pm a$, in agreement with our general discussion above. Rather than taking the limit of the shifted finite well solution it is much easier to start over again. Hence, we let

$$V(x) = \infty \quad \text{for} \quad |x| > a \quad , \quad V(x) = 0 \quad \text{for} \quad |x| \le a \ . \tag{7.25}$$

[37] Indeed, since $\epsilon \le w$, for $w \to 0$ necessarily also $\epsilon \to 0$ and then $\sqrt{w - \epsilon} \to 0$ and $\frac{\epsilon}{w} = \sin^2 \sqrt{w - \epsilon}$ becomes $\frac{\epsilon}{w} = w - \epsilon$ or $\epsilon(1 + w) = w^2$ which is solved as $\epsilon = w^2$ in the $w \to 0$ limit. One also checks that this has the correct sign to solve $k \tan ka = \alpha$. So this solution is $E = -\frac{2ma^2V_0^2}{\hbar^2}$.

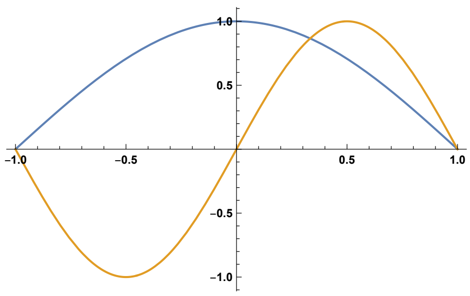
Then $\varphi(x) = 0$ for $|x| > a$ and since φ must be continuous (but not φ'), we have $\varphi(\pm a) = 0$. We set $k = \sqrt{2mE}/\hbar$ and then for $-a \leq x \leq a$ we have $-\varphi'' = \frac{2mE}{\hbar^2}\varphi = k^2\varphi$ with solutions $\varphi(x) = Be^{ikx} + Ce^{-ikx}$. The vanishing of φ at $x = \pm a$ implies $B = -Ce^{2ika}$ and $B = -Ce^{-2ika}$ which is compatible only if $e^{2ika} = \pm 1$ so that $2ika = in\pi$ with integer n. Hence, $k = \frac{n\pi}{2a} \equiv k_n$. For even n we have $B = -C$ and $\varphi_n(x) = 2iB \sin k_n x$, while for odd n we have $B = C$ and $\varphi(x) = 2B \cos k_n x$. Obviously, n and $-n$ result in wave-functions that only differ by an irrelevant sign, and $n = 0$ would lead to $\varphi(x) = 0$ which is not an eigenfunction. Let us summarise :

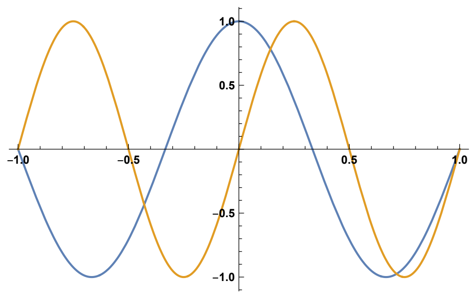
$$\begin{aligned} &k_n = \frac{n\pi}{2a} \ , \ n = 1, 2, \ldots \quad , \quad E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{8ma^2} \ , \\ &\text{even } n \ : \varphi_n(x) = \frac{1}{\sqrt{a}} \sin k_n x \quad , \quad \text{odd } n \ : \varphi_n(x) = \frac{1}{\sqrt{a}} \cos k_n x \ , \end{aligned} \tag{7.26}$$

where we have normalised the functions φ_n and also made some convenient choice of phase. Note that $L = 2a$ is the width of the well and one could rewrite these formula in terms of L as $k_n = \frac{n\pi}{L}$ and

$$\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \ , \ n = 1, 2, \ldots} \tag{7.27}$$

By well-known results about Fourier series, the set of φ_n forms a basis for the square-integrable functions on $[-a, a]$ that vanish at the boundaries. The figures show the first four wave-functions, φ_1 (blue) and φ_2 (yellow) on the left, and φ_3 (blue) and φ_4 (yellow) on the right, for $a = 1$.





In the previous section we have discussed whether $A = i\frac{\mathrm{d}}{\mathrm{d}x}$ is self-adjoint or only symmetric on the Hilbert space $L^2([0, 2\pi])$ and we had found that it is self-adjoint if $\mathcal{D}(A)$ (the domain of definition of A) is taken to be the periodic differentiable functions, but that it was only symmetric if $\mathcal{D}(A)$ is taken to be the differentiable functions that vanish at 0 and at 2π. In the latter case $A^\dagger$ had any complex number as eigenvalue while A had not a single eigenvalue. Naively, the present situation looks similar to this latter case but, of course, it is not. At present we should take as our Hilbert space $\mathcal{H}$ the square integrable functions on $[-a, a]$ that vanish at $x = \pm a$, so that these boundary conditions are already implemented for all elements of the Hilbert space. Then, for $A = i\frac{\mathrm{d}}{\mathrm{d}x}$ the domain of definition is simply the differentiable functions in $\mathcal{H}$ (which then automatically vanish at $x = \pm a$). The domain of $A^\dagger$ is also the differentiable functions in $\mathcal{H}$ and then $\mathcal{D}(A^\dagger) = \mathcal{D}(A)$ and A is self-adjoint. Similarly, $-\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ is a self-adjoint operator on $\mathcal{H}$.

7.5 Scattering by a potential well

Let us come back to the finite potential well. There, we only had finitely many eigenstates with $E < 0$ and, obviously, they alone cannot form a basis of $L^2(\mathbf{R})$. We must also consider the eigenfunctions for $E > 0$. As disussed before, in this case we do not expect any quantisation condition and the eigenvalues $E > 0$ form a continuum and the corresponding eigenfunctions are not normalisable. They are often called scattering states, for reasons that will become clear. We will set (recall $V_0 < 0$)

$$E > 0 \quad , \quad k_1 = \sqrt{2mE}/\hbar \quad , \quad k_2 = \sqrt{2m(E - V_0)}/\hbar > k_1 \ . \tag{7.28}$$

The solutions in the different regions are $Ae^{ik_1x} + A'e^{-ik_1x}$ for $x < -a$, $Be^{ik_2x} + Ce^{-ik_2x}$ for $-a \le x \le a$ and $De^{ik_1x} + D'e^{-ik_1x}$ for $x > a$. However, suppose we want to describe a situation where there is an incoming right-moving current of particles (coming in from $x = -\infty$ and moving towards the potential well). This does not mean that for $x < -a$ there should not be any left-moving current, since we expect reflection from the well. However, for $x > a$ we do not want to have any left-moving particles coming in from $x = +\infty$. The quantum mechanical description of these currents is the probability current j defined in (7.13). Since $\psi(t, x) = e^{-iEt/\hbar}\varphi(x)$ the $e^{-iEt/\hbar}$ drop out when computing j and we have for $x > a$:

$$j_{>a} = \frac{\hbar}{2im}\big(\varphi^*\varphi' - \varphi^{*\prime}\varphi\big) = \frac{\hbar k_1}{m}|D|^2 - \frac{\hbar k_1}{m}|D'|^2 \ , \tag{7.29}$$

where the cross terms $\sim D^*D'$ and $\sim D'^*D$ have dropped out. We interpret $\frac{\hbar k_1}{m}$ as a momentum divided by a mass, i.e. as a velocity, so that the first term corresponds to a probability density $|D|^2$ moving to the right with velocity $\frac{\hbar k_1}{m}$ and the second term to a probability density $|D'|^2$ moving to the left with velocity $-\frac{\hbar k_1}{m}$. If we do not want to have any current coming in from $+\infty$ and moving to the left (towards the well), we should set $D' = 0$. Then similarly, for $x < -a$ one has

$$j_{<a} = \frac{\hbar k_1}{m}|A|^2 - \frac{\hbar k_1}{m}|A'|^2 \ , \tag{7.30}$$

and we interpret the first piece as the incoming current and the second piece as the reflected current. Then one defines a reflexion coefficient R and a transmission coefficient T as

$$R = \frac{|A'|^2}{|A|^2} \quad , \quad T = \frac{|D|^2}{|A|^2} \ . \tag{7.31}$$

Again, one must now write the continuity conditions for φ and φ' at $x = -a$ and $x = a$, resulting in 4 equations for the 5 unknown coefficients A, A', B, C, D. But this time the goal is to express

A', B, C, D in terms of A, which is always possible, without having to impose any condition on the energy E. We see that E can then take any continuous (positive) value. Actually to obtain the transmission and reflection coefficients it is enough to eliminate B and C and express D and A' in terms of A. We leave this as an exercise :

Exercise 7.2 : *Complete the previous discussion by computing explicitly the ratios A'/A and D/A and obtain the reflexion and transmission coefficients R and T. Verify that $R+T=1$. Explain why $R+T=1$ must hold on general grounds. Does one observe any particular behaviour of R and T for certain values of the energy E ?*

7.6 Tunnel effect

Finally, we consider the situation where the potential vanishes for $|x|>a$ and equals $V_0>0$ for $|x|<a$, and we want to study what happens for $0<E<V_0$ for a current coming in from the left. Classically, the particles are all reflected by this potential barrier, but we will see that quantum mechanically there is a non-vanishing transmission probability. We set $k=\sqrt{2mE}/\hbar$ and $\alpha=\sqrt{2m(V_0-E)}/\hbar$ and start with the solutions

$$\begin{aligned}
\varphi(x) &= Ae^{ikx}+A'e^{-ikx} \quad , \quad x<-a \ , \\
\varphi(x) &= Be^{\alpha x}+Ce^{-\alpha x} \quad , \quad -a\le x\le a \ , \\
\varphi(x) &= De^{ikx} \quad , \quad x>a \ .
\end{aligned} \tag{7.32}$$

The continuity of φ and φ' yields the 4 conditions

$$\begin{aligned}
Ae^{-ika}+A'e^{ika} &= Be^{-\alpha a}+Ce^{\alpha a} \ , \\
ik(Ae^{-ika}-A'e^{ika}) &= \alpha(Be^{-\alpha a}-Ce^{\alpha a}) \ , \\
De^{ika} &= Be^{\alpha a}+Ce^{-\alpha a} \ , \\
ikDe^{ika} &= \alpha(Be^{\alpha a}-Ce^{-\alpha a}) \ .
\end{aligned} \tag{7.33}$$

Combining the first two equations in different ways yields

$$\begin{aligned}
(\alpha+ik)Ae^{-ika+\alpha a}+(\alpha-ik)A'e^{ika+\alpha a} &= 2\alpha B \ , \\
(\alpha-ik)Ae^{-ika-\alpha a}+(\alpha+ik)A'e^{ika-\alpha a} &= 2\alpha C \ .
\end{aligned} \tag{7.34}$$

Similarly, combining the last two equation in different ways yields

$$\begin{aligned}
(\alpha+ik)De^{ika-\alpha a} &= 2\alpha B \ , \\
(\alpha-ik)De^{ika+\alpha a} &= 2\alpha C \ .
\end{aligned} \tag{7.35}$$

Eliminating B and C between the two sets of equations gives

$$\begin{aligned}
Ae^{2(\alpha-ik)a}+rA'e^{2\alpha a} &= D \ , \\
Ae^{-2(\alpha+ik)a}+\frac{1}{r}A'e^{-2\alpha a} &= D \ ,
\end{aligned} \tag{7.36}$$

where we have introduced

$$r = \frac{\alpha - ik}{\alpha + ik} \ . \tag{7.37}$$

Obviously, $|r| = 1$. Eliminating D gives A' in terms of A, and then we also get D in terms of A :

$$\begin{aligned} A' &= -e^{-2ika}\,\frac{1}{r}\,\frac{1-e^{-4\alpha a}}{1-r^{-2}e^{-4\alpha a}}\,A \ , \\ D &= e^{-2\alpha a}e^{-2ika}\,r\,\frac{1-r^2}{1-r^{-2}e^{-4\alpha a}}\,A \end{aligned} \tag{7.38}$$

Recall the definition of the reflection and transmission coefficients in (7.31) and note that $|r| = 1$ implies $1/r = r^*$. Then

$$R = \left|\frac{1-e^{-4\alpha a}}{1-r^{-2}e^{-4\alpha a}}\right|^2 \quad , \quad T = e^{-4\alpha a}\left|\frac{1-r^2}{1-r^{-2}e^{-4\alpha a}}\right|^2 . \tag{7.39}$$

Let us verify that $T + R = 1$. To simplify the notation, set $x = e^{-4\alpha a}$. Indeed, then

$$R = \frac{1-2x+x^2}{(1-xr^{*2})(1-xr^2)} \quad , \quad T = \frac{x(2-r^2-r^{*2})}{(1-xr^{*2})(1-xr^2)} \quad \Rightarrow \quad T+R = \frac{1+x^2-xr^2-xr^{*2}}{(1-xr^{*2})(1-xr^2)} = 1 \ . \tag{7.40}$$

Let us have a closer look at the transmission coefficient T which represents the transmission probability (tunnel probability). We have $r = e^{-2i\theta}$ with $\tan\theta = \frac{k}{\alpha}$. Unless $k \ll \alpha$ ($E \ll V_0$), the phase θ will not be very small and then $1 - r^2$ will not be very small either, but of order one. One can then say that, up to a prefactor of order one, the tunnel probability is given by $T \simeq^{-4\alpha a}$. This can be rewritten in a form that is more generally valid also for non-constant potential barriers as

$$\boxed{T \simeq \exp\Big(-\frac{2}{\hbar}\int_{x_1}^{x_2} \mathrm{d}x\,\sqrt{2m(V(x)-E)}\Big) \ ,} \tag{7.41}$$

where x_1 and x_2 are the the classical turning points, i.e. the boundaries of the domain where $E < V(x)$.

Exercise 7.3 : *Check the computations leading to* (7.39).

Exercise 7.4 : *In the limit where $E \to V_0$ one has $\alpha \to 0$ and $r \to -1$ so that naively R and T are undetermined. Show more carefully that in this limit $R \to \frac{a^2k^2}{1+a^2k^2}$ and $T \to \frac{1}{1+k^2a^2}$.*

Exercise 7.5 *: Consider now an energy $E > V_0$. In this case one can study diffusion of an incoming beam of particles by this potential barrier. Proceeding similarly as before, determine the reflexion and transmission coefficients R and T.*