Week 3

PHY 303 Quantum Mechanics

Instructor: Sebastian Wüster, IISER Bhopal, 2021

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2 Solvable quantum problems in one dimension

We want to now apply our results on stationary states from section 1.6.5 to as many problems as possible and in doing so also understand how and why this tells us all we need to know about quantum mechanical problems. For simplicity we shall stick to a single spatial dimension x, i.e. working in 1D. We will see later (chapter 4), how to straightforwardly generalize most of these results to 3D. The problems in this section probably already almost exhaust the list of those where the quantum states and dynamics can be analytically found.

2.1 Free particle eigenstates

Let us first start to look at the simplest system, the free particle. Free particle means, that no force acts on the particle and hence the potential must be a constant $V(x) = V_0$. For simplicity V_0 is usually set to zero. We then have the

Free particle Hamiltonian, which is just $\hat{H} = \hat{p}^2/(2m)$, hence

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}. \tag{2.1}$$

This gives rise to the TISE

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi(x) = E\phi(x), \tag{2.2}$$

which we can write as

$$\frac{\partial^2}{\partial x^2}\phi(x) = -k^2\phi(x), \tag{2.3}$$

with constant $k = \sqrt{2mE}/\hbar$. You would have seen the differential equation (2.13) elsewhere, e.g. when dealing with the classical harmonic oscillator. Its general solution is $\phi(x) = A\sin[kx] + B\cos[kx]$, or equivalently $\phi(x) = Ce^{ikx} + De^{-ikx}$, linked though $C = B/2 + A/(2i)$ and $D = B/2 - A/(2i)$. In choosing one of the two forms, we shall be guided by something else we know about free particles: Their momentum should stay constant since they do not experience any force. We can see that the complex exponential function is a

Momentum eigenstate (plane wave solutions)

$$\phi(p,x) = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{p}{\hbar}x} \tag{2.4}$$

with $\hat{p}\phi(p,x) = p\phi(p,x)$,

using Eq. (1.30). Hence we shall pick the first of the two ways to write the general solutions. This solution works for <u>any energy E</u>, we call this a <u>continuous spectrum of a Hamiltonian</u>.

The states (2.4) have one draw-back, they cannot be normalized as in (1.27). Instead they have been chosen to fullfill the

Delta function normalisation

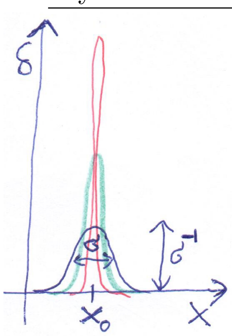
$$(\phi(p,x), \phi(p',x)) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dx\, e^{-i\frac{p}{\hbar}x} e^{i\frac{p'}{\hbar}x} = \delta(p-p'). \tag{2.5}$$

Here we made use of the

Dirac delta function: We define the object $\delta(x-x_0)$ such that

$$\int_{-\infty}^{\infty} dx\, f(x)\delta(x-x_0) = f(x_0), \tag{2.6}$$

for <u>any test-function</u> $f(x)$. In practice, you will ever only need Eq. (2.6).



left: You could loosely think of the delta-function as $= 0$ everywhere, except at x_0 where it is ∞. Clearly this definition is pathological. A better way is to think of it as the limit

$$\delta(x-x_0) = \lim_{\sigma\to 0} \frac{1}{\sqrt{\pi}\sigma} e^{-\frac{(x-x_0)^2}{\sigma^2}} \tag{2.7}$$

of an ever narrower Gaussian, as shown in the figure.

- The delta function is just a mathematical object, so its argument x can be any physical variable.
- Despite the name, the delta-function is not a genuine function, but mathematically a <u>distribution</u> or generalised function. That means we have to multiply it with a <u>test-function</u> and then integrate over it, to make sense of it, as we had seen above.

- The Delta function normalisation (2.5) now makes use of the important formula

$$(2\pi)\delta(x) = \int_{-\infty}^{\infty} dk\, e^{ikx}. \tag{2.8}$$

  See Griffith 59 for a refreshing discussion of this formula.

- An alternative normalisation also encountered is the box normalisation, where instead of an infinite space we assume (2.4) exists only within a volume $\mathcal{V}$ (in 1D interval), we write $\phi(p,x) = \frac{1}{\sqrt{\mathcal{V}}} e^{i\frac{p}{\hbar}x}$ and then see that these are normalised according to (1.27).

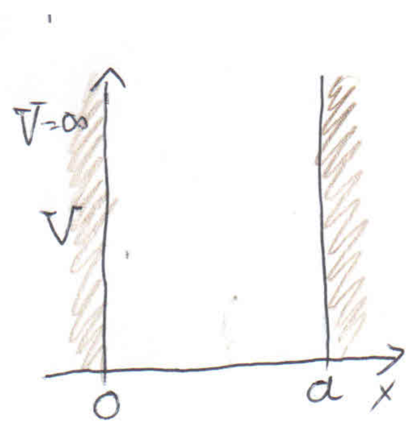
While the plane wave solutions (2.4) are straightforward to write down, the fact that they are not in the strict sense normalisable and form a continuous spectrum makes it harder to look at meaningful physics with them. We will thus defer a further discussion of the free particle to section 2.4, and first look at a few problems which are actually simpler to deal with, even though the Hamiltonian is seemingly more complicated.

2.2 Piecewise constant potentials

Just to group the problems logically, we will first consider potentials $V(x)$ that are piecewise constant, which is the next simpler setting compared to section 2.1. This means we can split space up at certain points x_k and write e.g.

$$\begin{aligned} V(x) &= V_- \text{ for } x \le x_0, \\ V(x) &= V_k \text{ for } x_k < x \le x_{k+1} \text{ with } k = 0, \cdots, N, \\ V(x) &= V_+ \text{ for } x > x_N. \end{aligned} \tag{2.9}$$

2.2.1 Infinite square well



left: We first consider the so-called infinite square well potential of width a, which is

$$\begin{aligned} V(x) &\to \infty \text{ for } x \le 0, \\ V(x) &= 0 \text{ for } 0 < x \le a, \\ V(x) &\to \infty \text{ for } x > a. \end{aligned} \tag{2.10}$$

If you are uncomfortable with the idea of an infinite potential, just set it to $V(x) = V_0$ outside the box, and then imagine the limit $V_0 \to \infty$.

Physically this implies the particle is free to move within $x = 0$ and $x = a$, but perfectly elastically reflects off the "walls" of that interval provided by the potential $V(x)$. We now want to solve the TISE (1.62) for this potential:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right]\phi_n(x)=\hat{H}\phi(x)=E_n\phi_n(x). \tag{2.11}$$

to try and find all finite energy eigenvalues E_n.

- First note, that a differential equation such as (1.62) essentially gives you a condition "for every x". That means we can first separately find its solution in each interval $x_k < x \leq x_{k+1}$ of (2.9).
- We have to then take special care of the connection points x_k, since the TISE contains a derivative and thus the condition does involve information from oth adjacent intervals at these points.
- Finally, even if the potential was smooth, the TISE is of second order in x and thus will in general have infinitely many solutions even for the same energy E_n, given by adjusting two unknown (complex) constants A, B (math courses). These are fixed by the requirement of normalisation 1.27 and what is called the boundary conditions. Those tell us how the function $\phi_n(x)$ at the edge of the solution interval, typically for $x \to \pm\infty$. In the end we find a unique solution $\phi_n(x)$, up to a complex phase (see discussion in section 1.6.1) for the eigenfunction $\phi_n(x)$ belonging to the specific energy eigenvalue E_n. However there can still be infinitely many different pairs $(\phi_n(x), E_n)$.

We shall now follow this program for the infinite box potential to see what it means.

(i) We first note that outside the box, we require $\phi_n(x) \equiv 0$. Suppose that was not the case for some finite interval $[p_1 p_2]$ outside the box. If we then take the expectation value of potential energy, we see

$$\langle V(\hat{x})\rangle \overset{Eq.~(1.41)}{=} \int_{-\infty}^{\infty} dx\, V(x)|\phi_n(x)|^2 > \int_{p_1}^{p_2} dx\, \underbrace{V(x)}_{\to\infty}|\phi_n(x)|^2 \to \infty. \tag{2.12}$$

Since the total energy $E_n > \langle V(\hat{x})\rangle$, it would be infinite, which does not make sense.

(ii) Inside the box, the TISE (2.11) can be written as before:

$$\frac{\partial^2}{\partial x^2}\phi_n(x) = -k_n^2\phi_n(x), \tag{2.13}$$

with constant $k_n = \sqrt{2mE_n}/\hbar$. This time we write the general solution is $\phi_n(x) = A\sin[k_n x] + B\cos[k_n x]$, because a subsequent step will then be easier. Here you see how the two constants mentioned before come in. We can fix these using

Continuity conditions for wavefunctions (for solutions of the TISE): For all x at which the potential $V(x)$ has at most a finite jump, the wavefunction $\phi_n(x)$ and its derivative $\frac{\partial}{\partial x}\phi_n(x)$ must be continuous. At x where the potential $V(x)$ has a infinite jump, only the wavefunction $\phi_n(x)$ must be continuous, the derivative may be discontinuous.

Proof: We form the TISE into $\phi_n(x)'' = -2m[E_n - V(x)]\phi_n(x)/\hbar^2$ and integrate both the LHS and RHS as in $\int_{x_0-\epsilon}^{x_0+\epsilon} dx \cdots$ over a small interval adjacent to the point x_0, taken as $[x_0-\epsilon, x_0+\epsilon]$, with infinitesimal ϵ:

$$\int_{x_0-\epsilon}^{x_0+\epsilon} dx\, \phi_n(x)'' = \left[\phi_n(x_0+\epsilon)' - \phi_n(x_0-\epsilon)'\right] = -\frac{2m}{\hbar^2}\int_{x_0-\epsilon}^{x_0+\epsilon} dx\, \underbrace{[E_n - V(x)]\phi_n(x)}_{=I(x)}. \tag{2.14}$$

Taking the limit $\epsilon \to 0$, we see that as long as $V(x)$ was finite everywhere, the integrand $I(x)$on the RHS is finite and thus $\lim_{\epsilon\to 0}\int_{x_0-\epsilon}^{x_0+\epsilon} dx I(x) = 0$. Then (2.14) implies that $\phi_n(x)'$ is continuous. If that is the case, we can redo a similar trick and write

$$\int_{x_0-\epsilon}^{x_0+\epsilon} dx\, \phi_n(x)' = \left[\phi_n(x_0+\epsilon) - \phi_n(x_0-\epsilon)\right], \tag{2.15}$$

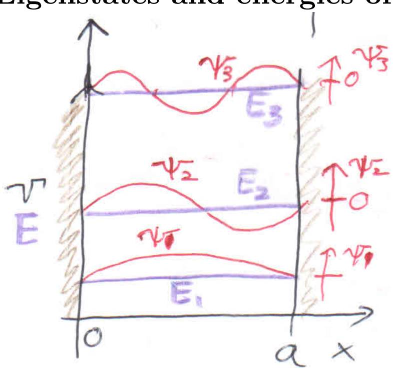
Again taking the limit $\epsilon \to 0$, we see that also $\phi_n(x)$ is continuous as long as $\phi_n(x)'$ is finite, which it is. If $V(x)$ is infinite or tends to infinite, the argument above does not hold, since we don't quite know what the RHS integral in (2.14) gives. We shall see an example later, where it can provide a finite answer and thus lead to a finite jump in the derivative $\phi_n(x)'$ at location x_0. However the wavefunction $\phi_n(x)$ itself always is continuous, even if the potential has an infinite jump.

(iii) We can now use the boundary conditions just derived to fix the constants A and B in teh solution above. Since the wavefunction vanishes outside the box, it being continuous means

$$\begin{aligned} 0 &= \phi_n(0) = B, \\ 0 &= \phi_n(a) = A\sin[k_n a] + B\cos[k_n a]. \end{aligned} \tag{2.16}$$

We reached $\sin[k_n a] = 0$, which is the case for $k_n a = n\pi$, for integer n. We can see that $n = 0$ is not normalizable and $n < 0$ gives nothing new compared to $n > 0$, then we reach

Eigenstates and energies of the particle in the infinite square well



left: Drawing of energies E_n (violet), potential $V(x)$ (black) and wavefunctions (red, read $\Psi_n \to \phi_n$)

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}, \text{ for } n = 1, 2, 3, \cdots \tag{2.17}$$

$$\phi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right). \tag{2.18}$$

- We have fixed the normalisation constant A through Eq. (1.6.1).
- There is an infinite number of solutions numbered by the quantum number n.

- Despite the crudeness of this potential, there is a lot of generally valid physics for quantum bound-states in it:

  (i) The smallest allowed energy E_1 is not zero.

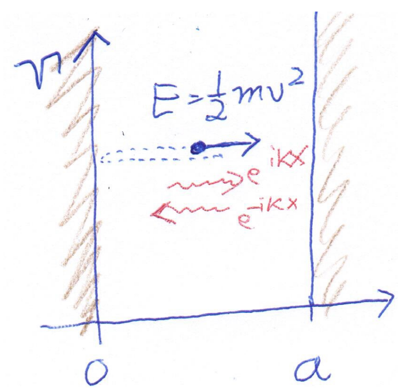
  (ii) The stronger the confinement (lower a), the larger the energy spacing $E_{n+1} - E_n$.

  (iii) The higher the mass, the smaller the energy spacing $E_{n+1} - E_n$.

- Solutions alternate between symmetric and anti-symmetric with respect to the box centre. The number of their nodes is $n - 1$. You can confirm that they are orthonormal (1.26) (exercise/Griffith), as expected from section 1.5.4, since the Hamiltonian is Hermitian.

- We also directly see that the eigenfunctions $\phi_n(x)$ form a basis of all functions in $[0, a]$, since $f(x) = \sum_n c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$ (See Eq. (1.18)) is exactly the Fourier series.

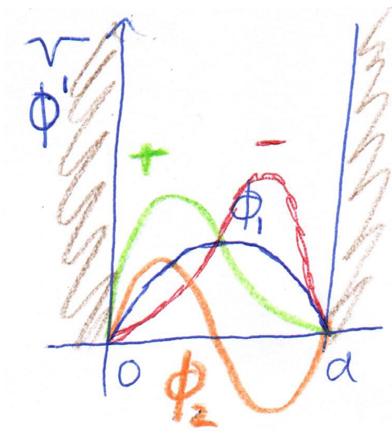
Example 13, Physical interpretation of particle in the box state:



left: Imagine what a classical particle in the box potential would do. Since there is no force between $[0, a]$ it would move there with constant velocity, only to experience a sudden elastic reflection when encountering the wall. It thus would bounce back and forth, with either momentum $p > 0$ or $p < 0$. As per our discussion in section 2.1, the corresponding momentum eigenstates are $e^{i\frac{p}{\hbar}x}$ and $e^{-i\frac{p}{\hbar}x}$, which add up to a cosine or sine, as in (2.18), depending on the sign with which we superimpose them. Now through the boundary conditions, we are selecting only a discretized set of these momenta p.

Now we can make use of the powerful statement Eq. (1.70) according to which the solutions of the TISE also dictate the time-evolution for cases with time-independent Hamiltonian (which clearly applies to the one in Eq. (2.11)).

Example 14, Particle in the box dynamics:



left: Consider the particle in state $\Psi(x, t = 0) = \frac{1}{\sqrt{2}}(\phi_1(x) + \phi_2(x)) = \phi_+$. We call this <u>superposition state</u>. As per Eq. (1.70), its time evolution is

$$\Psi(x,t) = \frac{1}{\sqrt{2}} e^{-i\frac{E_1}{\hbar}t}\left(\phi_1(x) + \underbrace{e^{-i\frac{(E_2-E_1)}{\hbar}t}}_{\equiv C(t)}\phi_2(x)\right) \tag{2.19}$$

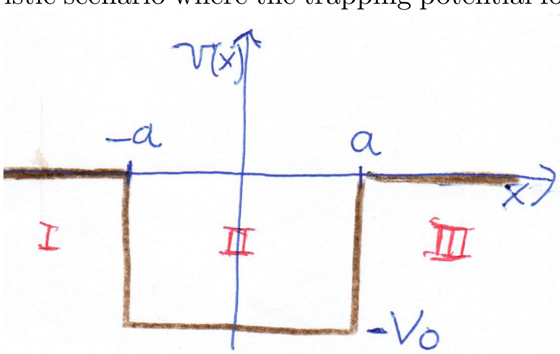
We know that at $t\frac{(E_2-E_1)}{\hbar} = (2n+1)\pi$ for integer n (odd multiples of π), the complex phase factor $C(t) = -1$, while at $t\frac{(E_2-E_1)}{\hbar} = (2n)\pi$ for integer n (even multiples of π) we have $C(t) = 1$.

We thus periodically cycle between a wavefunction ϕ_+ (green in figure) and $\phi_- = \Psi(x, t = 0) = \frac{1}{\sqrt{2}}(\phi_1(x) - \phi_2(x))$ (red in figure), up to the global phase $e^{-i\frac{E_1}{\hbar}t}$, which <u>does not</u> affect the position probability distribution. The corresponding probability densities $|\phi_\pm|^2$ would show a similar structure. This again corroborates the underlying classical picture of the particle bouncing back and forth between the wall. Now please checkout this online app. In contrast to PHY106, you should understand the meaning of <u>all its elements now</u>, after reading the documentation.

- When forming the probability density $|\Psi(x,t)|^2$ we see that the <u>global phase</u> $e^{-i\frac{E_1}{\hbar}t}$ drops out, as per our discussion in section 1.6.1. In contrast, the <u>relative phase</u> $C(t)$ between the states $\phi_{1,2}(x)$ turned out crucial, giving us all time dependence.

2.2.2 Finite square well

Instead of the slightly unsettling $V = \infty$ in the preceding section, we now consider the more realistic scenario where the trapping potential for the particle makes a finite jump by an energy V_0 only.



left: To follow Griffith's notation, we adjust the width and zero of energy slightly compared to Eq. (2.10):

$$\begin{aligned} V(x) &= 0 \text{ for } x \leq -a, \\ V(x) &= -V_0 \text{ for } -a < x \leq a, \\ V(x) &= 0 \text{ for } x > a, \end{aligned} \tag{2.20}$$

where $V_0 > 0$, see figure.

We are for now only looking for energies in the range $-V_0 < E_n < 0$. (You can show that $\min_x[V(x)] < E$, see Griffith problem 2.2.), and we will look at $E_n > 0$ in section 2.2.3.

As in section 2.2.1, we can treat all three regions separately and then worry about connection conditions. Let us again re-write the TISE as before:

$$\frac{\partial^2}{\partial x^2}\phi_n^{(r)}(x) = -{k_n^{(r)}}^2\phi_n^{(r)}(x), \tag{2.21}$$

for $(r) \in \{I, II, III\}$, where each region has its own wavenumber $k_n^{(r)} = \sqrt{2m[E_n - V(x)]}/\hbar$. We shall use the version where we write the general solution of the TISE in each region in the exponential form, as in section 2.1, with two so far unknown constants per region.

$$\begin{aligned}
\phi_n^{(I)}(x) &= Ae^{ik^{(I)}x} + Be^{-ik^{(I)}x}, \text{ for } x \le -a \\
\phi_n^{(II)}(x) &= Ce^{ik^{(II)}x} + De^{-ik^{(II)}x} \text{ for } -a < x \le a, \\
\phi_n^{(III)}(x) &= Fe^{ik^{(III)}x} + Ge^{-ik^{(III)}x} \text{ for } x > a.
\end{aligned} \tag{2.22}$$

Now note that, for the potential (2.20), $k_n^{(I)} = k_n^{(III)} = \sqrt{2mE_n}/\hbar = i\sqrt{-2mE_n}/\hbar \equiv i\kappa_n$, with real $\kappa_n > 0$. Since $E_n < 0$, these two wavenumbers must be imaginary, which we made explicit in the last step. In the second region $k_n^{(II)} = \sqrt{2m(E_n + V_0)}/\hbar \equiv \ell > 0$ is real. Inserting all that, the above Ansatz becomes

$$\begin{aligned}
\phi_n^{(I)}(x) &= Ae^{-\kappa x} + Be^{+\kappa x}, \\
\phi_n^{(II)}(x) &= Ce^{i\ell x} + De^{-i\ell x}, \\
\phi_n^{(III)}(x) &= Fe^{-\kappa x} + Ge^{+\kappa x}.
\end{aligned} \tag{2.23}$$

Now, in order for the wavefunction to be normalizable, we require $A = 0$ and $G = 0$, since the A term would blow up towards $x \to -\infty$ and the G term towards $x \to \infty$. Regarding C and D, note that the potential $V(x)$ is symmetric (even) under $x \leftrightarrow -x$, and you can show that in such cases all wavefunctions must be either even or odd (assignment). We do only the even ones for now, and thus reach

$$\phi_n(x) = \begin{cases} \phi_n^{(I)}(x) & = Be^{+\kappa x}, \text{ for } x \le -a. \\ \phi_n^{(II)}(x) & = C\cos\ell x \text{ for } -a < x \le a, \\ \phi_n^{(III)}(x) & = Be^{-\kappa x} \text{ for } x > a, \end{cases} \tag{2.24}$$

with continuity condition at e.g. $x = a$ given by

$$Be^{-\kappa a} = C\cos\ell a, \tag{2.25}$$

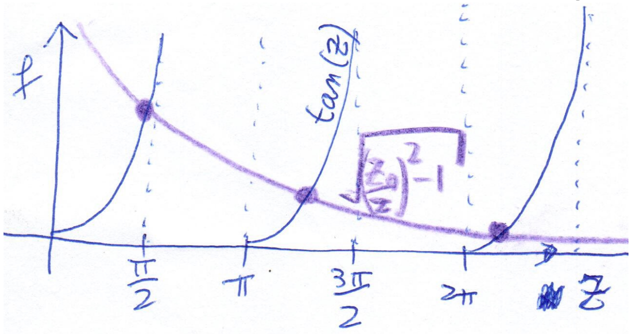
$$-\kappa Be^{-\kappa a} = -C\ell\sin\ell a. \tag{2.26}$$

Dividing Eq. (2.26) by Eq. (2.25) gives $\kappa = \ell\tan(\ell a)$. This is a transcendental equation[8], which typically is hard to solve. Since κ and ℓ contain the energy E_n, if we can find a solution for some E_n, we have found the eigenenergy. Grifitth discusses a bit how the renaming $z = la$ and $z_0 = a\sqrt{2mV_0}/\hbar$, allows us to recast the equation as

$$\tan z = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1},. \tag{2.27}$$

[8] As opposed to a polynomial one

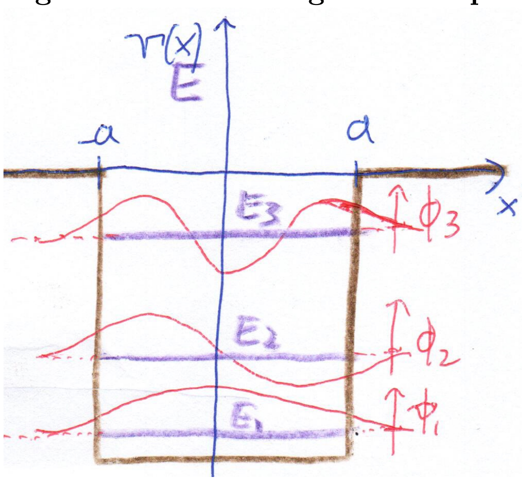
which allows us to understand the solutions graphically:



left: Drawing of $\sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$ (violet) and different branches of $\tan z$. Values of $z = a\sqrt{2m(E_n + V_0)}/\hbar$ with an intersect, give the allowed energies E_n.

Once we know an energy E_n, e.g. Eq. (2.25) will provide B in terms of C, and C can then finally be found from the normalisation. After also sorting out also the odd eigenstates, we finally reach the

Eigenstates and energies of the particle in the finite square well



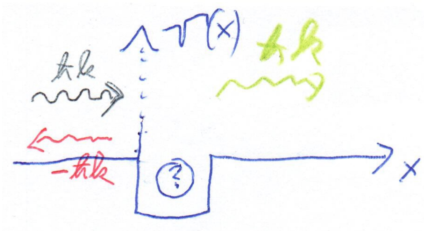
left: Eigenenergies and eigenstats in the finite box, in the same style as for the infinite one earlier.

- We see here one further key feature of quantum mechanics: The wavefunction "leaks" into the region where $E < V(x)$. Classical particles can't do this, since that would imply a negative kinetic energy.
- Another difference to section 2.2.1, that is apparent from the graphical solution of the equation for the eigenenergies, is that there is only a finite number of bound states.

For this problem, we now expect a new class of behavior for $E > 0$ (= energies higher than the height of the potential wall), which we shall discuss in the next section.

2.2.3 Scattering

For $E > 0$ we can again use (2.22) but this time all $k^{(r)}$ are real, with $k_n^{(I)} = k_n^{(III)} = \sqrt{2mE}/\hbar = k > 0$ and $k_n^{(II)} = \sqrt{2m(E+V_0)}/\hbar = \ell > 0$. For that reason, we cannot remove as many terms from (2.22) due to normalisation as before, but we set $G = 0$ due to the physical picture of scattering that we have in mind:



left: A particle is impinging on the square well with momentum $p = \hbar k$ from the left (black arrow). Due to the potential, it may then be scattered back (red arrow), due to energy conservation with momentum $-p$, or transmitted, keeping momentum p.

The Ansatz for the wavefunction is thus:

$$\phi_n^{(I)}(x) = Ae^{ikx} + Be^{-ikx}, \text{ for } x \le -a$$
$$\phi_n^{(II)}(x) = Ce^{i\ell x} + De^{-i\ell x} \text{ for } -a < x \le a,$$
$$\phi_n^{(III)}(x) = Fe^{ikx} \text{ for } x > a. \tag{2.28}$$

We can now set up 4 boundary conditions from (2.28) due to continuity of ϕ and ϕ' at $x = -a$ and $x = a$. This allows us in principle to eliminate 4 of the 5 remaining unknown constants A, B, C, D, F in Eq. (2.22). The last constant cannot be fixed by normalisation, since the Ansatz (2.22) cannot be normalized when all the wavenumbers are real, for the same reasons as discussed in section 2.1. This does not matter here, since we are interested in the question: If a particle is impacting the well from the left, what is its

Transmission probability given by

$$T = |F|^2/|A|^2. \tag{2.29}$$

- We can understand that using e.g. the concept of probability current in section 1.6.4. Applying Eq. (1.53) to Eq. (2.22) gives a probability current in region I of

$$\begin{aligned} J^{(I)} &= \frac{\hbar}{m}\mathfrak{Im}\big([A^*e^{-ikx} + B^*e^{ikx}][ikAe^{ikx} + (-ik)Be^{-ikx}]\big) \\ &= \frac{\hbar}{m}\mathfrak{Im}\Big(|A|^2(ik) - |B|^2(ik) + (ik)\underbrace{\left[B^*Ae^{2ikx} - BA^*e^{-2ikx}\right]}_{=2i\mathfrak{Im}[B^*Ae^{2ikx}]}\Big) \\ &= \frac{\hbar}{m}k\big(|A|^2 - |B|^2\big), \end{aligned} \tag{2.30}$$

  providing the interpretation of $|A|^2$ as ingoing and $|B|^2$ as reflected current density. Note $\hbar k/m = v$ is the velocity. Obtaining $|F|^2$ as transmitted current density is much easier.

Let us once explicitly go through the solution of the piecewise TISE for this problem, we will then only state the results for a few other applications later. Then you shall also practice it in an assignment for one of those problems. The 4 continuity conditions are:

$$Ae^{-ika} + Be^{ika} = Ce^{-i\ell a} + De^{i\ell a} \qquad \text{from continuity of } \phi_n \text{ at } x = -a, \tag{2.31}$$

$$Ce^{i\ell a} + De^{-i\ell a} = Fe^{ika} \qquad \text{from continuity of } \phi_n \text{ at } x = a, \tag{2.32}$$

$$(ik)Ae^{-ika} - (ik)Be^{ika} = (i\ell)Ce^{-i\ell a} - (i\ell)De^{i\ell a} \qquad \text{from continuity of } \phi_n' \text{ at } x = -a, \tag{2.33}$$

$$(i\ell)Ce^{i\ell a} - (i\ell)De^{-i\ell a} = (ik)Fe^{ika} \qquad \text{from continuity of } \phi_n' \text{ at } x = a, \tag{2.34}$$

We now first find C and D in terms of F, using Eq. (2.32)±Eq. (2.34)/(il) to reach

$$C = \frac{1}{2}Fe^{ia(k-\ell)}(1 + \frac{k}{\ell}), \tag{2.35}$$

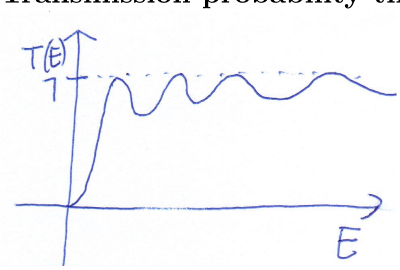
$$D = \frac{1}{2}Fe^{ia(k+\ell)}(1 - \frac{k}{\ell}), \tag{2.36}$$

We can now eliminate C and D, while taking Eq. (2.31)+ Eq. (2.33)/(ik) to reach

$$2Ae^{-2ika} = F\left[\cos(2la) - i(k/\ell + \ell/k)\sin(2la)\right]. \tag{2.37}$$

Alternatively, you can run these 4 equations for 5 unknowns into `mathematica` and hit `Solve[]`. Plugging the last line into (2.29), and expressing k and ℓ in terms of the relevant energies and potentials gives us the

Transmission probability through a finite square well



left: As shown on the left:

$$T = \frac{1}{1 + \frac{V_0^2}{4E(E+V_0)}\sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)} \tag{2.38}$$

- A first thing we notice is that $T \approx 0$ for small E. This is surprising, since $E > 0$ means the particle has more energy than the potential energy at <u>all x</u> and thus classically would pass with 100%. This is a manifestation of <u>quantum reflection</u>. The same would be true for a single potential step (where $V(x) = -V_0$ also at all $x > a$.

- From (2.38), $T = 1$ whenever $\frac{2a}{\hbar}\sqrt{2m(E+V_0)} = n\pi$ for $n \in \mathbb{Z}$ implying perfect transmission. We can reform this to give

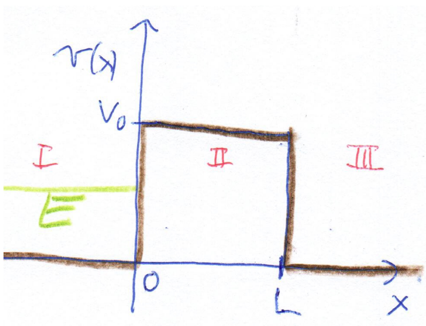
$$E_n + V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}, \tag{2.39}$$

  which are exactly the energies above zero where we would expect an eigenstate of the infinite box. We see that <u>resonances</u> with bound-states (or metastable states) significantly affect the scattering behaviour. This feature is crucial for experimental interrogation throughout, particularly in nuclear and particle physics. See also the section on Griffith, on the S-matrix (2.7).

- In this section, all values of $E > 0$ gave a solution of the TISE. Together with section 2.2.2 the finite well thus has a combination of a discrete spectrum $E_n < 0$ and a continuous spectrum, for $E > 0$. There are many other examples of this.

- The wavefunctions for $E > 0$ that reach all the way to $x \to \pm\infty$ are called scattering states.

2.2.4 Square barrier



left: We can invert the potential (2.20), by letting $V(x) > V_0 > 0$ within some range (now $x = 0$ to $x = L$). We then consider the same scattering Ansatz as proposed in section 2.2.3, which can be solved with the same techniques. Here we are mainly interested in the case $0 < E < V_0$. As you have learned in PHY106, this gives rise to

Quantum tunneling with transmission probability (2.29), in the limit $E \ll V_0$ and $\kappa L \gg 1$ given by

$$T = e^{-2\kappa L}, \text{ for } \kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}. \tag{2.40}$$

- You will learn how to derive the more general T for all cases in assignment 2.

- You can find this formula by applying the techniques of section 2.2.3 to this modified setting (exercise).

- Transmission through the barrier for $E < V_0$ is classically impossible, but allowed in quantum tunnelling.

- We had discussed the important points of (2.40) and physics examples where tunnelling is crucial quite extensively in PHY106, week9, hence we don't repeat that here.