

## Chapter 2

# Quantum mechanics in one dimension

Following the rules of quantum mechanics, we have seen that the state of a quantum particle, subject to a scalar potential  $V(\mathbf{r})$ , is described by the time-dependent Schrödinger equation,

$$i\hbar\partial_t\Psi(\mathbf{r}, t) = \hat{H}\Psi(\mathbf{r}, t), \quad (2.1)$$

where  $\hat{H} = -\frac{\hbar^2\nabla^2}{2m} + V(\mathbf{r})$  denotes the Hamiltonian. To explore its properties, we will first review some simple and, hopefully, familiar applications of the equation to one-dimensional systems. In addressing the one-dimensional geometry, we will divide our consideration between potentials,  $V(x)$ , which leave the particle free (i.e. unbound), and those that bind the particle to some region of space.

### 2.1 Wave mechanics of unbound particles

#### 2.1.1 Free particle

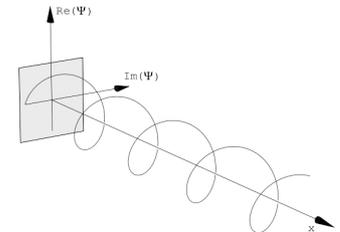
In the absence of an external potential, the time-dependent Schrödinger equation (2.1) describes the propagation of travelling waves. In one dimension, the corresponding complex wavefunction has the form

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

where  $A$  is the amplitude, and  $E(k) = \hbar\omega(k) = \frac{\hbar^2 k^2}{2m}$  represents the free particle energy dispersion for a non-relativistic particle of mass,  $m$ , and wavevector  $k = 2\pi/\lambda$  with  $\lambda$  the wavelength. Each wavefunction describes a plane wave in which the particle has definite energy  $E(k)$  and, in accordance with the de Broglie relation, momentum  $p = \hbar k = h/\lambda$ . The energy spectrum of a freely-moving particle is therefore continuous, extending from zero to infinity and, apart from the spatially constant state  $k = 0$ , has a two-fold degeneracy corresponding to right and left moving particles.

For an infinite system, it makes no sense to fix the amplitude  $A$  by the normalization of the total probability. Instead, it is useful to fix the flux associated with the wavefunction. Making use of Eq. (1.7) for the particle current, the plane wave is associated with a constant (time-independent) flux,

$$j(x, t) = -\frac{i\hbar}{2m} (\Psi^* \partial_x \Psi - \text{c.c.}) = |A|^2 \frac{\hbar k}{m} = |A|^2 \frac{p}{m}.$$



For a given value of the flux  $j$ , the amplitude is given, up to an arbitrary constant phase, by  $A = \sqrt{mj/\hbar k}$ .

To prepare a **wave packet** which is localized to a region of space, we must superpose components of different wave number. In an open system, this may be achieved using a Fourier expansion. For any function,<sup>1</sup>  $\psi(x)$ , we have the Fourier decomposition,<sup>2</sup>

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(k) e^{ikx} dk,$$

where the coefficients are defined by the inverse transform,

$$\psi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x) e^{-ikx} dx.$$

The normalization of  $\psi(k)$  follows automatically from the normalization of  $\psi(x)$ ,  $\int_{-\infty}^{\infty} \psi^*(k)\psi(k)dk = \int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = 1$ , and both can represent probability amplitudes. Applied to a wavefunction,  $\psi(x)$  can be understood as a wave packet made up of contributions involving definite momentum states,  $e^{ikx}$ , with amplitude set by the Fourier coefficient  $\psi(k)$ . The probability for a particle to be found in a region of width  $dx$  around some value of  $x$  is given by  $|\psi(x)|^2 dx$ . Similarly, the probability for a particle to have wave number  $k$  in a region of width  $dk$  around some value of  $k$  is given by  $|\psi(k)|^2 dk$ . (Remember that  $p = \hbar k$  so the momentum distribution is very closely related. Here, for economy of notation, we work with  $k$ .)

The Fourier transform of a normalized Gaussian wave packet,  $\psi(k) = (\frac{2\alpha}{\pi})^{1/4} e^{-\alpha(k-k_0)^2}$ , is also a Gaussian (exercise),

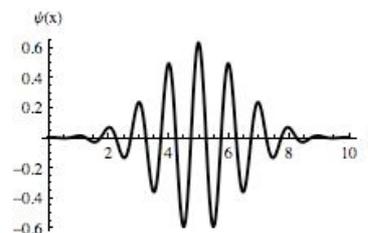
$$\psi(x) = \left(\frac{1}{2\pi\alpha}\right)^{1/4} e^{ik_0x} e^{-\frac{x^2}{4\alpha}}.$$

From these representations, we can see that it is possible to represent a *single* particle, localized in real space as a superposition of plane wave states localized in Fourier space. But note that, while we have achieved our goal of finding localized wave packets, this has been at the expense of having some non-zero width in  $x$  and in  $k$ .

For the Gaussian wave packet, we can straightforwardly obtain the width (as measured by the root mean square – RMS) of the probability distribution,  $\Delta x = (\langle(x - \langle x \rangle)^2\rangle)^{1/2} \equiv (\langle x^2 \rangle - \langle x \rangle^2)^{1/2} = \sqrt{\alpha}$ , and  $\Delta k = \frac{1}{\sqrt{4\alpha}}$ . We can again see that, as we vary the width in  $k$ -space, the width in  $x$ -space varies to keep the following product constant,  $\Delta x \Delta k = \frac{1}{2}$ . If we translate from the wavevector into momentum  $p = \hbar k$ , then  $\Delta p = \hbar \Delta k$  and

$$\Delta p \Delta x = \frac{\hbar}{2}.$$

If we consider the width of the distribution as a measure of the “uncertainty”, we will prove in section (3.1.2) that the Gaussian wave packet provides the minimum uncertainty. This result shows that we cannot know the position of a particle and its momentum at the same time. If we try to localize a particle to a very small region of space, its momentum becomes uncertain. If we try to



<sup>1</sup>More precisely, we can make such an expansion providing we meet some rather weak conditions of smoothness and differentiability of  $\psi(x)$  – conditions met naturally by problems which derive from physical systems!

<sup>2</sup>Here we will adopt an economy of notation using the same symbol  $\psi$  to denote the wavefunction and its Fourier coefficients. Their identity will be disclosed by their argument and context.

make a particle with a definite momentum, its probability distribution spreads out over space.

With this introduction, we now turn to consider the interaction of a particle with a non-uniform potential background. For non-confining potentials, such systems fall into the class of **scattering problems**: For a beam of particles incident on a non-uniform potential, what fraction of the particles are transmitted and what fraction are reflected? In the one-dimensional system, the classical counterpart of this problem is trivial: For particle energies which exceed the maximum potential, all particles are eventually transmitted, while for energies which are lower, all particles are reflected. In quantum mechanics, the situation is richer: For a generic potential of finite extent and height, some particles are always reflected and some are always transmitted. Later, in chapter 14, we will consider the general problem of scattering from a localized potential in arbitrary dimension. But for now, we will focus on the one-dimensional system, where many of the key concepts can be formulated.

### 2.1.2 Potential step

As we have seen, for a time-independent potential, the wavefunction can be factorized as  $\Psi(x, t) = e^{-iEt/\hbar}\psi(x)$ , where  $\psi(x)$  is obtained from the stationary form of the Schrödinger equation,

$$\left[ -\frac{\hbar^2 \partial_x^2}{2m} + V(x) \right] \psi(x) = E\psi(x),$$

and  $E$  denotes the energy of the particle. As  $|\Psi(x, t)|^2$  represents a probability density, it must be everywhere finite. As a result, we can deduce that the wavefunction,  $\psi(x)$ , is also finite. Moreover, since  $E$  and  $V(x)$  are presumed finite, so must be  $\partial_x^2 \psi(x)$ . The latter condition implies that

- ▷ both  $\psi(x)$  and  $\partial_x \psi(x)$  must be continuous functions of  $x$ , even if  $V$  has a discontinuity.

Consider then the influence of a potential step (see figure) on the propagation of a beam of particles. Specifically, let us assume that a beam of particles with kinetic energy,  $E$ , moving from left to right are incident upon a potential step of height  $V_0$  at position  $x = 0$ . If the beam has unit amplitude, the reflected and transmitted (complex) amplitudes are set by  $r$  and  $t$ . The corresponding wavefunction is given by

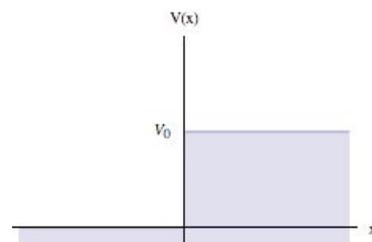
$$\begin{aligned} \psi_{<}(x) &= e^{ik_{<}x} + r e^{-ik_{<}x} & x < 0 \\ \psi_{>}(x) &= t e^{ik_{>}x} & x > 0 \end{aligned}$$

where  $k_{<} = \sqrt{\frac{2mE}{\hbar^2}}$  and  $k_{>} = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$ . Applying the continuity conditions on  $\psi$  and  $\partial_x \psi$  at the step ( $x = 0$ ), one obtains the relations  $1 + r = t$  and  $ik_{<}(1 - r) = ik_{>}t$  leading to the reflection and transmission amplitudes,

$$r = \frac{k_{<} - k_{>}}{k_{<} + k_{>}}, \quad t = \frac{2k_{<}}{k_{<} + k_{>}}.$$

The reflectivity,  $R$ , and transmittivity,  $T$ , are defined by the ratios,

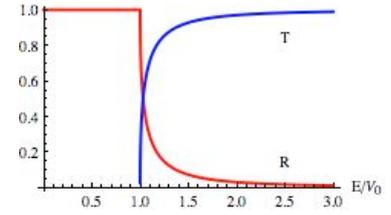
$$R = \frac{\text{reflected flux}}{\text{incident flux}}, \quad T = \frac{\text{transmitted flux}}{\text{incident flux}}.$$



With the incident, reflected, and transmitted fluxes given by  $|A|^2 \frac{\hbar k_{<}}{m}$ ,  $|Ar|^2 \frac{\hbar k_{<}}{m}$ , and  $|At|^2 \frac{\hbar k_{>}}{m}$  respectively, one obtains

$$R = \left| \frac{k_{<} - k_{>}}{k_{<} + k_{>}} \right|^2 = |r|^2, \quad T = \left| \frac{2k_{<}}{k_{<} + k_{>}} \right|^2 \frac{k_{>}}{k_{<}} = |t|^2 \frac{k_{>}}{k_{<}} = \frac{4k_{<}k_{>}}{(k_{<} + k_{>})^2}.$$

From these results one can confirm that the total flux is, as expected, conserved in the scattering process, i.e.  $R + T = 1$ .

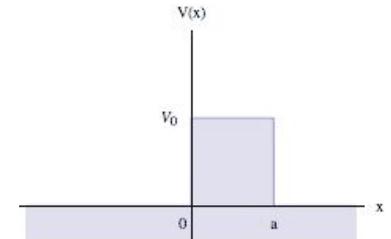


▷ EXERCISE. While  $E - V_0$  remains positive, show that the beam is able to propagate across the potential step (see figure). Show that the fraction of the beam that is reflected depends on the relative height of the step while the phase depends on the sign of  $V_0$ . In particular, show that for  $V_0 > 0$ , the reflected beam remains in phase with the incident beam, while for  $V_0 < 0$  it is reversed. Finally, when  $E - V_0 < 0$ , show that the beam is unable to propagate to the right ( $R = 1$ ). Instead show that there is an evanescent decay of the wavefunction into the barrier region with a decay length set by  $2\pi\sqrt{\hbar^2/2m(V_0 - E)}$ . If  $V_0 \rightarrow \infty$ , show that the system forms a standing wave pattern.

### 2.1.3 Potential barrier

Having dealt with the potential step, we now turn to consider the problem of a beam of particles incident upon a square potential barrier of height  $V_0$  (presumed positive for now) and width  $a$ . As mentioned above, this geometry is particularly important as it includes the simplest example of a scattering phenomenon in which a beam of particles is “deflected” by a local potential. Moreover, this one-dimensional geometry also provides a platform to explore a phenomenon peculiar to quantum mechanics – **quantum tunneling**. For these reasons, we will treat this problem fully and with some care.

Since the barrier is localized to a region of size  $a$ , the incident and transmitted wavefunctions have the same functional form,  $e^{ik_1x}$ , where  $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$ , and differ only in their complex amplitude, i.e. after the encounter with the barrier, the transmitted wavefunction undergoes only a change of amplitude (some particles are reflected from the barrier, even when the energy of the incident beam,  $E$ , is in excess of  $V_0$ ) and a phase shift. To determine the relative change in amplitude and phase, we can parameterise the wavefunction as



$$\begin{aligned} \psi_1(x) &= e^{ik_1x} + r e^{-ik_1x} & x \leq 0 \\ \psi_2(x) &= A e^{ik_2x} + B e^{-ik_2x} & 0 \leq x \leq a \\ \psi_3(x) &= t e^{ik_1x} & a \leq x \end{aligned}$$

where  $k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$ . Here, as with the step,  $r$  denotes the reflected amplitude and  $t$  the transmitted.

Applying the continuity conditions on the wavefunction,  $\psi$ , and its derivative,  $\partial_x \psi$ , at the barrier interfaces at  $x = 0$  and  $x = a$ , one obtains

$$\begin{cases} 1 + r = A + B \\ A e^{ik_2a} + B e^{-ik_2a} = t e^{ik_1a} \end{cases}, \quad \begin{cases} k_1(1 - r) = k_2(A - B) \\ k_2(A e^{ik_2a} - B e^{-ik_2a}) = k_1 t e^{ik_1a} \end{cases}.$$

Together, these four equations specify the four unknowns,  $r$ ,  $t$ ,  $A$  and  $B$ . Solving, one obtains (exercise)

$$t = \frac{2k_1 k_2 e^{-ik_1a}}{2k_1 k_2 \cos(k_2a) - i(k_1^2 + k_2^2) \sin(k_2a)},$$

translating to a transmissivity of

$$T = |t|^2 = \frac{1}{1 + \frac{1}{4} \left( \frac{k_1}{k_2} - \frac{k_2}{k_1} \right)^2 \sin^2(k_2 a)},$$

and the reflectivity,  $R = 1 - T$ . As a consistency check, we can see that, when  $V_0 = 0$ ,  $k_2 = k_1$  and  $t = 1$ , as expected. Moreover,  $T$  is restricted to the interval from 0 to 1 as required. So, for barrier heights in the range  $E > V_0 > 0$ , the transmissivity  $T$  shows an oscillatory behaviour with  $k_2$  reaching unity when  $k_2 a = n\pi$  with  $n$  integer. At these values, there is a conspiracy of interference effects which eliminate altogether the reflected component of the wave leading to perfect transmission. Such a situation arises when the width of the barrier is perfectly matched to an integer or half-integer number of wavelengths inside the barrier.

When the energy of the incident particles falls below the energy of the barrier,  $0 < E < V_0$ , a classical beam would be completely reflected. However, in the quantum system, particles are able to **tunnel** through the barrier region and escape leading to a non-zero transmission coefficient. In this regime,  $k_2 = i\kappa_2$  becomes pure imaginary leading to an evanescent decay of the wavefunction under the barrier and a suppression, but not extinction, of transmission probability,

$$T = |t|^2 = \frac{1}{1 + \frac{1}{4} \left( \frac{k_1}{\kappa_2} + \frac{\kappa_2}{k_1} \right)^2 \sinh^2 \kappa_2 a}.$$

For  $\kappa_2 a \gg 1$  (the weak tunneling limit), the transmittivity takes the form

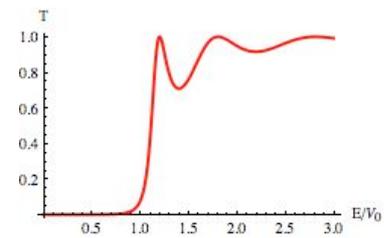
$$T \simeq \frac{16k_1^2 \kappa_2^2}{(k_1^2 + \kappa_2^2)^2} e^{-2\kappa_2 a}.$$

Finally, on a cautionary note, while the phenomenon of quantum mechanical tunneling is well-established, it is difficult to access in a convincing experimental manner. Although a classical particle with energy  $E < V_0$  is unable to penetrate the barrier region, in a physical setting, one is usually concerned with a thermal distribution of particles. In such cases, thermal activation may lead to transmission *over* a barrier. Such processes often overwhelm any contribution from true quantum mechanical tunneling.

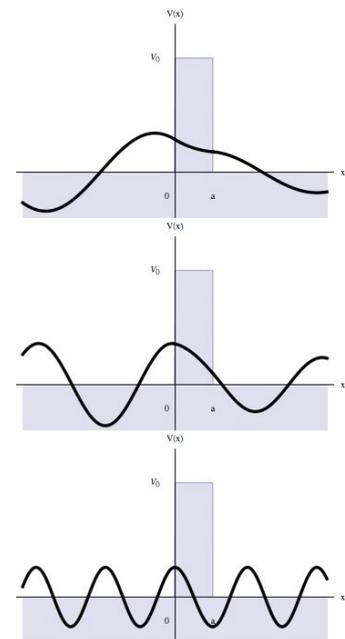
▷ **INFO. Scanning tunneling microscopy (STM)** is a powerful technique for viewing surfaces at the atomic level. Its development in the early eighties earned its inventors, Gerd Binnig and Heinrich Rohrer (at IBM Zürich), the Nobel Prize in Physics in 1986. STM probes the density of states of a material using the tunneling current. In its normal operation, a lateral resolution of 0.1 nm and a depth resolution of 0.01 nm is typical for STM. The STM can be used not only in ultra-high vacuum, but also in air and various other liquid or gas ambients, and at temperatures ranging from near zero kelvin to a few hundred degrees Celsius.

The STM is based on the concept of quantum tunnelling (see Fig. 2.1). When a conducting tip is brought in proximity to a metallic or semiconducting surface, a bias between the two can allow electrons to tunnel through the vacuum between them. For low voltages, this tunneling current is a function of the local density of states at the Fermi level,  $E_F$ , of the sample.<sup>3</sup> Variations in current as the probe passes over the surface are translated into an image. STM can be a challenging technique, as it requires extremely clean surfaces and sharp tips.

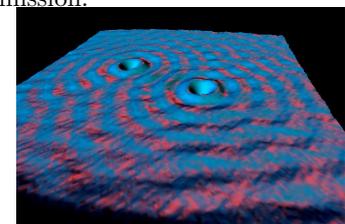
<sup>3</sup>Although the meaning of the Fermi level will be address in more detail in chapter 8, we mention here that it represents the energy level to which the electron states in a metal are fully-occupied.



Transmission probability of a finite potential barrier for  $\sqrt{2mV_0}a/\hbar = 7$ . Dashed: classical result. Solid line: quantum mechanics.



Real part of the wavefunction for  $E/V_0 = 0.6$  (top),  $E/V_0 = 1.6$  (middle), and  $E/V_0 = 1 + \pi^2/2$  (bottom), where  $mV_0 a^2/\hbar^2 = 1$ . In the first case, the system shows tunneling behaviour, while in the third case,  $k_2 a = \pi$  and the system shows resonant transmission.



STM image showing two point defects adorning the copper (111) surface. The point defects (possibly impurity atoms) scatter the surface state electrons resulting in circular standing wave patterns.

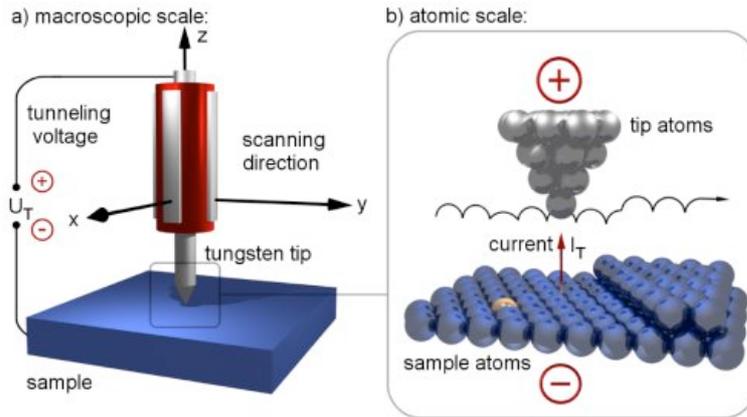


Figure 2.1: Principle of scanning tunneling microscopy: Applying a negative sample voltage yields electron tunneling from occupied states at the surface into unoccupied states of the tip. Keeping the tunneling current constant while scanning the tip over the surface, the tip height follows a contour of constant local density of states.

### 2.1.4 The rectangular potential well

Finally, if we consider scattering from a potential well (i.e. with  $V_0 < 0$ ), while  $E > 0$ , we can apply the results of the previous section to find a continuum of unbound states with the corresponding **resonance** behaviour. However, in addition to these unbound states, for  $E < 0$  we have the opportunity to find bound states of the potential. It is to this general problem that we now turn.

▷ EXERCISE. Explore the phase dependence of the transmission coefficient in this regime. Consider what happens to the phase as resonances (bound states) of the potential are crossed.

## 2.2 Wave mechanics of bound particles

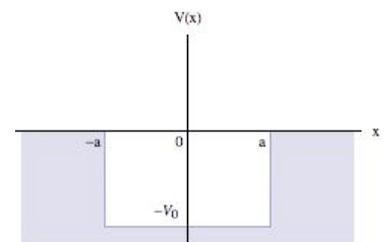
In the case of unbound particles, we have seen that the spectrum of states is continuous. However, for bound particles, the wavefunctions satisfying the Schrödinger equation have only particular quantized energies. In the one-dimensional system, we will find that all binding potentials are capable of hosting a bound state, a feature particular to the low dimensional system.

### 2.2.1 The rectangular potential well (continued)

As a starting point, let us consider a rectangular potential well similar to that discussed above. To make use of symmetry considerations, it is helpful to reposition the potential setting

$$V(x) = \begin{cases} 0 & x \leq -a \\ -V_0 & -a \leq x \leq a \\ 0 & a \leq x \end{cases},$$

where the potential depth  $V_0$  is assumed positive. In this case, we will look for bound state solutions with energies lying in the range  $-V_0 < E < 0$ . Since the Hamiltonian is invariant under **parity transformation**,  $[\hat{H}, \hat{P}] = 0$  (where  $\hat{P}\psi(x) = \psi(-x)$ ), the eigenstates of the Hamiltonian  $\hat{H}$  must also be



eigenstates of parity, i.e. we expect the eigenfunctions to separate into those symmetric and those antisymmetric under parity.<sup>4</sup>

For  $E < 0$  (bound states), the wavefunction outside the well region must have the form

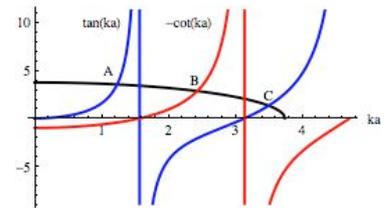
$$\psi(x < -a) = Ce^{\kappa x}, \quad \psi(x > a) = De^{-\kappa x},$$

with  $\kappa = \sqrt{-\frac{2mE}{\hbar^2}}$  while in the central well region, the general solution is of the form

$$\psi(-a < x < a) = A \cos(kx) + B \sin(kx),$$

where  $k = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$ . Once again we have four equations in four unknowns. The calculation shows that either  $A$  or  $B$  must be zero for a solution. This means that the states separate into solutions with even or odd parity.

For the even states, the solution of the equations leads to the quantization condition,  $\kappa = \tan(ka)k$ , while for the odd states, we find  $\kappa = -\cot(ka)k$ . These are transcendental equations, and must be solved numerically. The figure (right) compares  $\kappa a = (\frac{2mV_0a^2}{\hbar^2} - (ka)^2)^{1/2}$  with  $ka \tan(ka)$  for the even states and to  $-ka \cot(ka)$  for the odd states. Where the curves intersect, we have an allowed energy. From the structure of these equations, it is evident that an even state solution can always be found for arbitrarily small values of the binding potential  $V_0$  while, for odd states, bound states appear only at a critical value of the coupling strength. The wider and deeper the well, the more solutions are generated.



Comparison of  $\kappa a = (\frac{2mV_0a^2}{\hbar^2} - (ka)^2)^{1/2}$  with  $ka \tan(ka)$  and  $-ka \cot(ka)$  for  $\frac{2mV_0a^2}{\hbar^2} = 14$ . For this potential, there are a total of three solutions labelled A, B and C. Note that, from the geometry of the curves, there is always a bound state no matter how small is the potential  $V_0$ .

▷ EXERCISE. Determine the pressure exerted on the walls of a rectangular potential well by a particle inside. For a hint on how to proceed, see the discussion on degeneracy pressure on page 85.

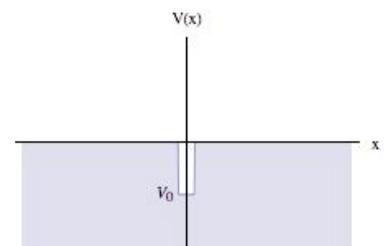
### 2.2.2 The $\delta$ -function potential well

Let us now consider perhaps the simplest binding potential, the  $\delta$ -function,  $V(x) = -aV_0\delta(x)$ . Here the parameter ‘ $a$ ’ denotes some microscopic length scale introduced to make the product  $a\delta(x)$  dimensionless.<sup>5</sup> For a state to be bound, its energy must be negative. Moreover, the form of the potential demands that the wavefunction is symmetric under parity,  $x \rightarrow -x$ . (A wavefunction which was antisymmetric must have  $\psi(0) = 0$  and so could not be influenced by the  $\delta$ -function potential.) We therefore look for a solution of the form

$$\psi(x) = A \begin{cases} e^{\kappa x} & x < 0 \\ e^{-\kappa x} & x > 0 \end{cases},$$

where  $\kappa = \sqrt{-2mE/\hbar^2}$ . With this choice, the wavefunction remains everywhere continuous including at the potential,  $x = 0$ . Integrating the stationary form of the Schrödinger equation across an infinitesimal interval that spans the region of the  $\delta$ -function potential, we find that

$$\partial_x \psi|_{+\epsilon} - \partial_x \psi|_{-\epsilon} = -\frac{2maV_0}{\hbar^2} \psi(0).$$



<sup>4</sup>Later, in section 3.2, we will discuss the role of symmetries in quantum mechanics.

<sup>5</sup>Note that the dimensions of  $\delta(x)$  are  $[\text{Length}^{-1}]$ .

From this result, we obtain that  $\kappa = maV_0/\hbar^2$ , leading to the bound state energy

$$E = -\frac{ma^2V_0^2}{2\hbar^2}.$$

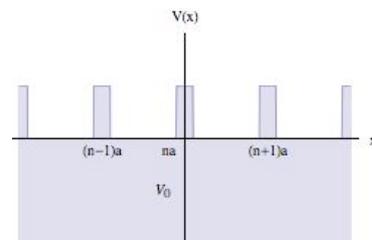
Indeed, the solution is unique. An attractive  $\delta$ -function potential hosts only one bound state.

▷ EXERCISE. Explore the bound state properties of the “molecular” binding potential  $V(x) = -aV_0[\delta(x+d) + \delta(x-d)]$ . Show that it consists of two bound states, one bonding (nodeless) and one antibonding (single node). How does the energy of the latter compare with two isolated  $\delta$ -function potential wells?

### 2.2.3 INFO: The $\delta$ -function model of a crystal

Finally, as our last example of a one-dimensional quantum system, let us consider a particle moving in a periodic potential. The **Kronig-Penney model** provides a caricature of a (one-dimensional) crystalline lattice potential. The potential created by the ions is approximated as an infinite array of potential wells defined by a set of repulsive  $\delta$ -function potentials,

$$V(x) = aV_0 \sum_{n=-\infty}^{\infty} \delta(x - na).$$



Since the potential is repulsive, it is evident that all states have energy  $E > 0$ . This potential has a new symmetry; a translation by the lattice spacing  $a$  leaves the potential unchanged,  $V(x+a) = V(x)$ . The probability density must therefore exhibit the same translational symmetry,

$$|\psi(x+a)|^2 = |\psi(x)|^2,$$

which means that, under translation, the wavefunction differs by at most a phase,  $\psi(x+a) = e^{i\phi}\psi(x)$ . In the region from  $(n-1)a < x < na$ , the general solution of the Schrödinger equation is plane wave like and can be written in the form,

$$\psi_n(x) = A_n \sin[k(x-na)] + B_n \cos[k(x-na)],$$

where  $k = \sqrt{2mE/\hbar^2}$  and, following the constraint on translational invariance,  $A_{n+1} = e^{i\phi}A_n$  and  $B_{n+1} = e^{i\phi}B_n$ . By applying the boundary conditions, one can derive a constraint on  $k$  similar to the quantized energies for bound states considered above.

Consider the boundary conditions at position  $x = na$ . Continuity of the wavefunction,  $\psi_n|_{x=na} = \psi_{n+1}|_{x=na}$ , translates to the condition,  $B_n = A_{n+1} \sin(-ka) + B_{n+1} \cos(-ka)$  or

$$B_{n+1} = \frac{B_n + A_{n+1} \sin(ka)}{\cos(ka)}.$$

Similarly, the discontinuity in the first derivative,  $\partial_x \psi_{n+1}|_{x=na} - \partial_x \psi_n|_{x=na} = \frac{2maV_0}{\hbar^2} \psi_n(na)$ , leads to the condition,  $k[A_{n+1} \cos(ka) + B_{n+1} \sin(ka) - A_n] = \frac{2maV_0}{\hbar^2} B_n$ . Substituting the expression for  $B_{n+1}$  and rearranging, one obtains

$$A_{n+1} = \frac{2maV_0}{\hbar^2 k} B_n \cos(ka) - B_n \sin(ka) + A_n \cos(ka).$$

Similarly, replacing the expression for  $A_{n+1}$  in that for  $B_{n+1}$ , one obtains the parallel equation,

$$B_{n+1} = \frac{2maV_0}{\hbar^2 k} B_n \sin(ka) + B_n \cos(ka) + A_n \sin(ka).$$

With these two equations, and the relations  $A_{n+1} = e^{i\phi}A_n$  and  $B_{n+1} = e^{i\phi}B_n$ , we obtain the quantization condition,<sup>6</sup>

$$\cos \phi = \cos(ka) + \frac{maV_0}{\hbar^2 k} \sin(ka).$$

As  $\hbar k = \sqrt{2mE}$ , this result relates the allowed values of energy to the real parameter,  $\phi$ . Since  $\cos \phi$  can only take values between  $-1$  and  $1$ , there are a sequence of allowed **bands** of energy with energy gaps separating these bands (see Fig. 2.2).

Such behaviour is characteristic of the spectrum of periodic lattices: In the periodic system, the wavefunctions – known as **Bloch states** – are indexed by a “quasi”-momentum index  $k$ , and a band index  $n$  where each Bloch band is separated by an energy gap within which there are no allowed states. In a **metal**, electrons (fermions) populate the energy states starting with the lowest energy up to some energy scale known as the **Fermi energy**. For a partially-filled band, low-lying excitations associated with the continuum of states allow electrons to be accelerated by a weak electric field. In a **band insulator**, all states are filled up to an energy gap. In this case, a small electric field is unable to excite electrons across the energy gap – hence the system remains insulating.

▷ **EXERCISE.** In the Kronig-Penney model above, we took the potential to be repulsive. Consider what happens if the potential is attractive when we also have to consider the fate of the states that were bound for the single  $\delta$ -function potential. In this case, you will find that the methodology and conclusions mirror the results of the repulsive potential: all states remain extended and the continuum of states exhibits a sequence of band gaps controlled by similar sets of equations.

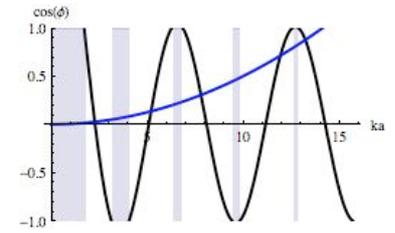


Figure 2.2: Solid line shows the variation of  $\cos \phi$  with  $ka$  over a range from  $-1$  to  $1$  for  $V_0 = 2$  and  $ma^2\hbar^2 = 1$ . The blue line shows  $0.01 \times E = (\hbar k)^2/2m$ . The shaded region represents values of  $k$  and energy for which there is no solution.

<sup>6</sup>Eliminating  $A_n$  and  $B_n$  from the equations, a sequence of cancellations obtains

$$e^{2i\phi} - e^{i\phi} \left( \frac{2maV_0}{\hbar^2 k} \sin(ka) + 2 \cos(ka) \right) + 1 = 0.$$

Then multiplying by  $e^{-i\phi}$ , we obtain the expression for  $\cos \phi$ .