

Quantum Mechanics I  
Case Studies

Oct. '03.  
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## 1. Piecewise Constant Potentials

Herein, we will consider some simple potentials in turn, and see to learn about some generic behavior of quantum systems.

### 1.1. Constant potential

The absolutely simplest potential of all is the constant one, which we may choose to be  $V(x) = 0$ . The corresponding force is of course zero, so that this corresponds to a ‘free’ particle. The (time independent) Schrödinger equation becomes

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right] \psi_E = E \psi_E, \quad (1.1)$$

or

$$\left[ \frac{d^2}{dx^2} + k^2 \right] \psi_E = 0, \quad (1.2)$$

where  $k = \frac{\sqrt{2mE}}{\hbar}$  is the *constant* wave-number (square-roots are always taken with the positive sign). The solutions of this simple 2nd order differential equation form a 2-parameter solution set which may be written as

$$\psi_E(x) = C_+ e^{ikx} + C_- e^{-ikx} = A \cos(kx) + B \sin(kx) = D \sin(kx + \delta). \quad (1.3)$$

The pair of constants  $C_{\pm}$  is easily related to  $A, B$  and to  $D, \delta$ ; one or the other or the third representation may be more advantageous in specific calculations, and the Student is required to know how to use and toggle between them all. Notice that there is no particular boundary condition<sup>1)</sup> on this type of wavefunctions, whence the parameters  $D, \delta, E$  remain constrained only by the (continuous) ortho-normalization condition:

$$\int_{-\infty}^{\infty} dx \psi_{E'}^* \psi_E = \delta(E - E'), \quad (1.4)$$

so that

$$\int_{-\infty}^{\infty} dE' \int_{-\infty}^{\infty} dx \psi_{E'}^* \psi_E = 1 \quad (1.5)$$

is well-defined<sup>2)</sup>.

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<sup>1)</sup> By ‘boundary’, here is meant ‘infinity’: when  $x \rightarrow \pm\infty$ ; such are also called ‘asymptotic conditions’.

<sup>2)</sup> Note that, strictly speaking, the integral (1.4) diverges for  $E' = E$ , but does so in a ‘tame’ enough manner, so that the double integral (1.5) is finite and may be used to normalize the overall amplitude of  $\psi_E$ .

Eq. (1.4), *i.e.*, (1.5) is a single condition on three variables,  $D, \delta, E$ , whence two of them remain free. Typically, the phase  $\delta$  and the energy  $E$ ; the condition (1.4) is used to fix the (overall) amplitude,  $D$ .

The physical meaning of the wave-function  $\psi_E(x) = C_+e^{ikx} + C_-e^{-ikx}$  is straightforward: upon multiplication with  $e^{i\omega t}$  of the first part,  $e^{ikx}$ , we obtain  $e^{ikx} \rightarrow e^{i(kx+\omega t)}$ , where  $\omega = E/\hbar = \hbar k^2/2m$ . Since  $e^{i(kx+\omega t)} = e^{i[k(x+\Delta x)+\omega(t+\Delta t)]}$  if  $\Delta x = +\omega\Delta t/k$ , this plane wave travels to the right. Similarly,  $e^{-ikx} \rightarrow e^{-i(kx-\omega t)}$  is a plane wave that travels to the left. So,  $\psi_E(x)$  is a linear combination of two traveling waves. Indeed, the right-moving probability current is

$$J_R = \frac{\hbar}{m} \Im m \left[ \psi_{E,R}^* \frac{d}{dx} \psi_{E,R} \right] = \frac{\hbar}{m} \Im m \left[ e^{-ikx} \frac{d}{dx} e^{ikx} \right] = \frac{\hbar k}{m}, \quad (1.6)$$

and the left moving one is

$$J_L = \frac{\hbar}{m} \Im m \left[ \psi_{E,L}^* \frac{d}{dx} \psi_{E,L} \right] = \frac{\hbar}{m} \Im m \left[ e^{ikx} \frac{d}{dx} e^{-ikx} \right] = -\frac{\hbar k}{m}, \quad (1.7)$$

in both cases being identifiable as the velocity of the particle described by the wave-function.

On the other hand,  $\psi_{E,S}(x) = A \cos(kx) + B \sin(kx) = D \sin(kx + \delta)$  is a standing wave, as the latter two representations show. Indeed, its probability current is

$$\begin{aligned} J_S &= \frac{\hbar}{m} \Im m \left[ \psi_{E,S}^* \frac{d}{dx} \psi_{E,S} \right] = \frac{\hbar}{m} \Im m \left[ D^* \sin(kx + \delta)^* \frac{d}{dx} D \sin(kx + \delta) \right], \\ &= \frac{\hbar}{m} \Im m \left[ |D|^2 \sin(kx + \delta) (-k \cos(kx + \delta)) \right], \\ &= -\frac{\hbar}{2m} |D|^2 k \Im m \left[ \sin(2kx + 2\delta) \right] = 0. \end{aligned} \quad (1.8)$$

In fact, it is easy to see that any essentially real wave-function (that is, where the function is real up to a multiplicative complex constant) yields a vanishing probability current.

Most importantly, this solution is *oscillatory*, with a constant wave number  $k$ , and momentum  $p = \hbar k$ . Thus, the left-moving plane wave corresponds to a particle with an infinitely well defined momentum, the spatial position of which is however spread all over: the probability density,  $|\psi_E(x)|^2$ , oscillates but is not significantly more or significantly less in any one region than elsewhere. Such states are typically called scattering states (which we'll study more in Chapter 8).

Note that the wave number ('spatial frequency', inverse wavelength) is proportional to the square-root of  $E - V(x)$ .

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We have tacitly assumed that  $E > V = 0$ . Imagine replacing  $E \rightarrow -E$  and consider the effect on the wave-functions (1.3). With negative  $E$ , the wave number becomes imaginary,  $k = i\kappa$  with  $\hbar\kappa = \sqrt{2m|E|}$ , and we can write

$$\psi_{-|E|} = D \sin(i\kappa x + \delta) = D \left[ \sin(\delta) \cosh(\kappa x) + i \cos(\delta) \sinh(\kappa x) \right]. \quad (1.9)$$

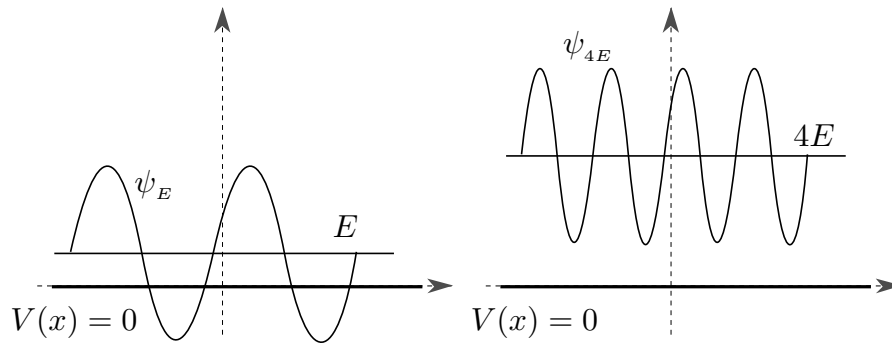


Fig. 1: The constant potential.

Note that this wave-function is no longer oscillatory, but is (almost) monotonous instead. However, such a wave-function cannot possibly be normalized, not even in the sense of Eqs. (1.4) or (1.5); the normalization integrals

$$|D'|^2 \int_{-\infty}^{\infty} dx |\sinh(kx - \delta')|^2 \quad (1.10)$$

and

$$|D'|^2 \int_{-\infty}^{\infty} dE' \int_{-\infty}^{\infty} dx |\sinh(kx - \delta')|^2 \quad (1.11)$$

are simply and incurably divergent for all nonzero  $D'$ .

### 1.2. Finite potential step

The next order of simplicity belongs to a simple ‘potential step’, where the potential is defined to be

$$V(x) = \begin{cases} 0, & \text{for } x < x_0; \\ V_0, & \text{for } x > x_0. \end{cases} \quad (1.12)$$

We note that for either  $x < x_0$  or for  $x > x_0$ , this looks like the previous case—the potential is constant, and we adopt the corresponding solutions. This is indeed the standard approach:

0. Fix the (next) value of  $E$  to be considered.
1. Divide the *domain* of  $x$  into contiguous regions where the energy is bigger than the potential:  $R_1 = \{x: E > V(x)\}$ , or smaller than the potential:  $R_2 = \{x: E < V(x)\}$ .
2. Find the general solution of the Schrödinger equation in each region.
3. Match the solutions across the interfacing boundaries between adjacent regions.
4. Enforce boundary conditions ‘at infinity’.
5. Normalize the wave-function.
6. Go back to item 0.

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Before we proceed with this task-list, we derive the general requirements to be used in step 3. To that end, consider the Schrödinger equation rewritten as

$$\frac{d^2\psi}{dx^2} \equiv \psi''(x) = \frac{m}{\hbar^2} [V(x) - E] \psi, \quad (1.13)$$

and think of it as determining the second derivative of the wave-function in terms of the wave-function itself and the square of the wave number. We know that  $E$  is a constant and that  $V(x)$  has a (finite) discontinuity; therefore,  $k^2 = \frac{2m}{\hbar^2} [E - V(x)]$  also has a (finite) discontinuity. If  $\psi$  is continuous,  $[V - E]\psi$  is discontinuous and so is  $\psi''$ . However, since this discontinuity is finite, upon integration:  $\psi' = \int dx \psi''$  has no discontinuity and then neither has  $\psi$ —consistent with our beginning assumption. Thus, we require:

$$\lim_{\epsilon \rightarrow 0} \psi(x_0 - \epsilon) = \lim_{\epsilon \rightarrow 0} \psi(x_0 + \epsilon), \quad (1.14a)$$

$$\lim_{\epsilon \rightarrow 0} \psi'(x_0 - \epsilon) = \lim_{\epsilon \rightarrow 0} \psi'(x_0 + \epsilon). \quad (1.14b)$$

*Alternatively*, once the equation (1.14a) has been enforced, we can divide the l.h.s. of Eq. (1.14b) by the l.h.s. of (1.14a), and the right-hand side of Eq. (1.14b) by the r.h.s. of (1.14a) to obtain:

$$\lim_{\epsilon \rightarrow 0} \frac{\psi'(x_0 - \epsilon)}{\psi(x_0 - \epsilon)} = \lim_{\epsilon \rightarrow 0} \frac{\psi'(x_0 + \epsilon)}{\psi(x_0 + \epsilon)}, \quad (1.14c)$$

$$\lim_{\epsilon \rightarrow 0} \ln(\psi(x_0 - \epsilon)) = \lim_{\epsilon \rightarrow 0} \ln(\psi(x_0 + \epsilon)).$$

*Conversely*: Assume now that  $\psi(x)$  has a (finite) discontinuity at  $x_0$ , as does the potential,  $V(x)$ . Then, the right-hand-side of Eq. (1.13), the product  $\frac{m}{\hbar^2} [V(x) - E] \psi(x)$ , would also have a (finite) discontinuity. However,  $\psi'(x)$  would have an (infinite) discontinuity at  $x_0$  (the slope is vertical!) and then  $\psi''(x_0)$ , on the left-hand-side of Eq. (1.13), would have to behave (at least) as badly as  $\delta(x - x_0)$  does—contradicting the established (finite) discontinuity of the equation's right-hand-side. To make this more obvious, notice that the integral of the left-hand-side, equal to  $\psi'(x)$ , would have an infinite discontinuity, whereas the integral of the right-hand-side,  $\frac{m}{\hbar^2} [V(x) - E] \psi(x)$ , would have no discontinuity at all!

This contradiction proves that  $\psi(x)$  cannot be discontinuous as long as  $V(x)$  has a discontinuity, including a finite or infinite “step” and even a  $\delta$ -function type behavior.

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**0.** Consider first the case **A**:  $E > V_0$ .

**A.1.** Following the above task-list, we define  $R_1 = [-\infty, x_0]$  and  $R_2 = [x_0, \infty]$ .

**A.2.** Adopting the solution of subsection 1.1, we can write:

$$\psi_1(x) = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x}, \quad k_1 = \sqrt{2mE}/\hbar; \quad (1.15a)$$

$$\psi_2(x) = A_2 e^{ik_2 x} + B_2 e^{-ik_2 x}, \quad k_2 = \sqrt{2m(E - V_0)}/\hbar. \quad (1.15b)$$

**A.3** Here, we need to ensure that

$$\psi_1(0) = \psi_2(0), \quad \psi'_1(0) = \psi'_2(0); \quad (1.16a)$$

$$A_1 + B_1 = A_2 + B_2, \quad ik_1 A_1 - ik_1 B_1 = ik_2 A_2 - ik_2 B_2. \quad (1.16b)$$

**A.4.** Both  $\psi_1$  and  $\psi_2$  oscillate (with so far undetermined but constant amplitudes), and there is no boundary condition “at infinity”.

**A.5** The normalization/orthonormality condition (1.11) becomes

$$\int_{-\infty}^{\infty} dE' \left[ \int_{-\infty}^0 dx \psi_{1,E'}^* \psi_{1,E} + \int_0^{\infty} dx \psi_{2,E'}^* \psi_{2,E} \right] = 1 . \quad (1.17)$$

Thus, we remain with three equations: two in Eq. (1.16b) and one in Eq. (1.17) (upon solving the integrals). These let us determine any three of the four constants  $A_1, B_1, A_2, B_2$ , thus leaving one of these and the energy,  $E$  as free parameters of the solution. In particular, having remained undetermined, the energy  $E$  can take on any one of continuously many values for  $E > V_0$ . Also, note that the probability density  $|\psi|^2$  does not diminish significantly outside any particular range of  $x$ . The solution for some particular value of  $E$  is sketched in the left part of the figure below.

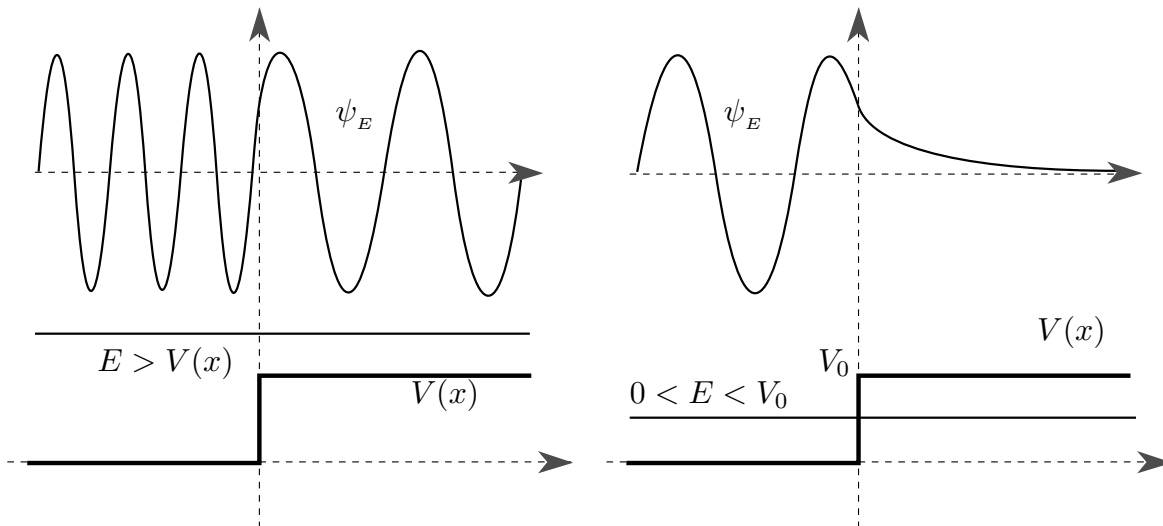


Fig. 2: The potential step.

Note that the probability current for the right-moving component of the wave-function evaluates to  $\hbar k_1/m$  for  $x < 0$  and  $\hbar k_2/m$  for  $x > 0$ ; these indeed are the speeds of the corresponding particle incoming from the left.

**0.** Consider next the case **B**:  $0 < E < V_0$ .

**B.1.** Following the above task-list, we keep  $R_1 = [-\infty, x_0]$  and  $R_2 = [x_0, \infty]$  from the previous part.

**B.2.** Adapting the solution of subsection 1.1, we can write:

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx} , \quad k = \sqrt{2mE}/\hbar ; \quad (1.18a)$$

$$\psi_2(x) = Ce^{\kappa x} + De^{-\kappa x} , \quad \kappa = \sqrt{2m(V_0 - E)}/\hbar . \quad (1.18b)$$

**B.3** Again, we need to ensure that

$$\psi_1(0) = \psi_2(0) , \quad \psi_1'(0) = \psi_2'(0) ; \quad (1.19a)$$

$$A + B = C + D , \quad ikA - ikB = \kappa C - \kappa D . \quad (1.19b)$$

**B.4.** Now  $\psi_1$  oscillates (with so far undetermined but constant amplitude), and there is no boundary condition for  $x \rightarrow -\infty$ . However,  $\psi_2$  is almost-monotonous and it is easy to see that the  $Ce^{\kappa x}$  term diverges as  $x \rightarrow \infty$ , which would prevent normalization. Thus, in view of this requirement, we must set  $C = 0$ .

**B.5** The normalization/orthonormality condition (1.11) becomes

$$\int_{-\infty}^{\infty} dE' \left[ \int_{-\infty}^0 dx \psi_{1,E'}^* \psi_{1,E} + \int_0^{\infty} dx \psi_{2,E'}^* \psi_{2,E} \right] = 1 . \quad (1.20)$$

Thus, we remain with three equations: two in Eq. (1.19b) and one in Eq. (1.20) (upon solving the integrals). These let us determine any three of the three constants  $A, B, D$ , thus leaving none of these free. The energy however does remain as a free parameter of the solution. In particular, having remained undetermined, the energy  $E$  can take on any one of continuously many values for  $0 < E < V_0$ . Note again that the probability density  $|\psi|^2$  does not diminish significantly outside any particular range of  $x < 0$ . The solution for some particular value of  $E$  is sketched in the right part of the figure above.

Note that the probability current for the right-moving component of the wave-function evaluates to  $\hbar k/m$  for  $x < 0$  but vanishes for  $x > 0$ . These indeed are the speeds of the corresponding particle incoming from the left: the particle isn't really allowed to travel inside the barrier, although the wave-function there is non-zero.

The last logical possibility,  $E < 0$  is excluded as the solution would turn out to be non-normalizable just as in subsection 1.1. In summary, the (energy) spectrum is as follows:

$$\begin{cases} E > V_0 , & E \text{ is continuous, } \psi(x) \text{ is oscillatory for all } x; \\ 0 < E < V_0 , & E \text{ is continuous, } \psi(x) \text{ oscillatory for } x < 0; \\ E < 0 , & \text{forbidden, since } \psi(x) \text{ would not be normalizable.} \end{cases}$$

### 1.3. Infinite discontinuities

By contrast, were the discontinuity in  $V$  (and so in  $k^2$ ) infinite, it would not have been possible to derive that  $\psi'$  should be continuous. Indeed, if we take the  $V_0 \rightarrow \infty$  limit, when also  $\kappa \rightarrow \infty$ , we obtain that:

- A. There is no analogue of the case **A** of the finite potential step: all (finite) energies  $E$  must be smaller than  $V_0 = \infty$ .
- B. Case **B** is the only allowed one. The wave-function for  $x > 0$  becomes  $\psi_2(x) \rightarrow 0$ , and so we obtain that  $\lim_{\epsilon \rightarrow 0} \psi(-\epsilon) = 0$ . This now becomes the new boundary condition.

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An interesting special case of potentials with infinite discontinuities is the case when the potential is  $V(x) = \lambda\delta(x)$ . Now we can actually integrate the Schrödinger equation between  $-\epsilon$  and  $+\epsilon$ :

$$0 = -\frac{\hbar^2}{2m} \int_{-\epsilon}^{\epsilon} dx \frac{d^2\psi}{dx^2} + \lambda \int_{-\epsilon}^{\epsilon} dx \delta(x)\psi - E \int_{-\epsilon}^{\epsilon} dx \psi, \quad (1.21a)$$

$$= -\frac{\hbar^2}{2m} [\psi'(+\epsilon) - \psi'(-\epsilon)] + \lambda\psi(0) - E[F(+\epsilon) - F(-\epsilon)], \quad (1.21b)$$

where  $F(x) \stackrel{\text{def}}{=} \int^x dy \psi(y)$ . Now, if  $\psi(x)$  is continuous at  $x = 0$ , so is  $F(x)$ . Then, taking the  $\epsilon \rightarrow 0$  limit, the terms in the right-most square bracket cancel, and we remain with

$$\lim_{\epsilon \rightarrow 0} [\psi(+\epsilon) - \psi(-\epsilon)] = 0, \quad \lim_{\epsilon \rightarrow 0} [\psi'(+\epsilon) - \psi'(-\epsilon)] = \frac{2m\lambda}{\hbar^2} \psi(0), \quad (1.22)$$

which are the boundary conditions for matching across a  $\delta$ -function potential. That is, the wave-functions must be continuous, but the first derivative has a discontinuity proportional to the product of  $\lambda$  (a.k.a. ‘opacity’) and the value of the wave-function at 0; the wave-function has a ‘breaking point’.

Now, if  $\lambda > 0$ , only  $E > 0$  levels are allowed (for  $E < 0$ , no solution is normalizable). Furthermore, the solutions to the left and to the right of the  $\delta$ -function are oscillatory with some finite and constant amplitudes. Thus there are no boundary conditions ‘at infinity’.

On the other hand, when  $\lambda < 0$ , both negative and positive values of  $E$  are allowed. For  $E > 0$ , the solutions look very similar to the ones in the  $\lambda > 0$  case (except now the discontinuity in  $\psi'$  has the opposite sign). For  $E < 0$ , however, a novel characteristic appears! We proceed following the above task-list and find:

$$\psi_-(x) = Ce^{\kappa x}, \quad x < 0, \quad (1.23a)$$

$$\psi_+(x) = De^{-\kappa x}, \quad x > 0, \quad (1.23b)$$

where we set  $D = 0$  in  $\psi_-$  since  $e^{-\kappa x}$  diverges for  $x \rightarrow -\infty$ , and similarly we set  $C = 0$  in  $\psi_+$  because  $e^{\kappa x}$  diverges as  $x \rightarrow \infty$ . The boundary conditions (1.22) imply that  $C = D$ , and that  $\kappa = m\lambda/\hbar^2$ . Since  $\kappa = \sqrt{2m(-E)}/\hbar$ , we obtain that  $E = -\frac{1}{2}m\lambda^2/\hbar^2$ . The wave-function of this state monotonically decays to both positive and negative infinity, and the probability density is non-negligible only around  $x = 0$ : this state is localized! Since this localization is bound by the location of the potential, such states are also called bound states. Below is a sketch of the wave-functions for a scattering and the bound state in this case.

In summary, the (energy) spectrum is as follows:

$$\begin{cases} E > 0, & E \text{ is continuous, } \psi(x) \text{ is oscillatory for all } x; \\ E = -\frac{1}{2}m\lambda^2/\hbar^2, & \text{a single value, separated from the continuous region, } E > 0, \\ & \psi(x) \text{ is exponentially decaying for } x \rightarrow \pm\infty. \end{cases}$$

In particular, notice the appearance of the nonvanishing energy gap, between the lowest lying energy value,  $E = -\frac{1}{2}m\lambda^2/\hbar^2$  and the continuous region,  $E > 0$ .

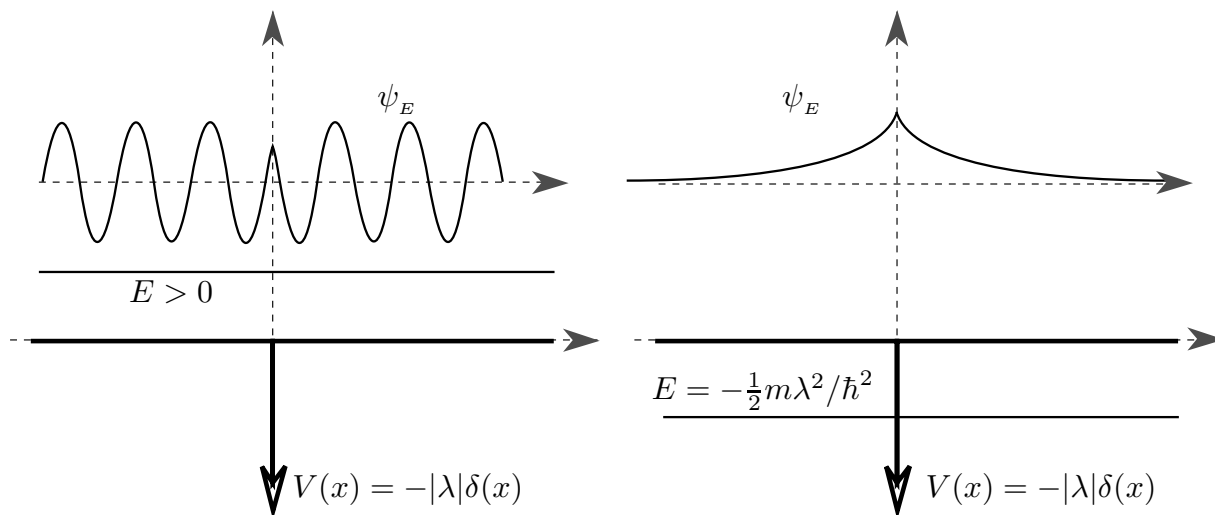


Fig. 3: The delta-function potential.

#### 1.4. Finite potential two-step

Consider now an iteration of the finite potential step: stepping back-and-forth. There are of course two possibilities, depicted in the figure below. In both cases, there are two possibilities for the value of  $E$ : either  $E > \max(V(x))$ , or  $\min(V(x)) < E < \max(V(x))$ . For the potential barrier (left part of the above figure), both types of states are oscillatory on both sides of the potential, have no boundary condition ‘at infinity’, and represent scattering states (continuous energy values).

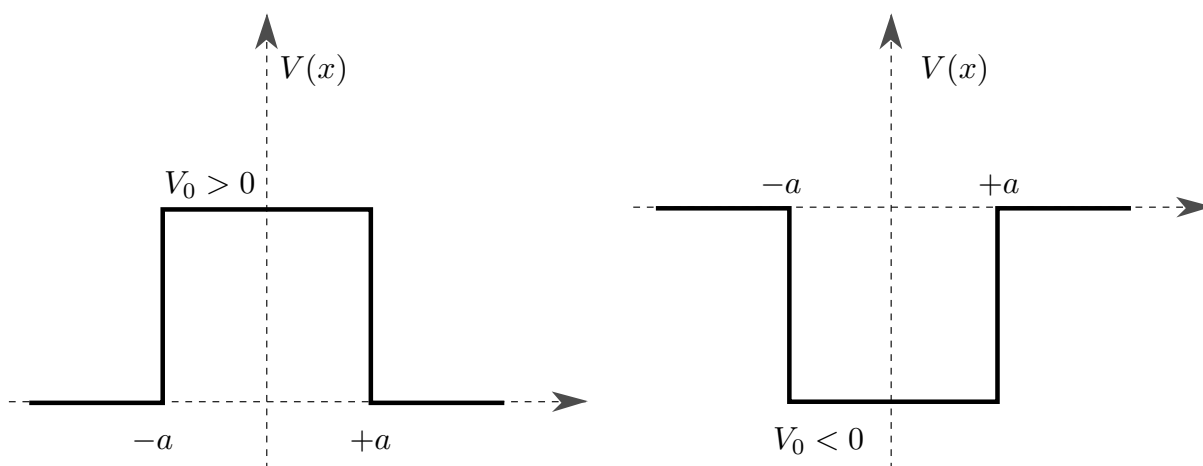


Fig. 4: The potential barrier (left), and well (right).

For the potential well (right part of the above figure), the states with  $E > 0$  are oscillatory throughout, no boundary conditions ‘at infinity’, and continuous values of energy.



However, the states with  $V_0 < E < 0$  are monotonous for  $|x| > a$ , and so must decay for  $x \rightarrow \pm\infty$ —which imposes two additional boundary conditions. Together with matching the wave-function and its derivative at  $\pm a$ , these are six boundary conditions; in addition, there is of course also the normalization condition. These are imposed on the solution which has two constants in the region  $R_1 = [-\infty, -a]$ , two for  $R_2 = [-a, +a]$ , and two for  $R_3 = [+a, +\infty]$ , and the energy level,  $E$ . This spells seven conditions on seven constants, whence all seven are determined. Thus, energy will again only be able to take some select values.

Let us work this out concretely. We write the solutions in the form:

$$\psi_1 = Ae^{\kappa x} , \quad x < -a , \quad (1.24a)$$

$$\psi_2 = B \sin(kx + \delta) , \quad |x| < a , \quad (1.24a)$$

$$\psi_3 = Ce^{-\kappa x} , \quad x > +a , \quad (1.24a)$$

with  $\kappa \stackrel{\text{def}}{=} \sqrt{2m|E|}/\hbar$  and  $k \stackrel{\text{def}}{=} \sqrt{2m(E - V_0)}/\hbar$ . The purpose for choosing these particular forms of the solution will become apparent as soon as we apply the boundary conditions. Indeed, let us focus on the logarithmic condition (1.14c):

$$\frac{A\kappa e^{-\kappa a}}{Ae^{-\kappa a}} = \frac{D[-k \cos(-ka + \delta)]}{D \sin(-ka + \delta)} , \quad @ x = -a \quad (1.25a)$$

$$\frac{D[-k \cos(ka + \delta)]}{D \sin(ka + \delta)} = \frac{C[-\kappa e^{-\kappa a}]}{Ce^{-\kappa a}} , \quad @ x = +a \quad (1.25b)$$

Lo, and behold! These expressions simplify *tremendously* into:

$$\kappa = -k \cot(-ka + \delta) , \quad @ x = -a \quad (1.26a)$$

$$k \cot(ka + \delta) = \kappa . \quad @ x = +a \quad (1.26b)$$

Noting that  $\cot(-x) = -\cot(x)$  and recalling that  $\cot(x)$  is periodic with period  $\pi$ , so that the inverse function is defined only up to the addition of an arbitrary integral multiple of  $\pi$ , this can be rewritten:

$$\cot^{-1}\left(\frac{\kappa}{k}\right) = ka - \delta + n_1\pi , \quad (1.27a)$$

$$\cot^{-1}\left(\frac{\kappa}{k}\right) = ka + \delta + n_2\pi , \quad (1.27b)$$

the sum and the difference of which, respectively, yield:

$$\cot^{-1}\left(\frac{k}{\kappa}\right) = ka + \frac{1}{2}(n_1 + n_2)\pi , \quad \delta = \frac{1}{2}(n_1 - n_2)\pi , \quad (1.28)$$

or, since  $\cot(x + \frac{N\pi}{2}) = -\tan(x)$  for odd  $N$  but  $\cot(x + \frac{N\pi}{2}) = \cot(x)$  for even  $N$ :

$$\frac{k}{\kappa} = \begin{cases} \tan(ka) & \text{for } (n_1 + n_2) \text{ even,} \\ -\cot(ka) = \frac{-1}{\tan(ka)} & \text{for } (n_1 + n_2) \text{ odd.} \end{cases} \quad (1.29)$$

Notice that these involve only the energy—not one of the other constants appear:

$$\sqrt{\frac{E-V_0}{E}} = \pm \left[ \tan \left( \sqrt{2m(E-V_0)} \frac{a}{\hbar} \right) \right]^{\pm 1}. \quad (1.30)$$

Clearly, this is a transcendental equation for  $E$ , and cannot be solved explicitly or in closed form. However, it can be solved graphically, by plotting the r.h.s. and the l.h.s. against  $E$ , and finding the values of  $E$  for which the graphs cross. Numerically, one can employ the halving method, the Newton-Raphson method, or any other method for finding the roots of the functions  $f_{\pm}(E) \stackrel{\text{def}}{=} \sqrt{\frac{E-V_0}{E}} \mp \left[ \tan \left( \sqrt{2m(E-V_0)} \frac{a}{\hbar} \right) \right]^{\pm 1}$ .

Without any calculation, it should be clear that the lowest value of  $E$  should be fairly close to  $V_0$ . Thus, one may expect to be able to estimate the ground state energy by expanding the tangent function treating  $\sqrt{\frac{E-V_0}{V_0}}$  as a small variable. To lowest nonzero order, the result from the ‘tan’ branch of (1.29) is  $E = \hbar^2/2ma^2$ , which is inconsistent as it is independent of  $V_0$ . To lowest nonzero order, the result from the ‘cot’ branch of (1.29) is  $E = (V_0 + \frac{\hbar^2}{4ma^2}) \pm \frac{\hbar}{a} \sqrt{\frac{V_0}{2m} + \frac{\hbar^2}{16m^2a^2}}$ . This at least has the correct behavior in the classical ( $\hbar \rightarrow 0$ ) limit: it becomes  $E = V_0$ . Otherwise, the shift from this value is obtained as a power series in  $\hbar$ , and is therefore expected to be near  $V_0$ .

Also without calculation, this model corresponds to there being no forces (equaling the negative gradient of the potential) at  $x \neq \pm a$  (the potential there being constant), and the forces at  $x = \pm a$  being ‘restorative’, *i.e.*, pushing the particle back into the well. The magnitude of these restorative forces at the boundary is proportional to the depth,  $V_0$ .

In summary, the (energy) spectrum is as follows (recall,  $V_0 < 0$ ):

$$\left\{ \begin{array}{ll} E > 0, & E \text{ is continuous, } \psi(x) \text{ is oscillatory for all } x; \\ V_0 < E < 0, & E \text{ is discrete, the values determined by Eq. (1.30),} \\ & \psi(x) \text{ oscillatory for } |x| < a \text{ but decays exponentially for } x \rightarrow \pm\infty; \\ E < V_0, & \text{forbidden, since } \psi(x) \text{ would not be normalizable.} \end{array} \right.$$

—o—

Now consider the infinite potential well, where we take the limit of  $V_0 \rightarrow -\infty$ . It would appear that the ground state energy also goes to  $-\infty$ , which hardly makes sense! In addition, the infinite potential well should physically correspond to no force inside the well (the potential there being constant), with infinitely strong restorative forces (the depth of the potential being infinite) at the boundary. Thus, the wave-function outside the potential well should be identically zero. Yet, the above calculations show a continuum of scattering states with  $E > 0$ ) which extend outside the well!

Both of these problems are remedied by formally shifting the Hamiltonian by  $+|V_0|$  before taking the  $V_0 \rightarrow -\infty$  limit. That is, we consider  $\hat{H}' = \hat{H} + |V_0|$  as the correct Hamiltonian, so that the new potential becomes

$$V'(x) = \begin{cases} +|V_0| & \text{for } |x| > a, \\ 0 & \text{for } |x| < a. \end{cases} \quad (1.31)$$

The above results for the wave-functions and the condition determining the energy are corrected in that now  $0 < E < |V_0|$ :

$$k = \sqrt{2mE}/\hbar, \quad \kappa = \sqrt{2m(|V_0| - E)}/\hbar, \quad (1.32)$$

and Eq. (1.30) becomes

$$\sqrt{\frac{E}{|V_0| - E}} = \tan\left(\sqrt{2mE} \frac{a}{\hbar}\right). \quad (1.33)$$

Now the  $V_0 \rightarrow -\infty$  limit can be taken safely. Physically, the potential outside  $|x| < a$  becomes infinitely big and prohibits the wave-functions there (the real exponentials decay infinitely fast as  $x$  becomes less than  $-a$  or more than  $+a$ ). Mathematically, the l.h.s. of Eq. (1.33) vanishes in the  $V_0 \rightarrow \infty$  limit, and we remain with the condition

$$\tan\left(\sqrt{2mE} \frac{a}{\hbar}\right) = 0, \quad \sqrt{2mE} \frac{a}{\hbar} = \frac{n\pi}{2}, \quad (1.34)$$

and so

$$E_n = \frac{n^2\pi^2\hbar^2}{8ma^2}. \quad (1.35)$$

This could also have been derived from the boundary conditions, as follows. Since the wave-functions must vanish for  $x \leq -a$  and so also at  $x = -a$ , write

$$\psi(x) = D \sin[k(x+a)]. \quad (1.36)$$

Since the wave-function also has to vanish for  $x \geq a$  and so also at  $x = a$ , we have that  $k(2a) = n\pi$ , which recovers Eq. (1.35).

In summary, the (energy) spectrum is as follows (recall,  $V_0 < 0$ ):

$$\begin{cases} E > 0, & E \text{ is discrete, the values determined by Eq. (1.35),} \\ & \psi(x) \text{ oscillatory for } |x| < a \text{ but vanishes for } |x| \geq a; \\ E < 0, & \text{forbidden, since } \psi(x) \text{ would not be normalizable.} \end{cases}$$

By the way, the replacement  $\hat{H} \rightarrow \hat{H}'$  before taking the  $V_0 \rightarrow \infty$  limit is called *renormalization*, and reflects the fact that energy is defined only up to an additive constant (determining the choice of  $E = 0$ ).

## 2. Continuous Potentials

In contrast with the previous section, we now assume that the potential is continuous in the area of concern. In particular, that implies that the potential crosses the energy level continuously—markedly unlike the cases in the previous section, whence also the matching conditions (1.14) will no longer apply.

In two special cases, we will be able to obtain an exact complete set of solutions: the (energy) spectrum and the corresponding Hilbert space. In full generality, however, we will obtain an approximate solution, which however often turns out to be quite accurate.

### 2.1. Linear potential

Consider the case where the potential is that of a constant force,  $V(x) = -F_0x$ , so that  $F \stackrel{\text{def}}{=} -\frac{d}{dx}V(x) = F_0 = \text{const.}$  Now the Schrödinger equation is:

$$\psi''(x) + \frac{2m}{\hbar^2}[F_0x + E]\psi(x) = 0. \quad (2.1)$$

Upon a Fourier transform and writing  $\tilde{\psi}(k) \stackrel{\text{def}}{=} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx e^{-ikx} \psi(x)$ , the Schrödinger equation becomes<sup>3)</sup>:

$$[(-ik)^2 \tilde{\psi}(k)] + \frac{2mF_0}{\hbar^2} [i\tilde{\psi}'(k)] - \frac{2mE}{\hbar^2} \tilde{\psi}(k) = 0,$$

which is only a first order differential equation, which we solve straightforwardly:

$$\tilde{\psi}(k) = \tilde{\psi}_0 \exp \left\{ i \left[ \frac{E}{F_0} k - \frac{\hbar^2 k^3}{2mF_0} \right] \right\},$$

and readily invert back:

$$\psi_E(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk e^{ikx} \tilde{\psi}(k) = \frac{\tilde{\psi}_0}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk e^{i[(x + \frac{E}{F_0})k - \frac{\hbar^2 k^3}{2mF_0}]}. \quad (2.2)$$

Note that  $\psi_{E+F_0a}(x) = \psi_E(x+a)$ . This is a result of the continuous symmetry of the problem (2.1):  $(E, x) \simeq (E - F_0a, x+a)$ , for all  $a \in \mathbb{R}$ . That is, the problem (2.1) and its solutions remain unchanged if we shift  $(E, x) \rightarrow (E - F_0a, x+a)$ , so that a translation  $x \rightarrow (x+a)$  is accompanied by an overall (global) re-zeroing of energy  $E \rightarrow (E - F_0a)$ . This is indeed a very simple example of a gauge-invariance, wherein the translation of a coordinate is compensated by re-gauging an observable (resetting the value of “zero energy” in this case).

For each fixed value of  $E$ , Eq. (2.2) provides an exact solution albeit given in integral form. It turns out to be oscillatory for  $x > -E/F_0$  (where  $E > V(x) = -F_0x$ ) and exponentially decaying for  $x < -E/F_0$ . The “other” solution of the 2nd order ODE (2.1) (which is of Sturm-Liouville type) is obtained using standard techniques. It is exponentially diverging for  $x < -E/F_0$  and so physically unacceptable. These two special functions (for each  $E$ ) are called the Airy functions, and are discussed in many texts on mathematical physics.

### 2.2. Quadratic potential

Another case for which exact solutions are obtained with relative ease is the so-called (linear) harmonic oscillator:  $V(x) = \frac{1}{2}m\omega^2x^2$ , where we used the classical mechanics result to write the spring constant as  $m\omega^2$  with  $\omega$  the natural frequency of the oscillator.

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<sup>3)</sup> Do work out  $\mathcal{F}[\psi''(x)]$  and  $\mathcal{F}[x\psi(x)]$  for yourself, please!

The Hamiltonian,  $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$  leads to a 2nd order ODE for stationary states in coordinate representation:

$$-\frac{\hbar^2}{2m}\psi''(x) + \frac{1}{2}m\omega^2x^2\psi(x) = E\psi(x) ,$$

which can be solved directly using Frobenius's method of series. However, we will solve this case herein using another method, exposing its algebraic structure.

We begin by changing variables:

$$\hat{a} \stackrel{\text{def}}{=} \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2m\omega\hbar}}\hat{p} , \quad \text{and} \quad \hat{a}^\dagger \stackrel{\text{def}}{=} \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2m\omega\hbar}}\hat{p} ,$$

and so also

$$\hat{x} = \sqrt{\frac{2\hbar}{m\omega}} \Re e(\hat{a}) = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}^\dagger + \hat{a}) , \quad \text{and} \quad \hat{p} = \sqrt{2\hbar m\omega} \Im m(\hat{a}) = i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a}^\dagger - \hat{a}) .$$

It is easy to verify that  $[\hat{x}, \hat{p}] = i\hbar$  implies

$$[\hat{a}, \hat{a}^\dagger] = \mathbf{1} , \tag{2.3a}$$

from which

$$\hat{a}\hat{a}^\dagger = \mathbf{1} + \hat{a}^\dagger\hat{a} , \quad \text{and} \quad \hat{a}^\dagger\hat{a} = \hat{a}\hat{a}^\dagger - \mathbf{1} . \tag{2.3b, c}$$

The (canonical) commutation relations (2.3) define the Heisenberg algebra

In terms of  $\hat{a}, \hat{a}^\dagger$ , we have that

$$\hat{H} = \frac{1}{2}\hbar\omega(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger) = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2}) .$$

This means that the Hamiltonian of the harmonic oscillator is a shift and a re-scale of the operator  $\hat{N} \stackrel{\text{def}}{=} \hat{a}^\dagger\hat{a}$ : eigenvalues of  $\hat{H}$ , *i.e.*, energies are  $E = \hbar\omega(\nu + \frac{1}{2})$  where  $\nu$  is the eigenvalue of  $\hat{N}$ , and eigenstates of  $\hat{N}$  are also eigenstates of  $\hat{H}$ :

$$\hat{N}|\nu\rangle = \nu|\nu\rangle \quad \Leftrightarrow \quad \hat{H}|\nu\rangle = \hbar\omega(\nu + \frac{1}{2})|\nu\rangle .$$

Our goal then is to determine the allowed values of  $\nu$ , and the corresponding states  $|\nu\rangle$ .

As all observables of the harmonic oscillator can be expressed in terms of  $\hat{a}$  and  $\hat{a}^\dagger$ , we start with determining how these operators act on the  $|\nu\rangle$ 's. In particular, consider the state  $\hat{a}|n\rangle$ , and determine if it is another eigenstate of  $\hat{N}$ :

$$\begin{aligned} \hat{N}(\hat{a}|\nu\rangle) &= \hat{a}^\dagger\hat{a}\hat{a}|\nu\rangle \stackrel{(2.3c)}{=} (\hat{a}\hat{a}^\dagger - 1)\hat{a}|\nu\rangle = \hat{a}\hat{a}^\dagger\hat{a}|\nu\rangle - \hat{a}|\nu\rangle , \\ &= \hat{a}\nu|\nu\rangle - \hat{a}|\nu\rangle = (n-1)(\hat{a}|\nu\rangle) , \end{aligned}$$

which means that  $\hat{a}|\nu\rangle$  is itself an eigenstate of  $\hat{N}$ , corresponding to the eigenvalue  $\nu-1$ , so that in fact  $\hat{a}|\nu\rangle \propto |\nu-1\rangle$ . A similar calculation proves that also  $\hat{a}^\dagger|\nu\rangle \propto |\nu+1\rangle$ .

Thus,  $\hat{a}$  and  $\hat{a}^\dagger$ , respectively decrease and increase  $\nu$  in units of 1. Since all observables are functions of  $\hat{a}, \hat{a}^\dagger$ , that means that the Hilbert space of the harmonic oscillator consists of  $|\nu\rangle$ 's with  $\nu$  changing in integral increments only. Furthermore, since  $E \geq \min(V(x)) = 0$ , we also know that

$$0 \leq E_\nu = \hbar\omega(\nu + \frac{1}{2}) \quad \text{implies} \quad \nu \geq -\frac{1}{2} .$$

Since  $\nu$  can change only in integral increments, we can write

$$\nu = \nu_0 + n, \quad \text{where} \quad -\frac{1}{2} \leq \nu_0 < \frac{1}{2} \quad \text{and} \quad n = 0, 1, 2, 3 \dots$$

and where  $\nu_0$  is a fixed constant. (The “initial” constant  $\nu_0$  can always be reduced to this interval by re-scaling  $n$  by an integer. conversely, all allowed values of  $\nu$  can be obtained using this parametrization.)

Now we turn to determine  $\nu_0$ . Since  $\hat{N}|\nu\rangle = \nu|\nu\rangle$ , we have that:

$$\begin{aligned} \langle \nu_0 | \hat{N} | \nu_0 \rangle &= \langle \nu_0 | \nu_0 | \nu_0 \rangle = \nu_0 \langle \nu_0 | \nu_0 \rangle = \nu_0, \\ &\parallel \\ \langle \nu_0 | \hat{a}^\dagger \hat{a} | \nu_0 \rangle &= (\hat{a} | \nu_0 \rangle)^\dagger (\hat{a} | \nu_0 \rangle) = |\hat{a} | \nu_0 \rangle|^2 \geq 0, \end{aligned}$$

so that  $\nu \geq 0$ . Thus, we have just halved the set of possible values of  $\nu_0$ , from  $-\frac{1}{2} \leq \nu_0 < \frac{1}{2}$  to  $0 \leq \nu_0 < \frac{1}{2}$ . But, if  $|\hat{a} | \nu_0 \rangle|^2 > 0$ , then  $(\hat{a} | \nu_0 \rangle)$  would be a state of positive norm, and would have to be included in the Hilbert space. This however cannot be the case, since  $(\hat{a} | \nu_0 \rangle) \propto | \nu_0 - 1 \rangle$  would have to have the energy

$$E_{\nu_0-1} = \hbar\omega((\nu_0-1) + \frac{1}{2}) = \hbar\omega(\nu_0 - \frac{1}{2}) < 0 = \min(V(x)),$$

since  $\nu_0 < \frac{1}{2}$ . Such states are not normalizable and must be excluded from the Hilbert space.

Therefore, only the value  $\nu_0 = 0$  remains a consistent choice. From now on, we will write  $|n\rangle$  in place of  $|\nu\rangle$ . Also, it follows that

$$\hat{a} | 0 \rangle = 0 \tag{2.4}$$

defines the state of the lowest energy,  $E_0 = \frac{1}{2}\hbar\omega$ , which we will call the “ground state” from now on.

—○—

Given  $|0\rangle$ , all the other states are created by iterative applications of  $\hat{a}^\dagger$ :

$$|1\rangle \propto \hat{a}^\dagger |0\rangle, \quad \dots \quad \text{so} \quad |n\rangle \propto (\hat{a}^\dagger)^n |0\rangle.$$

It remains to normalize these correctly. To that end, write  $|n\rangle = C_n (\hat{a}^\dagger)^n |0\rangle$  and note that

$$\begin{aligned} 1 &\stackrel{!}{=} \langle n | n \rangle = | |n\rangle |^2 = | C_n (\hat{a}^\dagger)^n |0\rangle |^2 = | C_n \hat{a}^\dagger \underbrace{(\hat{a}^\dagger)^{n-1} |0\rangle}_{C_{n-1}^{-1} |n-1\rangle} |^2 = \frac{|C_n|^2}{|C_{n-1}|^2} |\hat{a}^\dagger |n-1\rangle|^2, \\ &= \frac{|C_n|^2}{|C_{n-1}|^2} \langle n-1 | \hat{a} \hat{a}^\dagger |n-1\rangle = \frac{|C_n|^2}{|C_{n-1}|^2} \langle n-1 | [\hat{a}^\dagger \hat{a} + 1] |n-1\rangle, \\ &= \frac{|C_n|^2}{|C_{n-1}|^2} \langle n-1 | [(n-1) + 1] |n-1\rangle = \frac{|C_n|^2}{|C_{n-1}|^2} n \langle n-1 | n-1 \rangle = \frac{|C_n|^2}{|C_{n-1}|^2} n. \end{aligned}$$

so that (choosing the  $C_n$ 's to be real):

$$C_n = \frac{C_{n-1}}{\sqrt{n}}, \quad \Rightarrow \quad C_n = \frac{1}{\sqrt{n!}}.$$

Thus, all states  $|n\rangle$  for  $n = 1, 2, 3 \dots$  are completely determined from the ground state,  $|0\rangle$ . We note that

$$\hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle \quad \text{and} \quad \hat{a} |n\rangle = \sqrt{n} |n-1\rangle . \quad (2.5)$$

This then produces the whole Hilbert space,

$$\mathcal{H} = \{ |n\rangle, n = 0, 1, 2, 3 \dots : \langle n|n'\rangle = \delta_{n,n'} \ \& \ \sum_n |n\rangle \langle n| = \mathbf{1} \} .$$

and –since all observables,  $\hat{A}$ , can be expressed in terms of  $\hat{a}$  and  $\hat{a}^\dagger$ – the action of all observables on all states, and so also all matrix elements  $\langle n'|\hat{A}|n\rangle$  can be determined using this algebraic formalism.

It is of paramount importance to realize that the structure of the Hilbert space,  $\mathcal{H}$ , –and all results within it– are *completely!!!* determined by the Heisenberg algebra (2.3).

—○—

Furthermore, the formalism also permits to easily solve for the wave-functions of all  $|n\rangle$ . To that end, begin with rewriting Eq. (2.4) in the coordinate representation:

$$0 = \langle x|\hat{a}|0\rangle = \left[ \sqrt{\frac{m\omega}{2\hbar}} \hat{x} + \frac{i}{\sqrt{2m\omega\hbar}} \hat{p} \right] \psi_0(x) = \left[ \sqrt{\frac{m\omega}{2\hbar}} x + \frac{i}{\sqrt{2m\omega\hbar}} \frac{\hbar}{i} \frac{d}{dx} \right] \psi_0(x) ,$$

which may be simplified:

$$\psi_0'(x) = -\frac{m\omega}{\hbar} x \psi_0(x) , \quad \Rightarrow \quad \psi_0(x) = C_0 e^{-\frac{1}{2}\beta x^2} , \quad \beta = \frac{m\omega}{\hbar} .$$

Normalizing,

$$1 \stackrel{!}{=} \int_{-\infty}^{+\infty} dx |\psi_0(x)|^2 = 2|C_0|^2 \int_0^\infty dx e^{-\beta x^2} = |C_0|^2 \sqrt{\frac{\pi}{\beta}} ,$$

so that

$$\psi_0(x) = \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\frac{1}{2}\beta x^2} ,$$

and then

$$\psi_n(x) = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}} \psi_0(x) .$$

Up to normalization, the polynomials

$$H_n(x) \stackrel{\text{def}}{=} \frac{1}{\psi_0(x)\sqrt{n!}} (\hat{a}^\dagger)^n \psi_0(x)$$

are recognized to be the Hermite polynomials, obtained otherwise also through the Frobenius's method of series.

### 2.3. Solutions for a general potential: the WKB approximation

We seek a solution of the Schrödinger equation in the exponential form,  $\psi(x) = e^{\frac{i}{\hbar}u(x)}$ . By direct substitution, the Schrödinger equation becomes

$$\left[ \frac{1}{2m} \left( \frac{du}{dx} \right)^2 - \frac{i\hbar}{2m} \frac{d^2u}{dx^2} + [V(x) - E] \right] e^{\frac{i}{\hbar}u(x)} = 0 . \quad (2.6)$$

As  $e^{\frac{i}{\hbar}u(x)} \neq 0$ , this we rewrite as

$$i\hbar \frac{d^2u}{dx^2} = \left(\frac{du}{dx}\right)^2 - p^2, \quad p = p(x) \stackrel{\text{def}}{=} \sqrt{2m[E-V(x)]}. \quad (2.7)$$

This differential equation is definitely more complicated than the standard Schrödinger equation—it is neither linear nor homogeneous. However, precisely its nonlinearity enables us to set up an iterative solution in the form of a sequence  $\{u_0, u_1, \dots\}$  which hopefully converges to the true solution. Fortunately, at least in many cases of interest, already  $u_1(x)$  will turn out to be a quite useful (approximate) solution.

We begin the iteration by neglecting the second derivative (since  $\hbar$  is so small) and solve

$$0 = \left(\frac{du_0}{dx}\right)^2 - p^2, \quad (2.8)$$

which is easy:  $u_0 = \pm \int dx p(x) + C_0$ . Upon this, we will iteratively solve

$$\frac{du_{n+1}}{dx} = \pm \sqrt{i\hbar \frac{d^2u_n}{dx^2} + p^2}, \quad n = 0, 1, 2, \dots \quad (2.9)$$

Thus,

$$\frac{du_1}{dx} = \pm \sqrt{i \frac{d^2u_0}{dx^2} + p^2} = \pm \sqrt{i\hbar \frac{dp}{dx} + p^2} \approx \pm p \left(1 \pm \frac{i\hbar p'}{2p}\right), \quad (2.10)$$

which is solved by  $u_1 \approx \pm \int dx p + \frac{i\hbar}{2} \ln p$ . That is, we have ( $k \stackrel{\text{def}}{=} p/\hbar$ )

$$\psi_1(x) = \frac{A}{\sqrt{k(x)}} e^{i \int dx k(x)} + \frac{B}{\sqrt{k(x)}} e^{-i \int dx k(x)}, \quad V(x) < E, \quad (2.11)$$

which is called the WKB solution. Note that for constant  $V(x)$ ,  $k$  is also a constant, and upon redefining the constant and so far undetermined amplitudes to include  $1/\sqrt{k}$ , this becomes precisely the plane wave (exact!) solution of the previous section. Thus, heuristically, the WKB solution is expected to be accurate for ‘slowly varying’ potentials.

Of course, where the values of the potential are bigger than the energy level  $E$ , we substitute  $k \rightarrow i\kappa \stackrel{\text{def}}{=} i\sqrt{2m(V(x)-E)}/\hbar$ , and write the solution in the form

$$\psi_1(x) = \frac{C}{\sqrt{\kappa(x)}} e^{-\int dx \kappa(x)} + \frac{D}{\sqrt{\kappa(x)}} e^{\int dx \kappa(x)}, \quad V(x) > E, \quad (2.12)$$

#### 2.4. Matching conditions for a general potential

The trouble with deriving matching conditions is that both the oscillatory (2.11), and the monotonous solution (2.12) diverge at any classical turning point  $x_0$ , where  $V(x_0) = E$ . Thus, it does not make a lot of sense to compare the wave-functions and their derivatives at the turning point. Instead, one needs a ‘patch’—a well-defined wave-function which is a good approximation precisely at the turning point and in some small neighborhood around it. Such a ‘patching’ wave-function is found by approximating the potential by a linear function,  $V(x_0+\epsilon) \approx E + V_0'\epsilon$ . Substituting this into the Schrödinger equation yields the



Airy equation, and the required patching solutions are therefore the Airy functions. This is described in some detail on p.284–289 of Ref. [1]. Full details, and a slightly different derivation of the solutions (2.11) and (2.12), are found on p.164–170 of Ref. [2].

In any case, the matching conditions depend on whether the barrier (the region where  $V(x) > E$ ) is to the left or to the right. In the former case, with the barrier to the left, we have [3]:

$$A = \frac{1}{2}\vartheta C + \vartheta^* D , \quad B = \frac{1}{2}\vartheta^* C + \vartheta D . \quad (2.13)$$

For the barrier to the right, we have

$$A = \vartheta C + \frac{1}{2}\vartheta^* D , \quad B = \vartheta^* C + \frac{1}{2}\vartheta D . \quad (2.14)$$

**References**

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- [3] David Park: *Introduction to the Quantum Theory*, (McGraw-Hill, Inc., New York, 1992).