

## Chapter 4

### The Schrödinger Equation and two more Principles

In the previous chapter, we have studied spin-half and noticed that the measurement returns for any spin component are only two, namely  $\hbar/2$  and  $-\hbar/2$ . In the theory, this is mirrored by the fact that the operators for spin components have only those two eigenvalues. More generally, the set of eigenvalues for spin operators, what is called their “spectrum”, is finite and therefore discrete. However, there are other observables for which we would expect an infinite number of possible measurement returns. For example, a particle could be (almost) anywhere between two points, and therefore the spectrum of the position operator must be infinite. We begin this chapter by considering the observable ‘position’; to do that, we must introduce the notion of probability density.

#### 4.1. Probability Density

The mass density  $\delta$  of a body is mass per unit length. Consequently, if a wire’s density is constant at  $\delta = 1\text{kg}/\text{m}$  and its length is 3 meters, the wire’s total mass will be  $3\text{kg}$ , namely, the area of the figure between  $\delta$ ’s plot and the  $x$ -axis from 0 to 3 (Fig. 1).

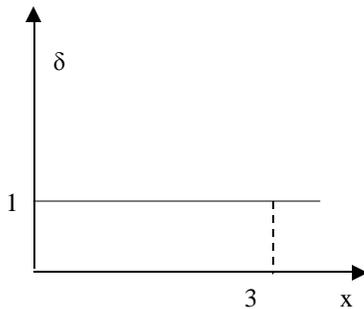


Figure 1

Even if the plot of the density is more complex than the one we just considered, the point remains the same: to determine the mass of the wire between 0 and 3, we reckon the area under  $\delta$  between 0 and 3.

Consider now a particle P moving to the right along the  $x$ -axis from 1 to  $l$ . At time  $t = 0$  P is at 1, and suppose that its speed is given as a function of position:

$$v = 1/x. \quad (4.1.1)$$

In other words, the farther ahead P moves, the slower its velocity according to (4.1.1).

Imagine taking snapshots at random times while P goes from 1 to  $l$ . Where will the bulk of the snapshots depict P to be? P starts with speed  $v_0 = 1$  and then slows down as it progresses to higher values of  $x$  until it gets to  $l$  with velocity  $1/l$ . Hence, if we divide the interval  $[l - 1]$  into equal intervals  $dx$ , P will spend less time in the early intervals (those closer to 1) and more in the later ones (those close to  $l$ ). Consequently, the snapshots will mostly depict P being closer to  $l$  than to 1.

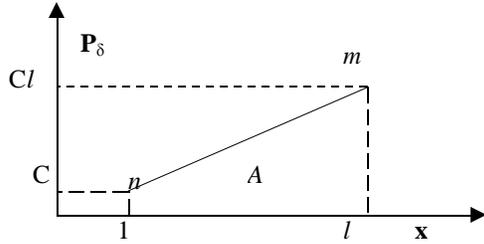
Let us make the previous considerations more precise. The probability that P will be observed in an interval  $dx$  is directly proportional to the amount of time P takes in traversing it. In other words, the probability that P will be observed in an interval  $dx$  is inversely proportional to the speed  $v$  with which P traverses it, and is therefore equal to

$C \frac{1}{v}$ , where  $C$  is a constant of proportionality. We express this by

$$P_\delta = C \frac{1}{v} = Cx, \quad (4.1.2)$$

where  $P_\delta$  is the position probability density. As mass density measures mass per unit of length, so position probability density measures probability per unit of length. The

former is proportional to the amount of matter per unit of length, the latter to the amount of time the particle spends in traversing a unit of length.



**Figure 2**

The probability that  $P$  is between 1 and  $l$  is given by the area  $A$  of the figure under  $nm$ , namely, the trapeze  $1lmn$  in figure 2. From classical geometry, we obtain

$$A = \frac{1}{2}(C + Cl)(l - 1). \quad (4.1.3)$$

However, the particle must be somewhere between 1 and  $l$ , and therefore  $A = 1$ . Hence,

$$C = \frac{2}{l^2 - 1}.^1 \quad (4.1.4)$$

Consequently,

$$P_\delta = \frac{2}{l^2 - 1} x. \quad (4.1.5)$$

The process whereby one determines the constant  $C$  is called “normalization”. It is demanded by the principle that the sum of all the mutually exclusive possibilities of a

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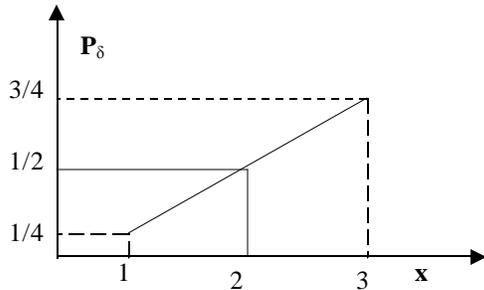
<sup>1</sup> That is,  $A = \frac{1}{2}(C + Cl)(l - 1) = \frac{1}{2}C(l^2 - 1)$ , from which (4.1.4) follows immediately.

situation must be equal to one. It is the same logical step requiring that the vector representing a quantum state be normalized.<sup>2</sup>

Now let us plug in some figures. Suppose that  $l = 3$ . Then, from (4.1.5) we obtain

$$P_{\delta} = \frac{1}{4}x. \quad (4.1.6)$$

Hence, the probability that P is between 1 and 2 is given by the area under  $P_{\delta}$  between 1 and 2 (Fig. 3).



**Figure 3**

Consequently,

$$\Pr(1,2) = \frac{3}{8}, \quad (4.1.7)$$

while the probability that P is between 2 and 3 is

$$\Pr(2,3) = \frac{5}{8}. \quad (4.1.8)$$

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<sup>2</sup> Of course, our example was artificially simple in that  $A$  was the area of a trapeze, a figure of classical geometry; typically, the area of the figure under  $P_{\delta}$  must be obtained by

using the integral  $A = \int_a^b P_{\delta} dx$ . However, the principle remains the same.

As we expected, since P slows down, it is more likely to be observed after the midpoint than before. Notice that  $\text{Pr}(1,2) + \text{Pr}(2,3) = 1$ , as it should be.

## 4.2 Schrödinger's Wave Function

Consider a particle moving along the  $x$ -axis. Quantum mechanics determines the probability of observing the particle in a given position at a given time by using the wave function  $\Psi(x,t)$  of the particle. One gets  $\Psi(x,t)$  by solving the Time Dependent Schrödinger Equation (TDSE),

$$i\hbar \frac{\partial}{\partial t} \Psi(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x,t) + V(x,t)\Psi(x,t) \quad (4.2.1)$$

where  $V$  is the (classical) potential energy determined by the physical system under investigation,  $m$  the mass of the particle, and  $\hbar$  (h-bar) is Planck's constant.<sup>3</sup> In other words, the wave function is a solution of TDSE. Setting up TDSE and solving it can be (and usually is) difficult. Fortunately, we need not attempt it. Suffice it to say that the relationship between the wave function, probability, and physical reality is given by Born's statistical interpretation:  $|\Psi(x,t)|^2$ , the squared modulus of the normalized wave function, is the probability density that upon observation the particle will be found at point  $x$  at time  $t$ .<sup>4</sup> For example, suppose that at time  $t_1$ ,  $|\Psi(x,t_1)|^2$  is the curve in figure 4.

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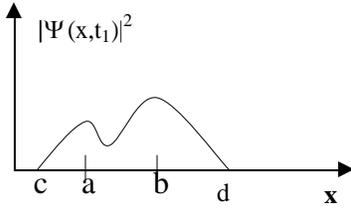
<sup>3</sup> Actually,  $\hbar$  is Planck's constant divided by  $2\pi$ .  $\frac{\partial}{\partial t}$  represents partial differentiation with

respect to  $t$  and  $\frac{\partial}{\partial x}$  partial differentiation with respect to  $x$ . For an explanation of

differentiation, see appendix 1.

<sup>4</sup> From now on, we shall assume that all the state vectors and all the wave-functions have

been normalized. As we know,  $|\Psi(x,t)|^2 = \Psi(x,t)^* \Psi(x,t)$ .



**Figure 4**

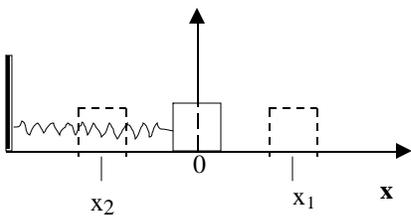
Then, the area under  $|\Psi(x, t)|^2$  between  $a$  and  $b$  is the probability that a position measurement at time  $t_1$  will return a value between  $a$  and  $b$ .<sup>5</sup> The key word here is “measurement”. That is, at least in the minimalist version we consider at this stage, quantum mechanics makes predictions only about measurement returns. In other words, all it tells us is what returns we shall have, and with what probability, if we perform such and such an experiment, without making any claims about quantum particles outside of the experimental setting.

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<sup>5</sup> From now on, to avoid clutter, at times we shall use “ $\Psi$ ” instead of “ $\Psi(x, t)$ ”. Often, not all the mathematical solutions to TDSE can satisfy the normalization requirement, in which case, being incompatible with the statistical interpretation, they do not represent particles. Of course, it is not enough to say that, after normalization,  $\int_a^b |\Psi|^2 dx$  (the area under  $|\Psi|^2$ ) is a probability; one must show that it satisfies the axioms of probability calculus. In fact, it can be shown that it does. See, for example, Ballentine, L. E., (1986). Note that normalization requires that the total area under  $|\Psi(x, t_1)|^2$ , to wit, that between  $c$  and  $d$ , must be equal to one.

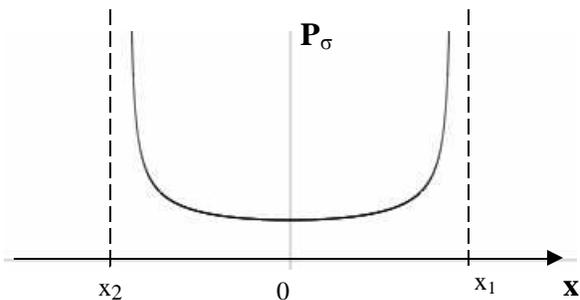
### 4.3 The Harmonic Oscillator

Consider a cube on a frictionless plane attached to a spring fixed to a wall. Suppose that the system is in an equilibrium position, corresponding to the relaxed length of the spring so that the box is at rest (Fig. 5). Let us take the origin 0 of the x-coordinate to be the position where the center of box is. Now, we stretch the spring to the right so that the center of the box is at  $x_1$  and then we let go. Obviously, the box will be pulled back by the spring, acquire energy which will be spent compressing the spring until its center reaches  $x_2 = -x_1$ . Then, it will be pushed again by the compressed spring to the position it had when we let the box go. In short, in the absence of friction or external forces the box will forever oscillate back and forth between  $x_1$  and  $x_2$  with simple harmonic motion. Such a system is a harmonic oscillator.



**Figure 5**

The probability density for the classical harmonic oscillator is plotted below (Fig. 6).



**Figure 6**

$x_1$  and  $x_2$  are called “turning points” because the center of the box cannot go beyond them: doing so would be contrary to the laws of mechanics. The plot tells us that if we take random snapshots of the box, the bulk of the snapshots will depict the box near the turning points. On reflection, this is how we would intuitively think it should be, since the box moves the slowest close to the turning points and the fastest close to point 0 in the middle of the run.

However, when we consider the quantum harmonic oscillator, we are in for some big surprises. First we need to plug the (classical) potential energy formula  $V(x) = \frac{1}{2}kx^2$  (where  $k$  is a constant measuring the springiness of the spring and  $x$  is the spring’s displacement) for the harmonic oscillator into TDSE. Once we have solved TDSE and obtained the wave function, we need to normalize the wave function. Although this is too complex for us to tackle, it turns out that the mathematics of normalization forces the *quantization* of energy. While the classical harmonic oscillator can have any energy level (between any two energy levels, one can always find a third), the quantum harmonic oscillator can only be found to have discrete and very definite energy levels  $E_0, E_1, E_2, \dots$ <sup>6</sup> In addition, while in the classical case the lowest energy level is zero (corresponding to the state in which the spring is relaxed and the box does not move), in the quantum case the measurement return for lowest possible energy (the energy of what is called “the ground state”) is

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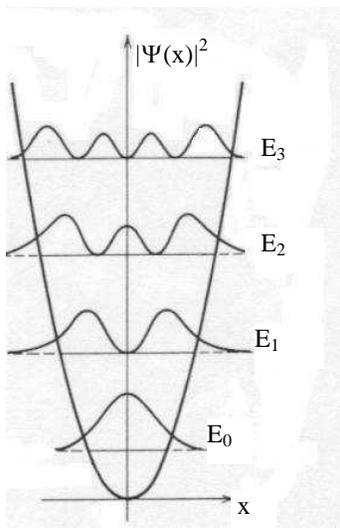
<sup>6</sup> In other words, it turns out that normalization compels the eigenvalues of the energy operator (of which more later) to form a discrete set.

$$E_0 = \frac{1}{2} \hbar \omega, \quad (4.3.1)$$

a quantity greater than zero, albeit a very small one.<sup>7</sup> The measurement returns of all the other possible energy levels (the energies of the excited states) are multiples of  $E_0$  according to the formula

$$E_n = (1 + 2n)E_0. \quad (4.3.2)$$

When it comes to position measurements, things are as strange, as we can gather from figure 7, which provides the plots of the probability densities for the first four energy levels. (The intersection points between each probability density and the parabola at an energy level are the classical turning points for that energy level).



**Figure 7**

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<sup>7</sup>  $\omega^2 = \frac{k}{m}$ , where  $k$  is a measure of the springiness of the spring, and  $m$  is the mass of the

cube. In other words, the stronger the force exercised by the spring, the larger  $\omega^2$  is, and the larger the mass of the cube, the smaller  $\omega^2$  is.

In an excited state  $E_n$ , there are  $n$  positions in the space between the turning points where the particle will never be found. In particular, in all odd states such as  $E_1$  or  $E_3$  the probability of finding the particle exactly in-between the turning points is zero. In addition, the probability of finding the particle outside the classically permitted range (beyond the turning points) is not zero, a phenomenon called “tunneling”. In fact, it turns out that the lower the energy, the greater the probability that the particle will tunnel: at the ground level, the probability of tunneling is slightly above 15%.

#### 4.4. Hilbert Spaces

There is a relation between the wave function and the state vectors we considered in the previous chapter, for it turns out that the wave function *is* a state vector. The basic idea is to construct a type of inner product vector space, called a “Hilbert space”, with particular functions as its elements by showing that they are really vectors. As one might expect, the functions in question turn out to be normalizable. They satisfy the vector requirements set out in the last chapter. The sum of two normalizable functions is also normalizable; addition on them is commutative and associative; multiplying a normalizable function by a scalar gives another normalizable function; there is a null function,  $f(x) = 0$ ; each function  $f(x)$  has a function  $-f(x)$  such that

$f(x) + [-f(x)] = 0$ ; the inner product of two normalizable functions is defined as

$$\langle f | g \rangle = \int f(x)^* g(x) dx, \text{ for appropriate limits of integration.}$$

We shall not construct the standard Hilbert space  $L_2$  here because it involves some (for us) unnecessary mathematical niceties. Suffice it to say that the wave function  $\Psi(x, t)$ , once normalized, becomes a normalized vector in  $L_2$ .

In the last chapter, we saw that observables are represented by Hermitian operators, and this remains true in Hilbert space. For example, the position operator is  $\hat{x}$ , and since it is Hermitian, its eigenfunctions (which can be treated as eigenvectors) are orthogonal and form a complete set. Hence, they constitute an orthonormal basis and any state function can always be expanded as a linear superposition of eigenfunctions of the position operator.<sup>8</sup> Other observables are expressed in position representation by operators; for example, momentum is represented by the operator  $-i\hbar\frac{\partial}{\partial x}$ .

We should note that state space does not have any intuitively satisfying relation to the ordinary 3-dimensional space of our experience. The reason is that the state space of a particle moving about is infinitely dimensional. As the particle could occupy an infinity of positions and the position operator is Hermitian, there must be an infinite number of relevant eigenvectors all orthogonal to each other, which is possible only in an infinitely dimensional space. Hence, it is important not to confuse the 3-dimensional space we share with atoms and electrons with the state vector space, which is an abstract mathematical entity.

What we said about position applies to any other observable: every operator expressing an observable has its own representation of any other operator expressing an observable. So, for example, the same state function and the same operator representing an observable can be expressed in energy representation, in position representation, in momentum representation, and so on. All these representations are equivalent, in the

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<sup>8</sup> The eigenfunctions in question are Dirac delta-functions. Their treatment, including normalization, involves mathematical subtleties that need not concern us.

sense that one does not contain any more information than the other: which representation one uses is a pure matter of convenience.<sup>9</sup>

Suppose now that at a given time a quantum state is expressed in position representation as  $\Psi(x)$  and in momentum representation as  $\phi(p)$ . Mathematically,  $\Psi(x,0)$  and  $\phi(p)$  enjoy a special relationship: they are Fourier transforms of each other. While any detailed account of this fact is unneeded here, we may note that it has a purely mathematical consequence *not* dependent on the physics of quantum mechanics, namely that their widths cannot both simultaneously be made arbitrarily small. In short, if one of the two functions spikes, the other gets correspondingly flat. So, if we measure position on a particle, then the attendant collapse turns  $\Psi(x)$  into a Dirac delta function (Figure 9 in exercise 4.3). Then, the plot of  $\phi(p)$  will be a horizontal line, and therefore so will be the momentum probability density  $|\phi(p)|^2$ , which entails that the momentum could take any value at all with the same probability. This is (a version of) the famous Heisenberg Uncertainty Principle, a special case of the Generalized Uncertainty Principle we shall prove later.

#### 4.5 Two More Principles

We can now add two more items to our list of principles of quantum mechanics, to wit:

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<sup>9</sup> One may think of the state function as a proposition that can be fully expressed in different languages, where a language is a representation space. The proposition “It rains” can be expressed in English, in German (“Es regnet”), in Italian (“Piove”), and so on.

5 (Commuting) quantum mechanical Hermitian operators bear to each other the same functional relationships obtaining among the classical observables they represent.

6 The time evolution of a quantum system is given by TDSE.

Let us comment on them. Principle (5) is best clarified by an example. In classical mechanics, the kinetic energy is

$$T = \frac{1}{2}mv^2 = \frac{1}{2}m\frac{p^2}{m^2} = \frac{p^2}{2m}, \quad (4.5.1)$$

where  $p = mv$  is the momentum. Principle (5) tells us that the same functional relation exists among the appropriate quantum mechanical operators. Hence, by substituting the momentum operator (in position representation) for  $p$ , we get

$$\hat{T} = \left(\frac{1}{2m} \frac{\hbar^2}{i^2} \frac{\partial^2}{\partial x^2}\right) = \left(\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}\right). \quad (4.5.2)$$

Similarly, the total mechanical energy is the sum of kinetic and potential energy. In quantum mechanics, the total energy of a system is represented by the energy operator  $\hat{H}$ , called “The Hamiltonian”. Hence, principle (5) tells us that in position representation,

$$\hat{H} = \left(\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}\right) + V(x).^{10} \quad (4.5.3)$$

Principle (6) tells us that the state vector representing a system changes in time according to the Schrödinger equation. TDSE has three important properties. First, it is

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<sup>10</sup> The Hamiltonian is very important in quantum mechanics; for one thing, we can now

write TDSE as  $i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi$ , which makes clear that the temporal evolution of the wave

function is driven by the Hamiltonian.

linear. Consequently, if in the temporal interval  $t_1 - t_2$  the state vector  $|\Psi\rangle$  evolves into  $|\Psi'\rangle$  and the state vector  $|\Xi\rangle$  into  $|\Xi'\rangle$ , then in the same time interval the state vector  $\alpha|\Psi\rangle + \beta|\Xi\rangle$  evolves into  $\alpha|\Psi'\rangle + \beta|\Xi'\rangle$ . Second, TDSE is first order with respect to time (the time derivative is first order). Hence, given the appropriate initial condition at time zero, TDSE totally determines the state vector for all future times. Third, TDSE preserves normalization: if a state vector is normalized at time zero, it stays normalized as it changes in time. In other words, in vector space the state vector changes its direction but not its length. We now consider a special type of operator that rotates vectors without altering their lengths and does the same job as TDSE.

#### 4.6 The Evolution Operator

In quantum mechanics, TDSE does two things: it provides us with the wave function  $\Psi(x,t)$  and it tells us how  $\Psi(x,t)$  evolves over time. Extracting the wave function from TDSE (that is, solving TDSE) is often mathematically very difficult and for us unnecessary. By contrast, understanding TDSE's second function is relatively easy. We may think of TDSE as a device in vector space that linearly transforms  $|\Psi(t_0)\rangle$ , the state vector at time zero, into  $|\Psi(t_n)\rangle$ , the state vector at a later time. There is a linear operator  $U(t, t_0)$ , the evolution operator, that does exactly the same thing, so that

$$U(t, t_0)|\Psi(t_0)\rangle = |\Psi(t)\rangle. \quad (4.6.1)$$

Note that since  $U(t, t_0)$  is linear,

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<sup>11</sup> It may be worth noting that if the system is conservative ( $H$  is time independent), then

$$U(t, t_0) = e^{\frac{-iH \cdot (t-t_0)}{\hbar}}.$$

$$U(t, t_0)[c_1|\psi_1(t_0)\rangle + c_2|\psi_2(t_0)\rangle] = c_1U(t, t_0)|\psi_1(t_0)\rangle + c_2U(t, t_0)|\psi_2(t_0)\rangle. \quad (4.6.2)$$

Linearity, embodied in (4.6.2), is a very important property of the evolution operator, that is, of how quantum systems evolve in time. We have already talked about it in the previous section, but its importance is such that we consider it again here. Suppose that at time  $t_0$  a system is in state  $|\Psi(t_0)\rangle = c_1|\psi_1(t_0)\rangle + c_2|\psi_2(t_0)\rangle$  and that at time  $t$  it has evolved into  $|\Psi(t)\rangle$ . Suppose also that had the system been in state  $|\psi_1(t_0)\rangle$ , at time  $t$  it would have evolved into  $|\psi_1(t)\rangle$ , and had the system been in state  $|\psi_2(t_0)\rangle$ , at time  $t$  it would have evolved into  $|\psi_2(t)\rangle$ . Then, (4.6.2) tells us that  $|\Psi(t)\rangle = c_1|\psi_1(t)\rangle + c_2|\psi_2(t)\rangle$ .

## Exercises

### Exercise 4.1

Suppose that in the density example case discussed in section 4.1, we skipped

normalization and instead of (4.1.5) we ended up with  $P_\delta = \frac{1}{v} = x$ . Calculate  $\text{Pr}(1,2)$ ,

$\text{Pr}(2,3)$  and explain why the result has to be wrong.

### Exercise 4.2

1. Consider two wave functions  $\Psi_1$  and  $\Psi_2$  that are the mirror image of each other with the  $x$ -coordinate providing the axis of symmetry. In other words, suppose that at time zero  $\Psi_1(x) = -\Psi_2(x)$ . Do they have the same physical meaning?
2. Suppose that  $\Psi' = e^{i\delta}\Psi$ , with  $\delta$  a real number (the factor  $e^{i\delta}$  is called a “global phase factor”). Do  $\Psi'$  and  $\Psi$  represent the very same physical state? [Hint:  $x^a x^b = x^{a+b}$  and  $x^0 = 1$ ]

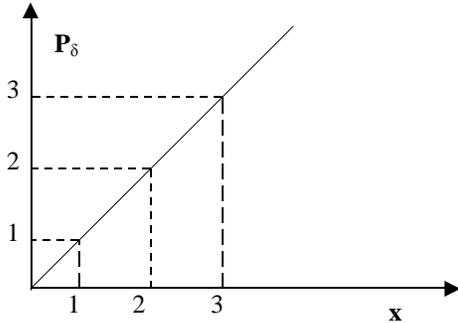
### Exercise 4.3

What must the plot of a Dirac delta-function look like? [Hint: Think about collapse and the fact that Dirac delta-functions are eigenfunctions of the position operator.]

## Answers to the Exercises

### Exercise 4.1

The plot of  $P_\delta = \frac{1}{v} = x$  is given in figure 8.



**Figure 8**

Hence,  $\text{Pr}(1,2) = \frac{1}{2}(1+2) \cdot 1 = \frac{3}{2}$  and  $\text{Pr}(2,3) = \frac{1}{2}(2+3) \cdot 1 = \frac{5}{2}$ , which is impossible

because a probability cannot be greater than 1. The only way to obtain probabilities again is to normalize the results by setting  $1 = C[\text{Pr}(1,2) + \text{Pr}(2,3)]$ , thus obtaining

$C = 1/4$ , and to multiply the pseudo-probabilities we obtained by  $C$ . The result are the correct probabilities of (4.1.7) and (4.1.8).

### Exercise 4.2

1. Since the only quantity with empirical relevance is the squared modulus of the wave function, and  $|\Psi(x)|^2 = |-\Psi(x)|^2$ , the answer is “Yes.”

2.  $|e^{i\delta}\Psi|^2 = (e^{i\delta}\Psi)^*(e^{i\delta}\Psi) = (e^{-i\delta}\Psi)(e^{i\delta}\Psi) = e^{i\delta-i\delta}|\Psi|^2 = |\Psi|^2$ . Hence,  $\Psi'$  and  $\Psi$  represent the very same physical state.

### Exercise 4.3

The plot of a Dirac delta-function must look like an infinitely tall and infinitesimally narrow spike at point  $a$  where the particle has been found and zero everywhere else, as in figure 9.

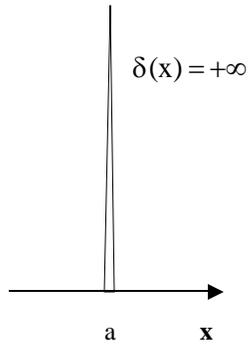


Figure 9