Introduction to Quantum Mechanics

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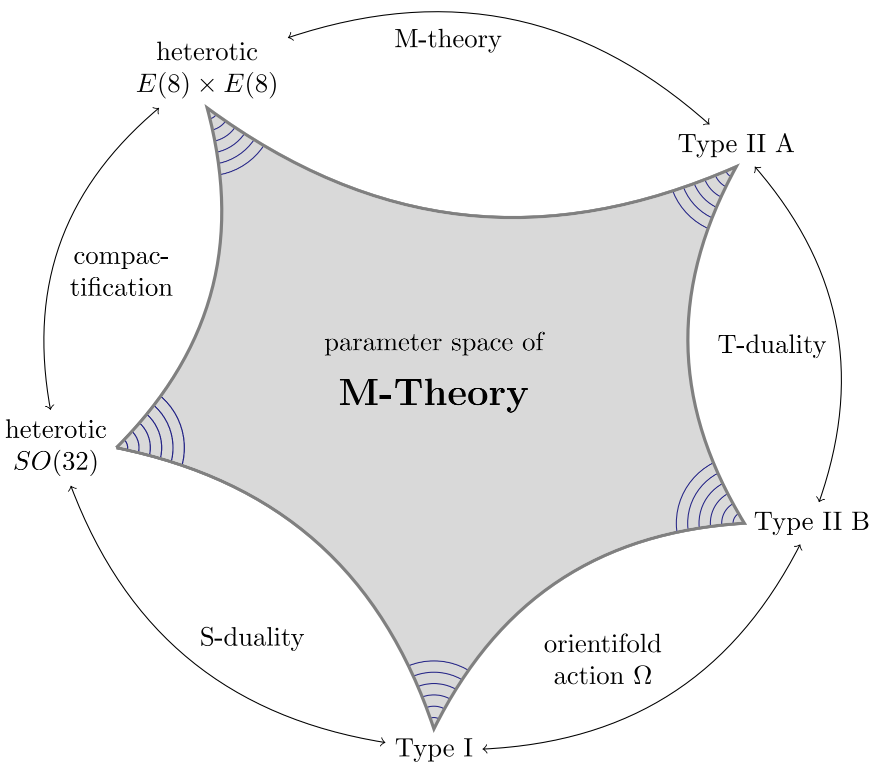
Adapted from *Introduction to Quantum Mechanics* 3rd ed. By David J. Griffiths



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1 The Wave Function

1.1 The Schrödinger Equation

Imagine a particle of mass m, constrained to move along the x axis, subject to move to some specified force $F(x,t)$. The program of *classical mechanics* is to determine the position of the particle at any given time $x(t)$. Once we know that, we can figure out the velocity ($v = \frac{dx}{dt}$), the momentum $p = mv$, the kinetic energy ($T = \frac{1}{2}mv^2$), or any other dynamical variable of interest. To determine $x(t)$, we apply Newton's Second Law: $F = ma$, or more specifically, $F = -\frac{\partial V}{\partial x}$, the derivative of a potential energy function, where $m\frac{\partial^2 x}{\partial t^2} = -\frac{\partial V}{\partial x}$. This together, with initial conditions, determines $x(t)$.

Quantum mechanics approaches this same problem a bit differently. In this case what we're looking for is the particles **wave function**, $\Phi(x,t)$, and we get it by solving the **Schrödinger Equation:**

Schrödinger Equation

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Phi}{\partial x^2} + V\Phi$$

Here i is the square root of -1, and $\hbar$ is Planck's constant - or rather, his *original* constant (h) divided by 2π:

$$\hbar = \frac{h}{2\pi} = 1.054573 \times 10^{-34} Js.$$

The Schrödinger equation plays a role logically analogous to Newton's second law.

1.2 The Statistical Interpretation

But what exactly *is* this wave function, and what does it do for you once you've *got* it? After all a particle by nature is a point, whereas the wave function (as its name suggests) is spread out in space (a function of x, for any given t).

How can such an object represent the state of a *particle*? The answer is provided by Born's **statistical interpretation**, which says that $|\Psi(x,t)|^2$ gives the *probability* of finding the particle at point x, at time t - or, more precisely,

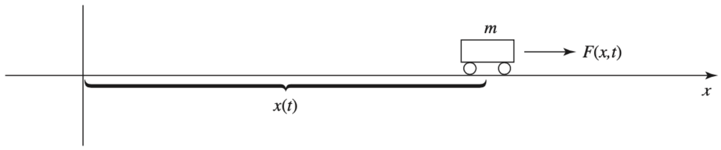

Figure 1: a "particle" constrained to move in one dimension under the influence of a specified force

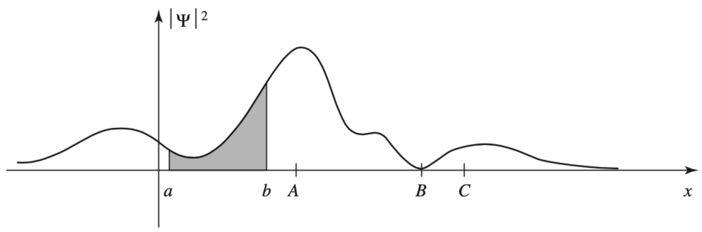

Figure 2: a typical wave function. the shaded area represents the probability of finding the particle between a and b. the particle would be relatively likely to be found near A, and unlikely to be found near B.

Born's Statistical Interpretation

$$\int_a^b |\Psi(x,t)|^2 \, dx = \{\text{probability of finding particle between } a \text{ and } b \text{, at time } t\ \}$$

Probability is the *area* under the graph of $|\Psi|^2$. For the wave function in the figure above, you would be quite likely to find the particle in the vicinity of point A, where $|\Psi|^2$ is large, and relatively unlikely to find it near point B.

The statistical interpretation introduces a kind of **indeterminacy** into quantum mechanics, for even if you know everything, the theory has to tell you about the particle, still you can't predict with certainty the outcome of a simple experiment to predict its position - all quantum mechanics has to offer is *statistical* information about *possible* results. It is natural to wonder whether this indeterminacy is a fact of nature, or a defect in the theory.

Suppose I *do* measure the position of the particle, and I find it to be a point C.

Question

Where was the particle just *before* I made the measurement?

Solution

There are three plausible answers

1. The **realist** position: The *particle was at C*. This certainly seems reasonable, and it is the response Einstein advocated. However, if this is true, quantum mechanics is an *incomplete* theory, since the particle *really was* at C, and yet quantum mechanics was unable to tell us so.

2. The **orthodox** position: The *particle wasn't really anywhere*. It was the act of measurement that forced it to "take a stand" (though how and why it chose the point C we dare not ask). This view is associated with Bohr and his followers. Among physicists it is the most widely accepted position. However, if it is correct, a century worth of debate about the act of measurement has done preciously little to illuminate.

The **agnostic** position: *Refuse to answer*. This is not as silly as it sounds - what sense can there be in making assertions about the status of a particle *before* a measurement. For decades this was the "fall-back" position of most physicists: they'd try to sell you the orthodox answer, but if you were persistent they'd retreat to the agnostic response, and terminate the conversation.

However, in 1964, John Bell astonished the physics community by showing that it makes an *observable* difference whether the particle had a precise (though unknown) position prior to the measurement or not. Bell's discovery effectively eliminated agnosticism as a viable option and made it an *experimental* question whether 1 or 2 was the correct choice.

What if I made a *second* measurement, immediately after the first? Would I get C again, or does the act of measurement cough up a completely new number each time? On this question everyone is in agreement:

A repeated measurement (on the same particle) must return the same value

Indeed, it would be tough to prove the particle was really at C in the first instance. How does the orthodox interpretation account for the fact that the second measurement is bound to yield the same result C? It must be that the first measurement radically alters the wave function, so that it now sharply peaked about C. We say that a wave function **collapses**, upon measurement, to a spike at the point C (it soon spreads out again, in accordance with the Schrödinger equation, so the second measurement must be made quickly). There are then, two entirely distinct kinds of

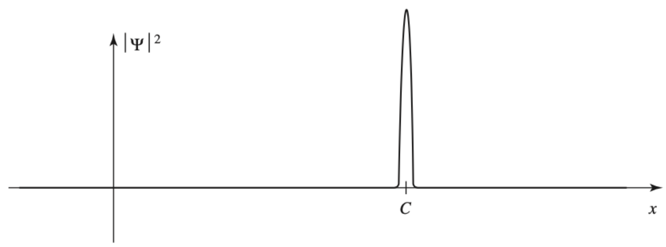

Figure 3: collapse of the wave function: graph of $|\Psi|^2$ immediately *after* a measurement has found the particle at point C.

physical processes: "ordinary" ones, in which the wave function evolves in a leisurely fashion under the Schrödinger equation, and "measurements," in which Ψ suddenly and discontinuously collapses.

1.2.1 Example 1.1

Electron Interference. How might we check that particles (electrons, for example) have a wave nature, encoded in Ψ?

The classic signature of a wave phenomena is *interference*: two waves *in phase* interfere constructively, and out of phase they interfere destructively. The wave nature of light wave confirmed in 1801 by Young's famous double slit experiment, showing interference "fringes" on a distant screen when a monochromatic beam passes through two slits. If essentially the same experiment is done with *electrons*, the same pattern develops, confirming the wave nature of electrons as more and more electrons collide with the screen.

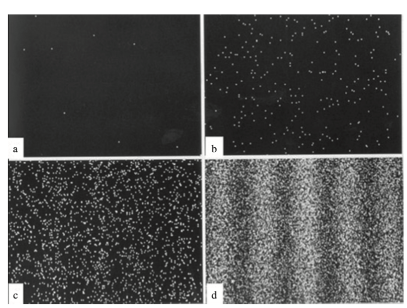

Figure 4: Build up of electron interference pattern. (a) Eight electrons, (b) 270 electrons, (c) 2000 electrons, (d) 160,000 electrons.

Of course, if you close off one slit, or somehow contrive to detect which slit each electron passes through, the interference pattern disappears; the wave function of the emerging particle is now entirely different.

2 Probability

2.1 Discrete Variables

Because of statistical interpretation, probability plays a central role in quantum mechanics, so I digress now for a brief discussion of probability theory. It is mainly a question of introducing some notation and terminology, and I shall do it in the context of a simple example:

Imagine a room containing 14 people, whose ages are:

one person aged 14
one person aged 15
three people aged 16
two people aged 22
two people aged 24
five people aged 25

If we let $N(j)$ represent the number of people of age j, then

$N(14) = 1$
$N(15) = 1$
$N(16) = 3$
$N(22) = 2$
$N(24) = 2$
$N(25) = 5$

while $N(17)$, for instance, is 0. The total number of people in the room is

$$N = \sum_{j=0}^{\infty} N(j).$$

Question If you selected one individual at random from this group, what is the **probability** that this person's age would be 15? ***Solution*** One chance in 14, since there are 14 possible choices,

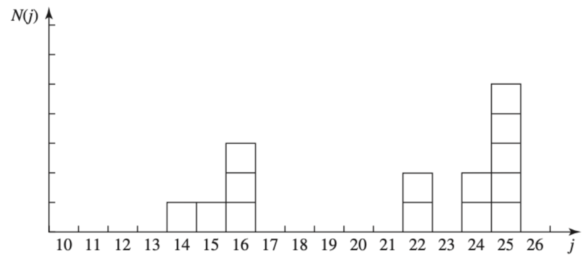

Figure 5: histogram of people

all equally likely, of whom only one is aged 14. If $P(j)$ is the probability of getting age j, then $P(14) = 1/14, P(15) = 1/14, P(16) = 3/14$, and so one. In general,

$$P(j) = \frac{N(j)}{N}.$$

Notice that the probability of getting *either* 14 or 15 is the *sum* of the individual probabilities (1/7). In particular, the sum of *all* probabilities is 1 - the person you select must have *some* age:

$$\sum_{j=0}^{\infty} P(j) = 1$$

Question

What is the **most probable** age?

Solution

25, obviously, the most probably j is the j for which $P(j)$ is a maximum.

Question

What is the **median** age?

Solution

23, for 7 people are younger than 23, and 7 people are older

Question

What is the **median** age?

Solution

$$\frac{14+15+3(16)+2(22)+2(24)+5(25)}{14} = \frac{294}{14} = 21.$$

In general, the average value of j, which we will write as $\langle j \rangle$ is

$$\langle j \rangle = \frac{\sum jN(j)}{N} = \sum_{j=0}^{\infty} jP(j).$$

In quantum mechanics the average is usually the quantity of interest; it is known as the **expectation value**.

Question

What is the average of the *squares* of the ages?

Solution

You could get $14^2 = 196$ with probability $1/14$, or $15^2 = 225$, with probability $1/14$, or $16^2 = 256$ with probability $3/14$, and so on. The average is then

$$\langle j^2 \rangle = \sum_{j=0}^{\infty} j^2 P(j)$$

In general, the average value of some *function* of j is given by

$$\langle f(j) \rangle = \sum_{j=0}^{\infty} f(j)P(j).$$

Beware: The average of the squares, $\langle j^2 \rangle$, is *not* equal, in general, to the square of the average, $\langle j \rangle^2$.

Now, there is a difference between the two histograms. The first is sharply peaked about the average, with the same number of elements, whereas the second is broad and flat. We need a numerical measure of the amount of "spread" in a distribution, with respect to the average. To get a value we can work with, we also square the value before average

$$\sigma^2 \equiv \langle (\Delta j)^2 \rangle.$$

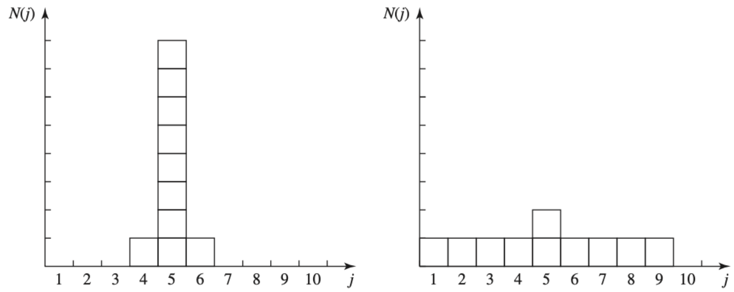

Figure 6: two histograms with the same median, mean, and same most probable value, but different standard deviations

This quantity is known as the **variance** of the distribution; σ itself is called the **standard deviation**, which measures the spread about $\langle j \rangle$. Taking the square root, the standard deviation can be written as

$$\sigma = \sqrt{\langle j^2 \rangle - \langle j \rangle^2}$$

2.2 Continuous Variables

So far we've only dealt with specific variables, not continuous and more realistic ones. The sensible thing to speak about is the probability of a variable existing in some *interval* - say, between 16 and 17 years old in the previous example. If the interval is sufficiently short, this probability is *proportional to the length of the interval.* Technically, we're talking about *infinitesimal* intervals.

$$\{\text{probability that an individual lies between } x \text{ and } (x + dx) \ \} = \rho(x)\, dx.$$

More specifically, the proportionality factor, $\rho(x)$ is better defined as **probability density**. The probability that x lies between a and b is given by the integral of $\rho(x)$:

$$P_{ab} = \int_a^b \rho(x)\, dx,$$

and the rules we deduced for discrete distributions translate in the obvious way:

$$\int_{-\infty}^{\infty} \rho(x)\, dx = 1$$
$$\langle x \rangle = \int_{-\infty}^{\infty} x\rho(x)\, dx,$$
$$\langle f(x) \rangle = \int_{-\infty}^{\infty} f(x)\rho(x)\, dx,$$
$$\sigma^2 \equiv \langle (\Delta x)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$$

2.2.1 Example 1.2

Suppose someone drops a rock off a cliff of height h. As it falls, I snap a million photographs at random intervals. On each picture I measure the distance the rock has fallen.

Question

What is the *average* of all these distances, or rather the *time average* of the distance traveled?

Solution

The rock starts out at rest, then falls so

$$x(t) = \frac{1}{2}gt^2$$

The velocity is $dx/dt = gt$ and the total flight time is $T = \sqrt{2h/g}$. The probability that a particular photograph was taken between t and $t + dt$ is dt/T, so the probability that is shows a distance in the range x to $x + dx$ is

$$\frac{dt}{T} = \frac{dx}{gt}\sqrt{\frac{g}{2h}} = \frac{1}{2\sqrt{hx}}dx.$$

Thus the probability *density* is

$$\rho(x) = \frac{1}{2\sqrt{hx}}, \quad (0 \leq x \leq h)$$

We can check this result,

$$\int_0^h \rho(x)\,dx = \frac{1}{2\sqrt{h}}(2x^{1/2})\Big|_0^h = 1$$

The *average* distance is

$$\langle x \rangle = \int_0^h x\frac{1}{2\sqrt{hx}}\,dx = \frac{1}{2\sqrt{h}}(\frac{2}{3}x^{3/2})\Big|_0^h = \frac{h}{3},$$

which is somewhat less than $h/2$, as anticipated. The image below shows the graph of $\rho(x)$, notice that the probability density can be infinite, though the probability itself must of course be finite, less than or equal to 1.

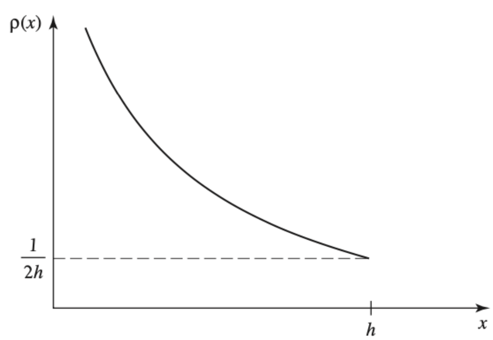

Figure 7: the probability density: $\rho(x) = 1/(2\sqrt{hx})$

2.2.2 Problem 1.1

For the distribution of ages in the example above:

(a) Compute $\langle j^2 \rangle$ and $\langle j \rangle^2$
(b) Determine Δj for each j and compute the standard deviation
(c) Use your results in (a) and (b) to check if the standard deviation makes sense.

14	1
15	1
16	3
22	2
24	2
25	5

a) $$\langle j^2 \rangle = \frac{14^2 + 15^2 + 3(16^2) + 2(22^2) + 2(24^2) + 5(25^2)}{14} = \boxed{459.571}$$

$$\langle j \rangle^2 = 21^2 = \boxed{441}$$

b) $\Delta j = j - \langle j \rangle$

j	Δj
14	-7
15	-6
16	-5
22	1
24	3
25	4

$$\sigma^2 = \langle (\Delta j)^2 \rangle$$

$$= \frac{1}{N} \sum (\Delta j)^2 N(j) = \frac{260}{14} = 18.571$$

$$\sigma = \sqrt{18.571} = \boxed{4.3}$$

c) $$\sigma = \sqrt{\langle j^2 \rangle - \langle j \rangle^2} = \sqrt{459.571 - 441} = \sqrt{18.571} = \boxed{4.3}$$

Figure 8: solutions for problem 1.1

2.2.3 Problem 1.2

(a) Find the standard deviation of the distribution in Example 1.2
(b) What is the probability that a photograph, selected at random, would show a distance x more than one standard deviation away from the average?

(a)

$$\rho(x) = \frac{1}{2\sqrt{hx}}$$

$$\langle x \rangle = \int_0^h x\rho(x)\,dx = \int_0^h x\frac{1}{2\sqrt{hx}}\,dx = \frac{1}{\sqrt{2h}}\int_0^h \frac{x}{\sqrt{x}}\,dx = \frac{1}{\sqrt{2h}}\int_0^h x^{1/2}\,dx = \frac{1}{\sqrt{2h}}\left(\frac{2}{3}x^{3/2}\right)\Big|_0^h = \underline{h/3}$$

$$\langle x \rangle^2 = \left(h/3\right)^2 = \underline{h^2/9}$$

$$\langle x^2 \rangle = \int_0^h x^2\rho(x)\,dx = \frac{1}{\sqrt{2h}}\int_0^h x^{3/2}\,dx = \frac{1}{\sqrt{2h}}\left(\frac{2}{5}x^{5/2}\right)\Big|_0^h = \frac{2}{5\sqrt{2h}}\left(h^{5/2}\right) = \underline{\frac{h^2}{5}}$$

$$\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 = \frac{h^2}{5} - \frac{h^2}{9} = \frac{4}{45}h^2 \Longrightarrow \boxed{\sigma = \frac{2h}{3\sqrt{5}}}$$

(b)

$$P_{ab} = \int_a^b \rho(x)\,dx$$

$$P_{photograph} = 1 - \int_{\langle x \rangle - \sigma}^{\langle x \rangle + \sigma} \frac{1}{2\sqrt{hx}}\,dx = 1 - \frac{1}{2\sqrt{h}}\int_{\langle x \rangle - \sigma}^{\langle x \rangle + \sigma} x^{-1/2}\,dx = 1 - \frac{1}{2\sqrt{h}}\left(2x^{1/2}\right)\Big|_{\langle x \rangle - \sigma}^{\langle x \rangle + \sigma}$$

$$\langle x \rangle + \sigma = \frac{h}{3} + \frac{2h}{3\sqrt{5}} = 0.6315h \Longrightarrow P = 1 - \frac{1}{\cancel{\sqrt{h}}}\left(\sqrt{0.6315\cancel{h}} - \sqrt{0.0352\cancel{h}}\right) = \boxed{0.393}$$

$$\langle x \rangle - \sigma = \frac{h}{3} - \frac{2h}{3\sqrt{5}} = 0.0352h$$

Figure 9: solutions to problem 1.2

2.2.4 Problem 1.3

Consider the **gaussian** distribution

$$\rho(x) = Ae^{-\lambda(x-a)^2},$$

where A, a and λ are positive real constants.

(a) Use the fact that $\int \rho(x)\,dx = 1$ to determine A
(b) Find $\langle x \rangle, \langle x^2 \rangle$ and σ
(c) Sketch $\rho(x)$

$\rho(x) = A e^{-\lambda(x-a)^2}$, A, a, λ positive real constants

(a)
$$\int_{-\infty}^{\infty} \rho(x)\,dx = 1 \implies \int_{-\infty}^{\infty} A e^{-\lambda(x-a)^2} dx = 1 \implies A\int_{-\infty}^{\infty} e^{-\lambda(x-a)^2} dx = 1$$

let $u = x-a$, $du = dx$
$$\implies A\int_{-\infty}^{\infty} e^{-\lambda(u)^2} dx = A\sqrt{\frac{\pi}{\lambda}} = 1 \implies \boxed{A = \sqrt{\frac{\lambda}{\pi}}}$$

(b)
$$\langle x \rangle = \int_{-\infty}^{\infty} x\sqrt{\frac{\lambda}{\pi}}\, e^{-\lambda(x-a)^2} dx = \sqrt{\frac{\lambda}{\pi}}\int_{-\infty}^{\infty} (u+a)\, e^{-\lambda(u)^2} dx$$
$$= \sqrt{\frac{\lambda}{\pi}}\left[\int_{-\infty}^{\infty} u e^{-\lambda u^2} du + a\int_{-\infty}^{\infty} e^{-\lambda(u)^2} dx\right] = A\left(0 + a\sqrt{\frac{\pi}{\lambda}}\right) = \boxed{a}$$

$$\langle x^2 \rangle = A\int_{-\infty}^{\infty} x^2 e^{-\lambda(x-a)^2} dx \implies A\left[\frac{1}{2\lambda}\sqrt{\frac{\pi}{\lambda}} + 0 + a^2\sqrt{\frac{\pi}{\lambda}}\right] = \boxed{a^2 + \frac{1}{2\lambda}}$$

(c)

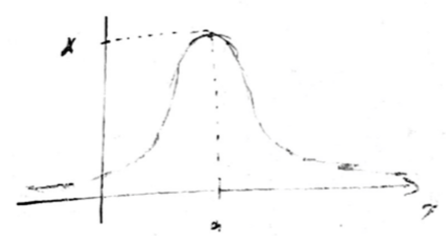

Figure 10: solution to problem 1.3

3 Normalization

We now return to the statistical interpretation of the wave function, which says that $|\Psi(x,t)|^2$ is the probability density for finding the particle at point x at time t. Therefore, i

$$\boxed{\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \, dx = 1}$$

However, $\Psi(x,t)$ must also be a solution to the Schrodinger equation, as that is how it is determined. A glance at the Schrodinger equation reveals that if $\Psi(x,t)$ is a solution, so too is $A\Psi(x,t)$, where A is any (complex)constant. This process of finding a constant A such that $\Psi(x,t)$ satisfies both the above integral and Schrodinger's Equation is known as **normalizing** the wave function. For some solutions to the Schrodinger equation, the integral above is infinite, in that case there exists no A that would make it 1. The same goes for the trivial solution $\Psi = 0$. Such **non-normalizable** solutions cannot represent particles, and are therefore rejected. Physically realizable states correspond to the **square-integrable** solutions to Schrodinger's Equation. But wait!. Suppose I have normalized the wave function at time $t = 0$. How do I know it will *stay* normalized as time goes on, and Ψ evolves? Fortunately Schrodinger's Equation has the remarkable property that it *preserves* the normalization of a wave function.

This is important, so let us prove it.

Proof

$$\frac{d}{dt}\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \, dx = \int_{-\infty}^{\infty} \frac{\partial}{\partial t}|\Psi(x,t)|^2 \, dx$$

*Note that the integral is only a function of t, so a normal derivative works. The integrand is a function of both x, t so we use a partial derivative. By the product rule,

$$\frac{\partial}{\partial t}|\Psi|^2 = \frac{\partial}{\partial t}(\bar{\Psi}\Psi) = \bar{\Psi}\frac{\partial \Psi}{\partial t} + \frac{\partial \bar{\Psi}}{\partial t}\Psi$$

Now the Schrodinger equation says that

$$\frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar}V\Psi$$

and hence also (taking complex conjugate)

$$\frac{\partial \bar{\Psi}}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \bar{\Psi}}{\partial x^2} - \frac{i}{\hbar}V\bar{\Psi}$$

so

$$\frac{\partial}{\partial t}|\Psi|^2 = \frac{i\hbar}{2m}\left(\bar{\Psi}\frac{\partial^2 \Psi}{\partial x^2} - \frac{\partial^2 \bar{\Psi}}{\partial x^2}\Psi\right) = \frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\bar{\Psi}\frac{\partial \Psi}{\partial x} - \frac{\partial \bar{\Psi}}{\partial x}\Psi\right)\right]$$

The original integral $\frac{d}{dt}\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \, dx$ can now be evaluated explicitly:

$$\frac{d}{dt}\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \, dx = \frac{i\hbar}{2m}\left(\bar{\Psi}\frac{\partial \Psi}{\partial x} - \frac{\partial \bar{\Psi}}{\partial x}\Psi\right)\Big|_{-\infty}^{\infty}$$

But $\Psi(x,t)$ must go to zero as x goes to ($\pm$) infinity - otherwise the wave function wouldn't be normalizable in the first place. It follows that

$$\frac{d}{dt}\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 0$$

and hence the integral is *constant* (independent of time); if Ψ is normalized at $t = 0$, it *stays* normalized for all future time.