Quantum Mechanics

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Preface

This notes has been written by B. Diez mainly from Introduction to Quantum Mechanics by David J. Griffiths and own knowledge.

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Chapter 1

The Wave Function

1.1 The Schrodinger Equation

Imagine a particle of mass m, constrained to move along the x-axis, subjet to some to specifies force F(x,t). The program of classical mechanics is to determine the position of the particle at any give time: x(t). Once we know that, we can figure out the velocity $(v=\mathrm{d}x/\mathrm{d}t)$, the momentum (p=mv), the kinetic energy $(T=(1/2)mv^2)$, or any other dynamical variable of interest. And how do we go about determining x(t)? We apply Newton's second law: F=ma. (For conservative systems—the only kins we shall consider, and, fortunately, the only kins that occur at the microscopic level—the force can be expressed as the derivative of a potential energy function 1 , $F=-\partial V/\partial x$, and Newton's law reads $m\mathrm{d}^2x/\mathrm{d}t^2=-\partial V/\partial x$) This, together with appropriate initial conditions (typically the position and velocity at t=0), determines x(t)

Quantum mechanics approaches this same problem quite differently. In this case what we're loocking for ir the particle's **wave function**, $\Psi(x,t)$, and we get it by solving the **Schrodinger equaation**:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$
 (1.1) Schrodinger equation

This equation plays a role logically analogous to Newton's second law: Given suitable initial conditions (typically, $\Psi(x,0)$), the Schrodignes equation determines $\Psi(x,t)$ for all future time, just as, in classical mechanics, Newton's law determines x(t) for all future time.

1.2 The Statistical Interpretation

What exactly is this "wave function"? Born's **statistical interpretation** of the wave function, says that $|\Psi(x,t)|^2$ gives the **probability** of finding the particle at point x, at time t, or more precisely

$$\int_a^b |\Psi(x,t)|^2 \mathrm{d}x = \text{probability of finding the particle between } a \text{ and } b \text{, at time } b$$
 (1.2) Statistical interpretation

¹Magnetic forces are an exception, but let's not worry about them just yet. By the eay, we shall assume for the moment that the motion is nonrelativistic ($v \ll c$)

Probability is the *area* inder the graph of $|\Psi(x,t)|^2$

Yhe statistical interpretation introduces a kind of **indeterminacy** into quantum mechanics, for even if you know evertything the theory has to tell you about the particle /to wit: its wave function, still you cannot predict with certainty the outcome of a simple experiment to measure its position— all quantum mechanics has to offer is *statistical* information about the *possible* results.

We say that the wave function **collapses**, upon measurement, to spike some point. There are, then, two entirely distinct kinds of physical processes: "ordinary" oenes, in which the wave function evolves in a leisurely fashion inder the Schrodinger equation, and "measurements", in which Ψ suddenly and discontinuously collapses 2 .

1.3 Probability

I will give some definitions. The total number is

$$N = \sum_{i=0}^{\infty} N(j) \tag{1.3}$$

The probability of getting j is

$$P(j) = \frac{N(j)}{N} \tag{1.4}$$

In particular, the sum of all the probabilities is 1:

$$\sum_{j=0}^{\infty} P(j) = 0 \tag{1.5}$$

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

$$< f(j) >= \sum_{j=0}^{\infty} f(j) P(j) \tag{1.6} \label{eq:1.6}$$
 Average value of a function

In quantum mechanics the average is usually the quantity of interest; in that context it has come to be called the **expectation value**.

Now we need a numerial measure of the amount of "spread" in a distribution, with respect to the aveerge. The most obvious way to do this would be to find out how far each individual deviates from de average,

$$\Delta j = j - \langle j \rangle \tag{1.7}$$

and compute the average of Δj . Trouble is, of course, that you get zero, by the nature of the avergae, Δj is as often negative as positive. To avoid this irritating problem you might decide

²The role of measurement in quantum mechanics is so critical and so bizarre that you may well be wondering what precisely constitutes a measurement. Does it have to do with the interaction between a miscroscopic (quantum) system and a mecorscopic (classical) measuring apparatus (as Bohr insisted), or is it intervention of a conscious "oberver" (as Wigner proposed)? For the moment let's take the naive view: A measurement is the kind of thing that a scientist does in the laboratory, with rules, stopwatches, and so on

to average de *absolute value* of Δj . But absolute values are nasty to work with; instead, we get around the sign problem by *squaring* before averaging:

$$\sigma^2 \equiv <(\Delta j)^2>$$
 (1.8) Variance

This quantity is known as the **variance** of the distribution; σ itsel is called the **standard deviation**.

There is a useful little theorem pn variances:

$$\sigma = \sqrt{\langle j^2 \rangle - \langle j \rangle^2} \tag{1.9}$$

1.4 Continous Variables

I hace assumed that we are dealing with a *discrete* variable—that is, one that can take on only isolated values. But it is simple enough to generalize to *continous* distributions. If the interval is sufficiently short, this probability is *proportional to the length of the interval*. This

probability that an individual lies between
$$x$$
 and $(x + dx) = \rho(x)dx$ (1.10)

Probabilty density

The proportionality factor $\rho(x)$, is often loosely called "the probability of gettinf x", but is sloopy lanuage; a better term is **probability density**. The probability that x lies between a and b (a finite interval) is given by the integral of $\rho(x)$:

$$P_{ab} = \int_{a}^{b} \rho(x) \mathrm{d}x \tag{1.11}$$

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

$$1 = \int_{-\infty}^{+\infty} \rho(x) \mathrm{d}x \tag{1.12}$$

$$\langle x \rangle = \int_{-\infty}^{+\infty} x \rho(x) dx$$
 (1.13)

$$\langle f(x) \rangle = \int_{-\infty}^{+\infty} f(x)\rho(x)\mathrm{d}x$$
 (1.14)

$$\sigma^2 \equiv <(\Delta x)^2> = < x^2> - < x>^2 \tag{1.15}$$

1.5 Normalization

We return now to the statistical interpretation of the wave function (1.2), which says that $|\Psi(x,t)|^2$ is the probability density for finding the particle at point x, at time t. It follows (1.5) that the integral of $|\Psi|^2$ must be 1 (the particle's got to be *somewhere*):

$$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 \mathrm{d}x = 1$$
 (1.16)

If $\Psi(x,t)$ is a solution of the Schrodinger equation , so too is $A\Psi(x,t)$, where A is any (complex) constant. What we must do, then, is pick this undetermined multiplicative factor so as to ensure that (1.16) is satisfied. This process is called **normalizing** the wave function. For some solutions to the Schrodinger equation the integral is *infinite*; in that case *no* multiplicative factor is going to make it 1. The same goes for the trivial solution $\Psi=0$. Shuch **non-normalizable** solutions cannot represent particles, and must be rejected. Physically realizable states correspond to the **square-integrable** solutions to Schrodinger equation.³

Fortunately, the Schrodinger equation has the remarkable property that it automatically preserves the normalization of the wave function.

1.6 Momentum

For a particle in state Ψ , the expectation value of x is

$$< x >= \int_{-\infty}^{+\infty} x |\Psi(x,t)|^2 \mathrm{d}x$$
 (1.17) Expectation value of x

What exactly does this mean? It emphatically does not meand that if you measure the position of one particle over and over, $\int x |\Psi 1^2 \mathrm{d}x$ is the average of the results you'll get. Rather, < x > is the average of measurements, performes on particles all in the satate Ψ , which means that either you must find some way to returning the particle to its original state after each measurement, or else you have to prepare a whole **ensamble** of particles, each in the same state Ψ , and measure the positions of all of them: < x > is the average of these results.

Now, as time goes on, < x > will cahnge (because of the time dependence of Ψ), ando we might be interested in knowing how fast ir moves. We see that

$$\frac{\mathrm{d} < x >}{\mathrm{d}t} = -\frac{i\hbar}{m} \int \Psi^* \frac{\partial \Psi}{\partial x} \mathrm{d}x \tag{1.18}$$

The expectations value of the velocity is equal to the time derivative of the expectation value of position:

$$\langle v \rangle = \frac{\mathrm{d} \langle x \rangle}{\mathrm{d}t} \tag{1.19}$$

(1.18) tell us, then, how to calculate $\langle v \rangle$ directly from Ψ .

Acually, it is customary to work with **momentum** (p = mv), rather than velocity:

$$= m \frac{\mathrm{d} < x >}{\mathrm{d}t} = -i\hbar \int \left(\Psi^* \frac{\partial \Psi}{\partial x} \right) \mathrm{d}x$$
 (1.20) Momentum

Let me write the expressions for < x > and in a more siggestive way:

$$\langle x \rangle = \int \Psi^*(x) \Psi \mathrm{d}x$$
 (1.21)

$$\langle p \rangle = \int \Psi^* \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right) \Psi dx$$
 (1.22)

³Evidently $\Psi(x,t)$ must go to zero faster than $1/\sqrt{|x|}$, as $|x|\to\infty$. Incidentally, normalization only fixed the *modulus* of A: the phase remains undetermiend. However, as we shall, the latter carries no physical significance anyway.

We say that the **operator** x "represents" position, and the operator $(\hbar/i)(\partial/\partial x)$ "represents" momentum, in quantum mechanics; to calculate expectation values we "sandwich" the appropriate operator between Ψ^* and Ψ , and integrate.

What about other quantities? The fact is, all classical dynamics variables can be expressed in terms of position and momentum.

To calculate the expectation value of any such quantity, Q(x,p), we simply replace every p by $(\hbar/i)(\partial/\partial x)$, insert the resulting operator between Ψ^* and Ψ , and integrate:

$$< Q(x,p) > = \int \Psi^* Q\left(x, \frac{\hbar}{i} \frac{\partial}{\partial x}\right) \Psi dx$$
 (1.23)

1.7 The Uncertaintly Principle

Teh wavelenght of Ψ is related to the *momentum* of the particle by the **de Broglie formula**:

$$p = \frac{\hbar}{\lambda} = \frac{2\pi\hbar}{\lambda} \tag{1.24}$$
 deBroglie formula

Thus a spread in *wavelength* corresponds to a spread in *momentum*, and our general observation now says that the more precisely determined a particle's position is, the ñedd precisely is its momentum. Quantitatively.

$$\sigma_x \sigma_p \geq rac{\hbar}{2}$$
 (1.25) Uncertanty principle

where σ_x es the standard deviation in x, and σ_p is the standard deviation in p.

Please understand what the uncertainty principle means: Like position measurements, momentum measurements yiled precise answers—the "spread" here refers to the fact that measurements on identically prepared systems do not yiled identical results. You can, if you want, construct a state such the repeated position measurements will be vey close together (bu making Ψ a localized "spike"), but you sill pay a price: Momentum measurements on this state will be widely scattered. Oer you can prepare a state with a reproducible momentum (by making Ψ a long sinusoidal wave), but in that case, position measurements will de widely scattered.

Chapter 2

Time-Independent Schrodinger Equation

2.1 Stationary States

Wa talked a lot about the wave function, and how you use it to calculare various quantities of interest. But, how do get $\Psi(x,t)$ in the first place? We need to solce the Schrodinger equation,

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi \tag{2.1}$$

for a specified potential V(x,t). In this chapter (and most of this book) I shall assume that V(x,t) is independent of t. In that case the Schrödinger equation can be solved by the method of separation of variables: We look for solutions that are simple products,

$$\Psi(x,t) = \psi(x)\varphi(t) \tag{2.2}$$

where ψ is a function of x alone, and φ is a function of t alone.

For separable solutions we have

$$\frac{\partial \Psi}{\partial t} = \psi \frac{\mathrm{d}\varphi}{\mathrm{d}t}, \qquad \frac{\partial^2 \Psi}{\partial x^2} = \frac{\mathrm{d}^2 \psi}{\mathrm{d}x^2} \varphi$$

(ordinaty derivatives, now), and Schrodinger equation reads

$$i\hbar \frac{\mathrm{d}\varphi}{\mathrm{d}t} = -\frac{\hbar^2}{2m} \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} \varphi + V\psi\varphi \tag{2.3}$$

Or, dividing through by $\psi\varphi$:

$$i\hbar \frac{1}{\varphi} \frac{\mathrm{d}\varphi}{\mathrm{d}t} = -\frac{\hbar^2}{2m} \frac{1}{\psi} \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V \tag{2.4}$$

Now, the left side is a function of t alone, and the right side is a function of x alone². The only way this can possibly be true is if both sides are in fact *constant* – otherwise, by varying

 $^{^{1}}$ It is tiresome to keep saying "potential energy function", so most people jus call V the "potential", even though this invites occasional confusion with electric potencial, which is actually potential energy per unit charge.

²Note that this would not be true if V were a function of t as well as x.

t, I could change the left side without touching the right side, and the two would no lonegr equal. For reasons that will appear in a moment, we shall call the separation constan E. Then

$$i\hbar \frac{1}{\varphi} \frac{\mathrm{d}\varphi}{\mathrm{d}t} = E$$

or

$$\frac{\mathrm{d}\varphi}{\mathrm{d}t} = -\frac{iE}{\hbar}\varphi$$

and

$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V = E$$
 (2.5)

or

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V\psi = E\psi$$
(2.6)

Timeindependent Schrodinger equation

Separation of variables hs turned a partial differential equation into two ordinary differential equations (2.1) and (2.6). The first, (2.1) is easy to solve (just multiply through by $\mathrm{d}t$ and integrate); the general solution is $C\exp(-iEt/\hbar)$, but we might as well absorb the constant C into ψ (since the quantity of interest is the product $\psi\varphi$). Then

$$\varphi(t) = e^{-iEt/\hbar} \tag{2.7}$$

The second equation (2.6) is called the *time-independent Schrodinger equation* we can go further with it until the potencial V(x) is specified.

The rest of thus chapter will be devoted to solving the time-independent Schrodinger equation, fot a variety of simple potentials. But before I get to that you have every right ask: What's so great about separable solutions? After all, most solutions so the (time dependent) Schrodinger equation do not take the form $\psi(x)\varphi(t)$. I offer three answers—two of them physical, and one mathematical:

1. They are **stationaty states**. Although the wave function itself,

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar} \tag{2.8}$$

does (obviously) depende on t, the probability density,

$$|\Psi(x,t)|^2 = \Psi^* \Psi = \psi^* e^{+iEt/\hbar} \psi e^{-iEt/\hbar} = |\psi(x)|^2$$
 (2.9)

does not—the time-dependence cancels out 3 . The same thing happens in calculate the expectation value of any dynamil variable; (1.23) reduces to

$$\langle Q(x,p) \rangle = \int \psi^* Q\left(x, \frac{\hbar}{i} \frac{\mathrm{d}}{\mathrm{d}x}\right) \psi \mathrm{d}x$$
 (2.10)

Every expectation value is constant in time; we might as well drop the factor $\varphi(t)$ altogether, and simply use ψ in place of Ψ . In particular, < x > is constant, and hence = 0 (See (1.20)). Nothing ever happens in a stationary state.

³For normalizable solutions, E must be real

2. They are states of *definite total energy*. In classical mechanics, the total energy (kinetic plus pontential) is called the **Hamiltonian**:

$$H(x,p) = \frac{p^2}{2m} + V(x)$$
 (2.11)

The corresponding Hamiltonian *operator*, obtained by the canonical substitution $p \to (\hbar/i)(\partial/\partial x)$, is therefore⁴

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \tag{2.12}$$

Thus the time-independent Schrodinger equation (2.6) can be written

$$\hat{H}\psi = E\psi \tag{2.13}$$

and the expectation value of the total energy is

$$\langle H \rangle = \int \psi^* \hat{H} \psi dx = E \int |\psi|^2 dx = E \int |\Psi|^2 dx = E$$
 (2.14)

(Notice that the normalization of Ψ entails the normalization of ψ .) Moreover,

$$\hat{H}^2 \psi = \hat{H}(\hat{H}\psi) = \hat{H}(E\psi) = E(\hat{H}\psi) = E^2 \psi$$

and hence

$$< H^2 > = \int \psi^* \hat{H}^2 \psi dx = E^2 \int |\psi|^2 dx = E^2$$

So the variance of H is

$$\sigma_H^2 = \langle H^2 \rangle - \langle H \rangle^2 = E^2 - E^2 = 0 \tag{2.15}$$

But remember, if $\sigma=0$, then every member of the sample must share the same value (the distribution has zero spread). Conclusion: A separable solution has the property that every measurement of the total energy is certain to return the value E.

3. The general solution is a **linear combiantion** of separable solutions. As we're about to discover, the time-independent Schrodinger equation (2.6) yields an infinite collection of solution $(\psi_1(x), \psi_2(x), ...)$, each with its assocaites value of the reparation constant $(E_1, E_2, ...)$; thus there is a different wave function for each **allowed energy**:

$$\Psi_1(x,t) = \psi_1(x)e^{-iE_1t/\hbar}, \qquad \Psi_2(x,t) = \psi_2(x)e^{-iE_2t/\hbar}, \dots$$

Now the time-dependent Schrodinger equation (2.1) has the property that any linear combination⁵ of solutions is itself a solution. Once we have found the separable solutions, then, we can immediately construct a much more general solution, on the form

$$f(z) = c_1 f_1(z) + c_2 f_2(z) + \cdots$$

where $c_1, c_2, ...$ are any (complex) constants.

⁴Whenever confusion might arise. I'll put a "hat" on the operator, to distinguish it from the dynamical variable it represents.

⁵A linear combination of the functions $f_1(z), f_2(z), ...$ is an expression of the form

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}$$
(2.16)

It so happens that *every* solution to the (time-dependent) Schrodinger equation can be written iun this form -it is simply a matter if finding the tight constants $(c_1, c_2, ...)$ so as to fit the initial conditions for the problem at hand.

Let me recapitulate, from a somewhat different persperctive. Here's the generic problem: You're given a (time-independent) potencial V(x) and the starting wave function $\Psi(x,0)$; your job is to find the wave function, $\Psi(x,t)$, for any subsequent time t. To do this you must solve the (time-dependent) Schrodinger equation (2.1); this yields, in general, an infinite set of solutions $(\psi_1(x),\psi_2(x),...)$, each with its own assocaited energy $(E_1,E_2,...)$. To fit $\Psi(x,0)$ you write down the general linear combination of these solutions:

$$\Psi(x,0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$
(2.17)

the miraacle os that you can always match the specified initial state by appropriate choice of the constants c_1, c_2, \ldots To construct $\Psi(x, t)$ you simply tack onto each term its characteristic time dependence, $\exp(-iE_n t/\hbar)$:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar} = \sum_{n=1}^{\infty} c_n \Psi_n(x,t)$$
(2.18)

The separable solutions themselves,

$$\Psi_n(x,t) = \psi_n(x)e^{-iE_nt/\hbar} \tag{2.19}$$

are stationary states, in the sense that all probabilities and expectation values are independent of time, but this property is emphatically *not* shared by the general solution (2.18); the enrgies are different, for different stationary states, and the exponentials do not cancel, when you calculate $|\Psi|^2$.

2.2 The Infinite Square Well



Figure 2.1: The infinte square well potential (2.20)

Suppose

$$V(x) = \begin{cases} 0 & , 0 \le x \le a \\ \infty & , \text{otherwise} \end{cases}$$
 (2.20)

Fig. (2.1). A particle in this potential is completely free, except at two ends (x = 0 and x = a), where an infinte force prevents it from escaping.

Outside the well, $\psi(x)=0$ (the probability of findig the particle there is zero) Inside the well, where V=0, the time-independent Schrodinger equation (2.6) reads

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi\tag{2.21}$$

or

$$\frac{\mathrm{d}^2 \psi}{\mathrm{d}x^2} = -k^2 \psi, \qquad \text{where } k \equiv \frac{\sqrt{2mE}}{\hbar}$$
 (2.22)

(By writinf it in this way, I have tacitly assumed that $E \ge 0$.) Equation (2.22) is the classical **simple harmonic oscilaltor** equation; the general solution is

$$\psi(x) = A\sin kx + B\cos kx \tag{2.23}$$

where A and B are arbitraty constants. Tipically, these constants are fixed by the **boundary conditions** of the problem. What are the appropiate boundary conditions for $\psi(x)$? Ordinatily, both ψ and $\mathrm{d}\psi/\mathrm{d}x$ are continuous, but where the potential goes to infinity only the first of these applies.

Continuity of $\psi(x)$ requieres that

$$\psi(0) = \psi(a) = 0 \tag{2.24}$$

so as to join onto the solution outisde the well. What does this tell us about A and B? Well,

$$\psi(0) = A\sin 0 + B\cos 0 = B$$

so B=0, and hence

$$\psi(x) = A\sin kx \tag{2.25}$$

Then $\psi(a)=A\sin ka$, so either A=0 (in which case we're left with the trivial –non-normalizable–solution $\psi(x)=0$), or else $\sin ka=0$, which means that

$$ka = 0, \pm \pi, \pm 2\pi, \pm 3\pi, \dots$$
 (2.26)

But k=0 is no good (again, that would imply $\psi(x)=0$), and the negative solutions give nothing new, since $\sin(-\theta)=-\sin(\theta)$ andw e can absorb the minus sign into A. So the distinct solutions are

$$k_n = \frac{n\pi}{a}, \quad \text{with } n = 1, 2, 3, \dots$$
 (2.27)

Curiously, the boundary condition at x=a does not determine the constant A, but rather the constant k, and hence the possible values of E:

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$
 (2.28) Possible values of E

In radical contrast to the classical case, a quantum particle in the infinite square well cannot have just any old energy—it has be one of these special **allowed** values⁶. To find A we normalize ψ :

$$\int_{a}^{a} |A|^{2} \sin^{2}(kx) dx = |A|^{2} \frac{a}{2} = 1, \quad \text{so } |A|^{2} = \frac{2}{a}$$

This only determines the agnitude if A, but it is simples to pick the positive real root: $A = \sqrt{2/a}$ (the phase of A carries no physical significance anyway). Inside the well, the solutions are

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \tag{2.29}$$

As a collection, the functions $\psi_n(x)$ have some interesting and important properties:

- 1. They are alternately **even** and **odd**, with respecto to the center of the well: ψ_1 is even, ψ_2 is odd, ψ_3 is even, and so on.
- 2. As you go up in energy, each successive state has one more **node** (zero-crossing): ψ_1 has one (the end points don't count), ψ_4 has one, ψ_3 has two, and so on.
- 3. They are mutually orthogonal, in the sense that

$$\int \psi_m(x)^* \psi_n(x) \mathrm{d}x = 0 \tag{2.30}$$

whenever $m \neq n$ We can combine orthogonality and normalization into a single satatement⁷:

$$\left| \int \psi_m(x)^* \psi_n(x) dx = \delta_{mn} \right| \tag{2.31}$$

We say that the ψ 's are **orthonormal**.

4. They are **complete**, in the sense that any other function, f(x), can be expressed as a linear combination of them:

$$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi}{a}x\right)$$
 (2.32)

(2.32) is nothing but the **Fourier series** for f(x), and the fact that any function can be expanded in this way is sometimes called **Dirichlet's theorem** The coefficients c_n can be evaluated—for a given f(x)—by a method I call **Fourier's trick**, which beautifully exploits the orthonormality of $\{\psi_n\}$: Multiply both sides of (2.32) by $\psi_m(x)^*$, and integrate

$$\psi_m(x)^* f(x) dx = \sum_{n=1}^{\infty} c_n \int \psi_m(x)^* \psi_n(x) dx = \sum_{n=1}^{\infty} c_n \delta_{nm} = c_n$$
 (2.33)

⁶Notice that the quantization of energy emerged as a rather technical consequence of the boudnary conditions on solutions to the time-independent Schrodinger equation

⁷In this case the ψ 's are real, so the * on ψ_m is unnecessary, but for future purposes it's a good idea to get the habir of putting it there.

Thus the *n*th coefficient in the expansion of f(x) is

$$c_n = \int \psi_n(x)^* f(x) dx$$
(2.34)

Completeness holds for all the potentials you are likely to encounter, but the proofs tens to be nasty and laborious.

The stationary states (2.19) of the infinite square well are evidently

$$\Psi_n(x,t) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-i(n^2\pi^2\hbar/2ma^2)t}$$
 (2.35)

I claimed (2.18) that the most general solution to the (time-dependent) Schrodinger equation is a linear combinations of stationary states:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-i(n^2\pi^2\hbar/2ma^2)t}$$
(2.36)

It remais only for me to demosntrate that I can fit any prescribed initial wave function, $\Psi(x,0)$, by appropriate choice of the coefficients c_n :

$$\Psi(x,0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

The completeness of the ψ 's guarantees that I can always express $\Psi(x,0)$ in this way, and their orthonormality licenses the use of Fourier's trick to determine the actual coefficients:

$$c_n = \sqrt{\frac{2}{a}} \int_a^a \sin\left(\frac{n\pi}{a}x\right) \Psi(x,0) dx$$
 (2.37)

That does it: Given the initial wave function, $\Psi(x,0)$, we first compute the expansion coefficients c_n using (2.37), and the plug these into (2.36) to obtain $\Psi(x,t)$.

Loosely speaking, c_n tells you the "amount of ψ_n that is contained in Ψ ". Some people like to say that $|c_n|^2$ is the "probability of finding the particle in the nth stationary state", but this is a bad language; the particle is in the state Ψ , not Ψ_n , and, anuhow, in the laboratory you don't "find a particle to be in a particular state" —you measure some observable, and what you get is a number. As we'll see next, what $|c_n|^2$ tells you is the probability that a measurement of the energy would yield the value E_n (a competent measurement will always return one og the "allowed" values—hebce the name—and $|c_n|^2$ is the probability of getting the particular value E_n).

Of course, the sum of these probabilities shoul be 1,

$$\sum_{n=1}^{\infty} |c_n|^2 = 1 \tag{2.38}$$

Indeed, this follows follows from the normalization of Ψ .

Moreover, the expectation value of the energy must be

$$< H> = \sum_{n=1}^{\infty} |c_n|^2 E_n$$
 (2.39) Expectation value of the energy

Notice that the probability of getting a particular energy is independent of time, and so, a fortiori, is the expectation value of H. This is a manifestation of **conservatio of energy** in quantum mechanics.

2.3 The Harmonic Oscillator

The paradigm for a classical harmonic oscillator is a mass m attached to a spring of force constant k. The motion is governed by **Hooke's law**,

$$F = -kx = m\frac{\mathrm{d}^2x}{\mathrm{d}t^2}$$

(ignoring friction), and the solution is

$$x(t) = A\sin(\omega t) + B\cos(\omega t)$$

where

$$\omega \equiv \sqrt{\frac{k}{m}} \tag{2.40}$$

is the (angular) frequency of the oscillation. The potential energy is

$$V(x) = \frac{1}{2}kx^2 (2.41)$$

its graph is a parabola.

Virtually any oscillatory motion is approximately simple harmonic, as long as the aplitude is small.

The quantum problem is to solve the Schrodinger equation for the potential

$$V(x) = \frac{1}{2}m\omega^2 x^2 \tag{2.42}$$

(it it customary to eliminate the spring constant in favor of the classical frequency, using (2.40)). As we have seen, it suffices to solve the time-independent Schrodinger equation:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2x}{\mathrm{d}t^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi$$
 (2.43)

In the literature you will find two entirely different approaches to this problem. The first is a straightforward "brute force" solution to the differential equation, usin the **power series method**; it has the virtue that the same strategy can be applied to many other potentials. The second is a diabolically clever algebraic technique, using so-called **ladder operator**. We'll se the algebraic methos first, because it is quicker and simpler (and a lot more fun)⁸.

⁸We'll encounter some of the same strategies in the theory og angular momentum, and the technique generalizes to a broad class of potentials in **super-symmetric quantum mechanics**

2.3.1 Algebraic Method

To begin with, let's rewrite (2.43) in a more suggestive form:

$$\frac{1}{2m}[p^2 + (m\omega x)^2]\psi = E\psi$$
 (2.44)

where $p \equiv (\hbar/i) d/dx$ is, of course, the momentum operator. The basic idea is to *factor* the Hamiltonian,

$$H = \frac{1}{2m} [p^2 + (m\omega x)^2]$$
 (2.45)

If these were *numbers*, it would be easy:

$$u^{2} + v^{2} = (iu + v)(-iu + v)$$

Here, however, it's not quite so simple, because p and x are *operators*, and operators do not, in general, **commute** (xp is not de same as px). Still, this does motivate us to examine the quantities

$$a_{\pm} \equiv \frac{1}{\sqrt{2\hbar m\omega}} (\mp ip + m\omega x)$$
 (2.46)

(the factor in front is just there to make the final result look nicer).

Well, what is the product a_-a_+ ?

$$a_{-}a_{+} = \frac{1}{2\hbar m\omega}(ip + m\omega x)(-ip + m\omega x)$$
$$= \frac{1}{2\hbar m\omega}[p^{2} + (m\omega x)^{2} - im\omega(xp - px)]$$

As anticipated, there's an extra term, involving (xp-px). We call this the **commutator** of x and p; it is a measure of how badly the *fail* to commute. In general the commutator of operators A and B (written with brackets) is

$$[A, B] \equiv AB - BA \tag{2.47}$$

In this notation,

$$a_{-}a_{+} = \frac{1}{2\hbar m\omega} [p^{2} + (m\omega x)^{2}] - \frac{i}{2\hbar} [x, p]$$
 (2.48)

We need to figure out the commutator of x and p. Warning: Operators are notoriously slippery to work with in the abstract, and you are bound to make mistakes unless you give them a "test function", f(x), to act on. At the end you can throw away the test function, and you'll be left with an equation involving the operators alone. In the present case we have:

$$[x,p]f(x) = \left[x\frac{\hbar}{i}\frac{\mathrm{d}f}{\mathrm{d}x} - \frac{\hbar}{i}\frac{\mathrm{d}xf}{\mathrm{d}x}\right] = \frac{\hbar}{i}\left(x\frac{\mathrm{d}f}{\mathrm{d}x} - x\frac{\mathrm{d}f}{\mathrm{d}x} - x\right) = i\hbar f(x) \tag{2.49}$$

Dropping the test function, which has served its purpose,

This lovely and obiquitous result is known as the **cannonical commutation relation**⁹. With this, (2.48) becomes

$$a_{-}a_{+} = \frac{1}{\hbar\omega}H + \frac{1}{2} \tag{2.51}$$

or

$$H = \hbar\omega \left(a_- a_+ - \frac{1}{2} \right) \tag{2.52}$$

Evidently the Hamiltonian does not factor perfectly—there's that extra -1/2 on the right. Notice that the orderinf of a_+ and a_- is important here; the same argument, with a_+ on the left, yields

$$a_{+}a_{-} = \frac{1}{\hbar\omega}H - \frac{1}{2} \tag{2.53}$$

In particular,

$$[a_{-}, a_{+}] = 1 (2.54)$$

So the Hamiltonian can equally well be written

$$H = \hbar\omega \left(a_+ a_- + \frac{1}{2} \right) \tag{2.55}$$

In terms of a_{\pm} , then, the Schrodinger equation ¹⁰ for the harmonic oscillator takes the form

$$\hbar\omega \left(a_{\pm}a_{\mp} \pm \frac{1}{2}\right)\psi = E\psi \tag{2.56}$$

(in equations like this you rrad the upper signs all the way across, or else the lower signs).

Now, here comes the crucial step: I claim that if ψ satisfies the Schrodinger equations with enrgy E, (that is: $H\psi=E\psi$), then $a_+\psi$ satisfies the Schrodinger equations with energy $(E+\hbar\omega):H(a_+\psi)=(E+\hbar\omega)(A_+\psi)$

By the same token, $a_-\psi$ is a solution with energy $(E-\hbar\omega)$

$$H(a_+\psi) = (E + \hbar\omega)(a_+\psi H(a_-\psi)) \qquad = (E - \hbar\omega)(a_-\psi)$$

Here, then is a wonderful machine for generating new solution, with higer and lower energies—if we could just find *one* solution, to ger started! We call a_{\pm} ladder operators, because they allow us to climb up and doen in energy; A_{+} is the raising operator, and a_{-} the lowering operator.

But wait! What if I apply the lowering operator repeatedly? Eventually I'm going to reach a state with energy less than zero, which does not exist! At some point the machine must fail. How can that happen? We know that $a_-\psi$ is a new solution to the Schrodinger equation, but there is no guarantee that it will be normalizable—it might be zero, or its square-integral might be infinite. In practice it is the forme: There occurs a "lowest rung" (call it ψ_0) such that

$$a_{-}\psi_{0} = 0 \tag{2.57}$$

⁹In deep sense all of the mysteries of quantum mechanics can be traced to the fact that position and momentum do not commute. Indeed, some authors take the cannoncial commutation relation as an *axiom* of the theory, and use ir to *derive* $p = (\hbar/i) d/dx$

¹⁰I'm getting tired of writing "time-independent Schrodinger equation", so when it's clear from the context which one I mena, I'll just call it the "S equation".

We can use this to determine $\psi_0(x)$:

$$\frac{1}{\sqrt{2\hbar m\omega}} \left(\hbar \frac{\mathrm{d}}{\mathrm{d}x} + m\omega x \right) \psi_0 = 0$$

or

$$\frac{\mathrm{d}\psi_0}{\mathrm{d}x} = -\frac{m\omega}{\hbar}x\psi_0$$

The differential equation is easy to solve:

$$\int \frac{\mathrm{d}\psi_0}{\psi_0} = -\frac{m\omega}{\hbar} \int x \mathrm{d}x \quad \Rightarrow \quad \ln \psi_0 = -\frac{m\omega}{2\hbar} x^2 + \text{ constant}$$

SO

$$\psi_0(x) = Ae^{-\frac{m\omega}{2\hbar}x^2}$$

We might as well normalize it right away:

$$=|A|^2 \int_{-\infty}^{\infty} e^{-m\omega x^2/\hbar} dx = |A1|^2 \sqrt{\frac{\pi\hbar}{m\omega}}$$

so $A^2 = \sqrt{m\omega/\pi\hbar}$, and hence

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$
 (2.58)

To determine the energy of this satte we plug it into the Schrodinger equation (in the form of (2.56)), $\hbar\omega(a_+a_-+1/2)\psi_0=E_0\psi_0$. and exploit the fact that $a_-\psi_0=0$:

$$E_0 = \frac{1}{2}\hbar\omega \tag{2.59}$$

With our foot now securely planted on the bottom rung (the ground state of the quantum oscillator), we simply apply the raising operator (repeatedly) to generate the excited states, increasing the energy by $\hbar\omega$ with each step:

$$\psi_n(x) = A_n(a_+)^n \psi_0(x), \quad \text{with } E_n = \left(n + \frac{1}{2}\right) \hbar \omega$$
 (2.60)

where A_n is the normalization constant. By applying the raising operator (repeatedly) to ψ_0 , then, we can (in principle) construct all the stationary states of the harmonic oscillator. Meanwhile, without ever doing that explicitly, we have determined the allowed energies.

You can even get the normalization algebraically, but it takes some fancy foorwork, wo watch closely. we know that $a_{\pm}\psi_n$ is proportional to $\psi_{m\pm1}$,

$$a_{+}\psi_{n} = c_{n}\psi_{n+1}, \qquad a_{-}\psi_{n} = d_{n}\psi_{n-1}$$
 (2.61)

but what are the proportionality factors, c_n and d_n ? First note that for "any" functions f(x) and g(x),

$$\int_{-\infty}^{\infty} f^*(a_{\pm}g) dx = \int_{-\infty}^{\infty} (a_{\mp}f)^* g dx$$
 (2.62)

(In the language of linear algebra, a_{\pm} is the **hermitian conjuagte** of A_{\pm}). In particular,

$$\int_{-\infty}^{\infty} (a_{\pm}\psi_n)^* (a_{\pm}\psi_n) dx = \int_{-\infty}^{\infty} (a_{\mp}a \pm \psi_n)^* \psi_n dx$$

But (invoking (2.56) and (2.60))

$$a_{+}a_{-}\psi_{n} = n\psi_{n}, \qquad a_{-}a_{+}\psi_{n} = (n+1)\psi_{n}$$
 (2.63)

SO

$$\int_{-\infty}^{\infty} (a_{+}\psi_{n})^{*}(a_{+}\psi_{n}) dx = |c_{n}|^{2} \int_{-\infty}^{\infty} |\psi_{n+1}|^{2} dx = (n+1) \int_{-\infty}^{\infty} |\psi_{n}|^{2} dx$$
$$\int_{-\infty}^{\infty} (a_{-}\psi_{n})^{*}(a_{-}\psi_{n}) dx = |d_{n}|^{2} \int_{-\infty}^{\infty} |\psi_{n-1}|^{2} dx = n \int_{-\infty}^{\infty} |\psi_{n}|^{2} dx$$

But since ψ_n and $\psi_{n\pm 1}$ are normalized, it follows that $|c_n|^2=n+1$ and $|d_n|^2=n$ and hence.

$$a_{+}\psi_{n}\sqrt{n+1}\psi_{n+1}, \qquad a_{-}\psi_{n} = \sqrt{n}\psi_{n-1}$$
 (2.64)

Thus

$$\psi_1 = a_+ \psi_0, \qquad \psi_2 = \frac{1}{\sqrt{2}} a_+ \psi_1 = \frac{1}{\sqrt{2}} (a_+)^2 \psi_2$$

$$\psi_3 = \frac{1}{\sqrt{3}} a_+ \psi_2 = \frac{1}{\sqrt{3 \cdot 2}} (a_+)^3 \psi_0, \qquad \psi_4 = \frac{1}{\sqrt{4}} a_+ \psi_3 = \frac{1}{\sqrt{4 \cdot 3 \cdot 2}} (a_+)^4 \psi_0$$

and so on .Clearly

$$\boxed{\psi_n = \frac{1}{\sqrt{n!}} (a_+)^n \psi_o} \tag{2.65}$$

which is to say that the normalization factor in (2.60) is $A_n = 1/\sqrt{n!}$.

As in the case of the infinite square well, the stationary states if the harmonic oscillator are orthogonal:

$$\int_{-\infty}^{\infty} \psi_m^* \psi_n \mathrm{d}x = \delta_{mn} \tag{2.66}$$

This can be proved usign (2.63) and (2.62) twice—first moving a_+ and then moving a_- :

$$\int_{-\infty}^{\infty} \psi_m^*(a_+ a_-) \psi_n dx = n \int_{-\infty}^{\infty} \psi_m^* \psi_n dx$$

$$= \int_{-\infty}^{\infty} (a_- \psi_m)^* (a_- \psi_n) dx = \int_{-\infty}^{\infty} (a_- a_- \psi_m)^* \psi_n dx$$

$$= m \int_{-\infty}^{\infty} \psi_m^* \psi_n dx$$

Unless m=n, then, $\int \psi_m^* \psi_n \mathrm{d}x$ must be zero. Orthonomality means that we can again use Forier's trcik (2.34) to evaluate the coefficients, when we expand $\Psi(x,0)$ as a linear combination of stationary states (2.17), and $|c_n|^2$ is again the probability that a measurement of energy would yield the vakue E_n .

2.3.2 Analytic Method

We return now to the Schrodinger equation for the harmonic oscillator,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi = E\psi$$
 (2.67)

and solve it directly, by the series method. Thing loock a little cleanes if we introduce the dimensionless variable

$$\xi \equiv \sqrt{\frac{m\omega}{\hbar}}x\tag{2.68}$$

in terms of ξ the Schrodinger equation reads

$$\frac{\mathrm{d}^2 \psi}{\mathrm{d}\xi^2} = (\xi^2 - K)\psi \tag{2.69}$$

where K is the energy, in units of $(1/2)\hbar\omega$:

$$k \equiv \frac{2E}{\hbar\omega} \tag{2.70}$$

Our problem is to solve (2.69), and in the process obtain the "allowed" values of K (and hence of E).

To begin with, note that at very large ξ (which is to say, at very large x), ξ^2 completely dominates over the constant K, so in this regime

$$\frac{\mathrm{d}^2 \psi}{\mathrm{d}\xi^2} \approx \xi^2 \psi \tag{2.71}$$

which has the approximate solution

$$\psi(\xi) \approx Ae^{-\psi^2/2} + Be^{+\xi^2/2} \tag{2.72}$$

The B term is clearly not normalizable (it blows up as $|x| \to \infty$); the physically acceptable solutions, then, have the asymptoic form

$$\psi(\xi) \to ()e^{-\xi^2/2}, \qquad \text{at large } \xi \tag{2.73}$$

This suggests that we "peel off" the exponential part,

$$\psi(\xi) = h(\xi)e^{-\xi^2/2} \tag{2.74}$$

in hopes that what remains, $h(\xi)$, has a simplier functional form than $\psi(\xi)$ itself. Differentiating (2.74)

$$\frac{\mathrm{d}\psi}{\mathrm{d}\xi} = \left(\frac{\mathrm{d}h}{\mathrm{d}\xi} - \xi h\right) e^{-\xi^2/2}$$

and

$$\frac{\mathrm{d}^2 \psi}{\mathrm{d}\xi^2} = \left(\frac{\mathrm{d}^2 h}{\mathrm{d}\xi^2} - 2\xi \frac{\mathrm{d}h}{\mathrm{d}\xi} + (\xi^2 - 1)h\right) e^{-\xi^2/2}$$

so the Schrodinger equation (2.69) becomes

$$\frac{\mathrm{d}^2 h}{\mathrm{d}\xi^2} - 2\xi \frac{\mathrm{d}h}{\mathrm{d}\xi} + (K - 1)h = 0 \tag{2.75}$$

I propose to look fot solutions to (2.75) in the form of *power series* in ξ^{11} :

$$h(\xi) = a_0 + a_1 \xi + a_2 \xi^2 + \dots = \sum_{j=0}^{\infty} a_j \xi^j$$
 (2.76)

Differentiating the seris term by term,

$$\frac{\mathrm{d}h}{\mathrm{d}\xi} = a_1 + 2a_2\xi + 3a_3\xi^2 + \dots = \sum_{j=0}^{\infty} ja_j\xi^{j-1}$$

and

$$\frac{\mathrm{d}^2 h}{\mathrm{d}\xi^2} = 2a_2 + 2 \cdot 3a_3\xi + 3 \cdot 4a_4\xi^2 + \dots = \sum_{j=0}^{\infty} (j+1)(j+2)a_{j+2}\xi^j$$

Putting these into (2.75), we find

$$\sum_{j=0}^{\infty} [(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j]\xi^j = 0$$
(2.77)

It follows (from the uniqueness of power series expansions) that the coefficient of each power of ξ must vanish,

$$(j+1)(j+2)a_{j+1} - 2ja_j + (K-1)a_j = 0$$

and hence that

$$a_{j+2} = \frac{(2j+1-K)}{(j+1)(j+2)}a_j \tag{2.78}$$

This **recursion formula** is enterely equivalent to the Schrodinger equation. Starting with a_0 , it generates all the even-numbered coefficients

$$a_2 = \frac{(a-K)}{2}a_0$$
 $a_4 = \frac{(5-K)}{12}a_2 = \frac{(5-K)(1-K)}{24}a_0$, ...

and starting with a_2 , it generates the odd coefficients:

$$a_3 = \frac{(3-K)}{6}a_1$$
, $a_5 = \frac{(7-K)}{20}a_3 = \frac{(7-K)(3-K)}{120}a_1$, ...

We write the complete solution as

$$h(\xi) = h_{\mathsf{even}}(\xi) + h_{\mathsf{odd}}(\xi) \tag{2.79}$$

¹¹This is known as the **Frobenius method** for solving a differential equation. According yo Taylor's theorem, any reasonably well-behaven function can be expressed as a power series, so (2.76) ordinarily involver no loss of generality.

where

$$h_{\text{even}}(\xi) \equiv a_0 + a_2 \xi^2 + a_4 \xi^4 + \cdots$$

is an even fucntion of ξ , built on a_0 , and

$$h_{\text{odd}}(\xi) \equiv a_1 \xi + a_3 \xi^3 + a_5 \xi^5 + \cdots$$

is an odd function, built on a_1 (2.78) determines $h(\xi)$ in terms of two arbitrary constants (a_0 and a_1)—which is just what we would expect, for a second-order differentual equation.

However, not all the solutions so obtained are *normalizable*. Fot at very large j, the recursion formula becomes (approximayely)

$$a_{j+2} \approx \frac{2}{i} a_j$$

with the (approximate) solution

$$a_j \approx \frac{C}{(j/2)!}$$

for some constant C, and this yields (at large ξ , where the higher powers dominate)

$$h(\xi) \approx C \sum \frac{1}{(j/2)!} \xi^j \approx C \sum \frac{1}{j!} \xi^{2j} \approx C e^{\xi^2}$$

Now, if h goes like $\exp(\xi^2/2)$, then ψ (remember ψ ?—that's what we're trying to calculate) goes like $\exp(\xi^2/2)$ (2.74), which is precisely the asymtotic behavior we didn's want¹². There is only one way to wiggle out of this: For normalziable solutions the *power series must terminate*. There must occur some "highest" j (call it n), such that the recursion formula spits out $a_{a+2}=0$ (this woll truncate either series $h_{\rm even}$ or the series $h_{\rm odd}$; the other one must be zero from that start: $a_1=0$ if n is even, and $a_0=0$ if n is odd). For physically acceptable solutions, then, (2.78) requires that

$$K = 2_n + 1$$

for some non-neagtive integer n, which is to say (referring to (2.74)) that the energy must be

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad \text{for } n = 0, 1, 2, \dots$$
 (2.80)

Thus we recover, by a completely different method, the fundamental quantization condition we found algebraically in (2.60).

¹²It's no surprise that the ill-behaven solutions are still in (2.78):this recursion relation is equivalent to the Schrodinger equation, so it's got to include both the asymtotic forms we found in (2.72)

Chapter 3

Formalism

3.1 Hilbert Space

The purpose of this chapter is to recast the theory in a more powerful form.

Quantum theory is based on two constructs: wave functions and operators. The state of a system is represented by its wave function, obervables are represented by operators. Mathematically, weave functions satisfy the defining conditions for abstract **vectors**, and operators act on them as **linear transformations**. So the natural language of quantum mechanics is **linear algebra**.

But it is not, I suspect, a form of linear algebra with which you are immediately familiar. In an N-dimensional space it is simplest to represent a vector $|\alpha\rangle$, by the N-tuple of its components, $\{a_n\}$, with respect to a specified orthonormal basis:

$$|\alpha\rangle \to \boldsymbol{a} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix}$$
 (3.1)

The **inner product**, $\langle \alpha | \beta \rangle$, of two vectors (generalizing the dot product in three dimensions) is the complex number,

$$\langle \alpha | \beta \rangle = a_1^* b_1 + a_2^* b_2 + \dots + a_N^* b_N$$
 (3.2)

Linear transformations, T, are represented by **matrices** (with respect to the specified basis), which act on vectors (to produce new vectors) by the ordinary rules of matrix multiplication:

$$|\beta\rangle = T |\alpha\rangle \to \mathbf{b} = \mathbf{Ta} = \begin{pmatrix} t_{11} & t_{12} & \cdots & t_{1N} \\ t_{21} & t_{22} & \cdots & t_{2N} \\ \vdots & \vdots & \vdots & \vdots \\ t_{N1} & t_{N2} & \cdots & t_{NN} \end{pmatrix}$$
(3.3)

But the "vectors" we encounter in quantum mechanics are (for the most specified) functions, and they live in infinite-dimensional spaces. For them the N-tuple/matrix notation is awkward, at best, and manipulations that are well-behaved in the finite dimensional case can be problematic. (The underlying reason is that whereas the finite sum in (3.2) always exists, an

infinite sum—or a integral— may not converge, in which case the inner product does not exists, and any argument involving inner products is immediately suspect.).

The collection of all functions of x constitutes a vector space, but fot our purposes it is much too latge. To represent a possible physical state, the function Ψ must be normalized:

$$\int |\Psi|^2 \mathrm{d}x = 1$$

The set of all **square-integrable functions**, on a specified ineterval¹,

$$f(x)$$
 such that
$$\int_{a}^{b} |f(x)|^{2} dx < \infty$$
 (3.4)

constitutes a (much smaller) vector space. Mathematicians call it $L_2(a,b)$; physicist call it **Hilbert space**. In quantum mechanics then

We define the **inner product of two functions**, f(x) and g(x), as follows:

$$\langle f|g\rangle \equiv \int_{a}^{b} f(x)^{*}g(x)\mathrm{d}x$$
 (3.6)

If f and g are both square-integrable (that is, if they are both in hilber spaces), their inner product is guaranteed to exist. This follows from the integral **Schwartz inequality**:

$$\left| \int_{a}^{b} f(x)^{*} g(x) dx \right| \leq \sqrt{\int_{a}^{b} |f(x)|^{2} dx} \int_{a}^{b} |g(x)|^{2} dx$$
 (3.7)

Notice in particular that

$$\langle g|f\rangle = \langle f|g\rangle^* \tag{3.8}$$

Moreover, the inner product of f(x) with itself.

$$\langle f|f\rangle = \int_{a}^{b} |f(x)|^{3} \mathrm{d}x \tag{3.9}$$

is real and and non-negative; it's zero only when f(x) = 0.

A function is said to be **normalized** if its inner product with itself is 1; two functions are **orthogonal** of their inner product is 0; and a set of functions, $\{f_n\}$, is **orthonormal** of they are normalized and mutually orthogonal

$$\langle f_m | f_n \rangle = \delta_{mn} \tag{3.10}$$

Finally, a set of functions is **compelte** if any other function (in Hilbert space) can be expreded as a linear combination of them:

$$f(x) = \sum_{n=1}^{\infty} c_n f_n(x) \tag{3.11}$$

If rge functions $\{f_n(x)\}\$ are orthonormal, the coefficients are given by Fourier's trick

$$c_n = \langle f_n | f \rangle \tag{3.12}$$

¹Fot is, the limits (a and b) will almost always be $pm\infty$, but we might as well keep thing more general for the moment

3.2 Obervables

3.2.1 Hermitian Operators

The expectation value of an observable Q(x,p) can be expressed very neatly in inner-product notation:

$$\langle Q \rangle = \int \Psi^* \hat{Q} \Psi dx = \langle \Psi | \hat{Q} \Psi \rangle$$
 (3.13)

Now, the outcome of a measurement has got to be *real*, and so, a fortiori, is the average of many measurements:

$$\langle Q \rangle = \langle Q \rangle^* \tag{3.14}$$

But the complex conjugate of an inner product reverses the order (3.8), so

$$\left\langle \Psi \middle| \hat{Q}\Psi \right\rangle = \left\langle \hat{Q}\Psi \middle| \left| \Psi \right\rangle$$
 (3.15)

and this must hold true for any wave function Ψ . Thus operators representing *obervables* have the very special property that

$$\left\langle f\middle|\hat{Q}f\right\rangle = \left\langle \hat{Q}f\middle|f\right\rangle \qquad \text{for all } f(x)$$
 (3.16)

We call such operators **hermitian**.

The essentiak point is that a hermitian operator can be applied either to the first member of an inner product or to the second, with the same result, and hermitian operators naturally arise in quantum mechanics because their expectations values are real:

Is the momentum operator, for example, hermitian?

$$\langle f|\hat{p}g\rangle = \int_{-\infty}^{\infty} \frac{\hbar}{i} \frac{\mathrm{d}g}{\mathrm{d}x} \mathrm{d}x = \frac{\hbar}{i} f^* g \Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \left(\frac{\hbar}{i} \frac{\mathrm{d}f}{\mathrm{d}x}\right)^* g \mathrm{d}x = \langle \hat{p}f|g\rangle \tag{3.18}$$

Notice if f(x) and g(x) are squared integrable, they must go to zero at $\pm \infty$.

3.2.2 Determinate States

Ordinarily, when you measure an obervable Q on an ensamble of identically prepared system, all in the same state Ψ , you do not ger the same reuslt each time—this is the indeterminancy of quantum mechanics. Question: Would it be possible to prepare a state such that every measurement of Q is certain to return the same value (call it a)? This would be, if younlike, a determinate state, for the obervable Q (Actually, we already know one example: Stationary states are dterminate states of Hamiltonian; a measurement of the total enery, on a particle in the stationary state Ψ_n , is certain to yield the corresponding "allowed" energy E_n).

Well, the standard deviation of Q, in a determiante state, would to be zero, shich is to say,

$$\sigma^2 = \langle (\hat{Q} - \langle Q \rangle)^2 \rangle = \langle \Psi | (\hat{Q} - q)^2 \Psi \rangle = \langle (\hat{Q} - q) \Psi | (\hat{Q} - q) \Psi \rangle = 0$$
 (3.19)

But the only function whose inner product with itself vanishes is 0, so

$$\hat{Q}\Psi = q\Psi \tag{3.20}$$

This is the **eigenvalue equation** for the operator \hat{Q} ; Ψ is an **eigenfunction** of \hat{Q} , and q is the corresponding **eigenvalue**. Thus

Determiante states are eigenfunctions of
$$\hat{Q}$$
 (3.21)

Measurements of Q ajon such states is certain to yield the eigenvalue, q.

Note that the eigenvalue is a number (not a operator or a function). You can multuply any eigenfunction by a constant, and it is still an eigenfunction, with the same eigenvalue. Zero does not count as an eigenfunction. But there's nothing wrong with zero as an eigenvalue. The collection of all the eigenvalues of an operator is called its **specturm**. Sometimes two (or more) linearly independent eigenfunctions share the same eigenvalue; in that case the spectrum is said to be **degenerate**.

3.3 Eigenfunctions of a Hermitian Operator

Our attention is thus directed to the *eigenfunction of hermitian operators* (physically: determine states of obervables). These fall into two categories: If the spectrum is **discrete** (i.e., the eigenvalues are separated from one another) then the eigenfunctions lie in Hilbert space and they constitute physically realizable states. If the spectrum is **contonuous** (i.e., the eigenvalues fill out an entire range) then the eigenfunctions are non normalizable, and they do not represent possible wave functions (*though linear cominations* of them–involving neccessarily a spread in eigenvalues—may be normalizable). Some operator have a discrete spectrum only (for example, the Hamiltonian for the harmonic oscillator). some have only a continuous spectrum (for example, the free partivle Hamiltonian), and some have both discrete part and a continuous part (for example, the Hamiltonian for a finite square well). The discrete case is easier to handle. because the relevant inner product are guaranteed to exist—in fact, it is very similar to the finite-dimensional theory (the eigenvectors of a hermitian matrix). I'll treat the discrete case first, and then the continuous one:

3.3.1 Discrete Spectra

Mathematically, the normalizable eigenfunctions of a hermitian have two important properties:

Theorem 1 Their egigenvalues are real.

This is comforting: If you measure an obervable on a particle ina dterminate state, you will at least get a real number.

Theorem 2 Eigenfunctions belonging to distinct eigenvalues are orthogonal.

In a *finite*-diemsnional vector space the eigenvectos of a hermitian matrix have a third fundamental property: The span the space (every vector can be expressed as a linar combination of them). Unfortunately, the proof does not generalize to infinite-dimensional spaces. But the property itslef is essential to the internal consistency of quantum mechanics, so we will take it as an *axiom* (or, more precisely, as a restriction on the class of hermitian operators that can represent obervables):

Axiom 1 The eigenvalues of an obervable operator are compelte: Any function (in Hilber space) can be expressed as a linear combination of them.

3.3.2 Continuous Spectra

If the spectrum of a hermitian operator is *continuous*, the eigenfunctions are not normalizable, and the proofs of Theorems 1 and 2 fail, because the inner products may not exists. Nevertheless, there is a sense in which the three essential properties (reality, orthogonality, and complereness) still hold. I think it's best to approach this subtle case through specific examples.

Example 1 Find the eigenfunctions and eigenvalues of the momentum operator

Solution 1

Let $f_p(x)$ be the eigenfunction and p the eigenvalue:

$$\frac{\hbar}{i} \frac{\mathrm{d}}{\mathrm{d}x} f_p(x) = p f_p(x) \tag{3.22}$$

The general solution is

$$f_p(x) = Ae^{ipc/\hbar}$$

This is not square-integrable, for any (complex) value of p-the momentum operator has no eigenfunctions in Hilbert space. And yet, if we restrict ourselves to real eigenvalues. we do recover a kind of ersatz "orthonormality". ...

3.3.3 Generalized Statistical Interpretation

Generalized statistical interpretation: If you measure an obervable Q(x,p) on a particle in the state $\Psi(x,t)$, you are certain to get *one of the eigenvalues* of the hermitian operator $\hat{q}(x,-i\hbar\mathrm{d}/\mathrm{d}x)$. If the spectrum of \hat{Q} is discrete, the probability of getting the particular eigenvalue q_n associated with the orthonormalized eifengunction $f_n(x)$ is

$$|c_n|^2$$
, where $c_n = \langle f_n | \Psi \rangle$ (3.23)

If the sprectrum is continuous, with real eigenvalues q(z) and associated Dirac-orthonormalized eigenfunctions $f_z(x)$, the probability of gettin a result in the range $\mathrm{d}z$ is

$$|c(z)|^2 dz$$
 where $c(z) = \langle f_z | \Psi \rangle$ (3.24)

Upon measurement, the wave function "collapses" to the corresponding eigenstate.

The statistical interpretation is raadically different from anything we encounter in classical physics. A somewhat different persperctive helps to make it plausible: The eigenfunctions of an observable operator are *complete*, so the wave function can be written as a linear combination of them:

$$\Psi(x,t) = \sum_{n} c_n f_x(x) \tag{3.25}$$

(For simplicity, I'll assume that the spectrum is discrete; it's easy to generalise this argument to the continuous case.) Because the eigenfucntions are *orthonormal*, the coefficients are given by Fourier's trick:

$$c_n = \langle f_n | \Psi \rangle = \int f_n(x)^* \Psi(x, t) dx$$
 (3.26)

Qualitatively, c_n tells you "how much f_n is contained in Ψ ", and given that a mesuremnet has to return one of the eigenvalues of \hat{Q} , it seems reasonable that the probability of getting the particular eigenvalue q_n would be determined by the "amount of f_n " in Ψ . But because probabilities are determined by the absolute square of the wave function, the precise measure is actually $|c_n|^2$. That's the essential burden of the generalized statistical interpretation.

Of course, the total probability (summed over all outcomes) has got to be one:

$$\sum_{n} |c_n|^2 = 1 \tag{3.27}$$

Similarly, the expectation value of Q should be the sum over all possibles outcomes of the eigenvalue times the probability of getting the eigenvalue:

$$\langle Q \rangle = \sum_{n} q_n |c_n 1^2$$
 (3.28)

The momentum space wave function, $\Phi(p,t)$. It is essentially the *Fourier transform* of the (**position space**) wave function $\Psi(x,t)$ —which, by Plancherel'stheorem, is its *inverse* Fourier transform:

$$\Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \Psi(x,t) dx$$
 (3.29)

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{ipx/\hbar} \Phi(p,t) dp$$
 (3.30)

According to the generalized statistical interpretationm, the probability that a measurement of momentum would yiled a result in the range dp is

$$|\Phi(p,t)|^2 \mathrm{d}p \tag{3.31}$$

3.4 The Uncertaintly Principle

3.5 Dirac Notation

Imagine an ordinary vactor \mathbf{A} in two dimensions. How would you describe this vector to someone? The most convenient way is to set up catesian axes, x and y, and specify the components of \mathbf{A} : $a_x = \hat{i} \cdot \mathbf{A}$, $A_y = \hat{j} \cdot \mathbf{A}$. Of course, your sister might have drawn a different set of axed, x' and y', and she would report differen components: $A_x' = \hat{i}' \cdot \mathbf{A}$, $A_y' = \hat{j}' \cdot \mathbf{A}$. But it's all the same vector—we're simply expressing it with respecto to two different bases $(\{\hat{i},\hat{j}\})$ and $\{\hat{i}',\hat{j}'\}$. The vector itself lives "out there is space", independent of anybody's (arbitraty) choice of coordinates.

The same is true for the state of a system in quantum mechancis. It is represented by a vector, $|s(t)\rangle$, that lives "out there in Hilbert space", but we can express it with respecto

to any number of different bases. The wave function $\Psi(x,t)$ is actually the coefficient in the expansion of $|s(t)\rangle$ in the basis of position eigenfunctions:

$$\Psi(x,t) = \langle x|s(t)\rangle \tag{3.32}$$

(with $|x\rangle$ standing fot the eigenfunctions of \hat{x} with eigenvalue x), whereas the momentum sapce wavefunction $\Phi(x,t)$ is the expansion of $|s\rangle$ in the absis of momentum eigenfunctions:

$$\Phi(p,t) = \langle p|s(t)\rangle \tag{3.33}$$

(with $|p\rangle$ standing for the eigenfunction of \hat{p} with eigenvalue p). Or we could expand $|s\rangle$ in the basis of energy eigenfunctions (supposing for simplicity that the spectrum is discrete):

$$c_n(t) = \langle n|s(t)\rangle \tag{3.34}$$

(with $|n\rangle$ standing for thr nth eigenfunction of \hat{H})–(3.26). But it's all the same state; the functions Ψ and Φ , and the collection of coefficients $\{c_n\}$, contain exactly the same information—they are simply three different ways of describing the same vector:

$$\Psi(x,t) = \int \Psi(y,t)\delta(x-y)dy = \int \Phi(p,t)\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}dp$$
$$= \sum c_n e^{-iE_nt/\hbar}\psi_n(x)$$
(3.35)

Operators (representing obervables) are linear transformations—they "transform" one vector into another:

$$|\beta\rangle = \hat{Q} |\alpha\rangle \tag{3.36}$$

Just as vectors are represented, with respect to a particular basis $\{|e_n\rangle\}^2$, by their components,

$$|\alpha\rangle = \sum_{n} a_n |e_n\rangle$$
, with $a_n = \langle e_n | \alpha \rangle$: $\beta = \sum_{n} b_n |e_n\rangle$, with $b_n = \langle e_n | \beta \rangle$ (3.37)

operators are represented (with respect to a particular basis) by their matrix elements³

$$\langle e_m | \hat{Q} | e_n \rangle \equiv Q_{mn} \tag{3.38}$$

In this notations (3.36) takes the form

$$\sum_{n} b_n |e_n\rangle = \sum_{n} a_n \hat{Q} |e_n\rangle \tag{3.39}$$

or, taking the inner product with $|e_m\rangle$,

$$\sum_{n} b_n \langle e_m | e_n \rangle = \sum_{n} a_n \langle e_m | \hat{Q} | e_n \rangle \tag{3.40}$$

 $^{^{2}\}Gamma$ ll assume the basis is discrete: otherwise n becomes a continuous index and the syms are replaced by integrals

³Tjis terminology is inspired, obviously, by the finite-dimensinal case, but the "matrix" will now typically have an infinite (maybe even uncountable) number of elements.

and hence

$$b_m = \sum_n Q_{mn} a_n \tag{3.41}$$

Thus the matrix elements tell you how the components transform.

Later on we will encounter sysrem that admit only a finite number (N) of linearly independet states. In that case $|s(t)\rangle$ lives un an N-dimensional vector space; it can be represented as a column of (N) components (with respecto to a given bases), and operators take the form of ordinary $(N\times N)$ matrices. These are the simplest quantum systems—none of the subtleties associted with infinite-dimensional vector spaces arise.

Dirac proposed to chop the bracket notation for the inner product, $\langle \alpha | \beta \rangle$, into two pieces, which he called **bra**, $\langle \alpha |$, and **ket** $|\beta \rangle$. The latter is a vector, but what exactly is the former? It's a *linear function* of vectors, in the sense that when it hits a vector (to its right) it yields a (complex) number—the inner product. (When an *operator* hits a vector, it delivers another vector; when a *bra* hits a vector, it delivers a number.) In a function space, the bra can be thought of as an instruction to integrate:

$$\langle f| = \int f^*[\cdots] \mathrm{d}x$$

with the ellipsis $[\cdot]$ waiting to be filled by whatever function the bra encounters in the jet to its right. In a finite-dimensional vector space, with the vectors expressed as columns,

$$|\alpha\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} \tag{3.42}$$

the corresponding bra is a row vector:

$$\langle \alpha | = \left(a_1^* a_2^* \cdots a_n^* \right) \tag{3.43}$$

The collection of all bras constitutes another vector space—the so-called **dual space**.

The license to treat bras as separate entities in their own right allows for some powerful and pretty notation. For example, if $|\alpha\rangle$ is a normalized vector, the operator

$$\hat{P} \equiv |a\rangle\langle a| \tag{3.44}$$

picks out the portion of any vector that "lies along" $|\alpha\rangle$:

$$\hat{P} |\beta\rangle = \langle \alpha | \beta \rangle |\alpha\rangle$$

we call it the **projection operator** onto the one-dimensional subspace spanned by $|\alpha\rangle$. If $\{|e_n\rangle\}$ is a discrete orthonormal basis,

$$\langle e_m | e_n \rangle = \delta_{mn} \tag{3.45}$$

then

$$\sum_{n} |e_n\rangle\langle e_n| = 1 \tag{3.46}$$

(the identity operator). For if we les this operator act on any vector $|\alpha\rangle$, we recover the expansion of $|\alpha\rangle$ in the $\{|e_n\rangle\}$ basis:

$$\sum_{n} |e_n\rangle \langle e_n|\alpha\rangle = |\alpha\rangle \tag{3.47}$$

Similarly, if $\{|e_z\rangle\}$ is a $\it Dirac$ orthonormalized continuous basis,

$$\langle e_a | e_{z'} \rangle = \delta(z - z')$$
 (3.48)

then

$$\int |e_z\rangle\langle e_z| \,\mathrm{d}z = 1 \tag{3.49}$$

(3.46) and (3.49) are the tidiest ways ti express completeness.

Chapter 4

Quantum Mechanics In Three Dimensions

4.1 Angular Momentum

Classically, the angular momentum of a particle (with respecto to the origin) is given by the formula

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \tag{4.1}$$

which os to say,

$$L_x = yp_z - zp_u, \quad L_y = zp_x - xp_z, \quad L_z = xp_y - yp_x$$
 (4.2)

The corresponding quantum operators are obtained by the standard prescription $p_x \to -\hbar\partial/\partial x, p_y \to -i\hbar\partial/\partial y, p_z \to -\hbar\partial/\partial z.$

Eigenvalues

The operators L_x and L_y do not commute; in fact¹

$$[L_x, L_y] = [yp_z - zp_y, zp_x - xp_z]$$

= $[yp_z, zp_x] - [yp_z, zp_z] - [zp_y, zp_x] + [zp_y, xp_z]$ (4.3)

From the canonical commutation relations² we know that the inly operators here that *fail* to commute are x with p_x , y with p_y , and z with p_z . So the two middles terms drop out, leaving

$$[L_x, L_y] = y p_x [p_z, z] + x p_y [z, p_z] = i\hbar (x p_y - y p_x) = i\hbar L_z$$
(4.4)

Of course, we could have started out with $[L_y,L_z]$ or $[L_z,L_x]$, but there is no need to calculate these separately—we can get them immediately by cyclic permutation of the indices $(x \to y, y \to z, z \to x)$

$$\begin{bmatrix}
[L_x, L_y] = i\hbar L_z; & [L_y, L_z] = i\hbar L_x; & [L_z, L_x] = i\hbar L_y
\end{bmatrix}$$
(4.5)

Fundamental commutation relations for angular momentum

¹Note that all the operators we encounter in quantum mechanics are distributive with respect to addition: A(B+C) = AB + AC. In particular, [A, B+C] = [A, B] + [A, C].

²The cannonical commutation relations are $[r_i, p_j] = -[p_i, r_j] = i\hbar \delta_{ij}$ $[r_i, r_j] = [p_i, p_j] = 0$

These are the fundamental commutation relations for angular momentum; everything else follows from them.

Notice that L_x, L_y and L_z are *incompatible* obervables. According to the generalized uncertainty principle (??)

$$\sigma_{L_x}^2 \sigma_{L_y}^2 \ge \left(\frac{1}{2i} \left\langle i\hbar L_z \right\rangle\right)^2 = \frac{\hbar^2}{4} \left\langle L_z \right\rangle^2$$

or

$$\sigma_{L_x}\sigma_{L_y} \ge \frac{\hbar}{2} |\langle L_z \rangle| \tag{4.6}$$

It would therefore be fuitle to look for states that are simultaneously eigenfunctions of L_x and L_y . On the other hand, the square of the total angular momentum,

$$L^2 \equiv L_x^2 + L_y^2 + L_z^2 \tag{4.7}$$

does commute with L_x :

$$\begin{split} [L^2,L_x] &= [L_x^2,Lx] + [L_y^2,L_x] + [L_z^2,Lx] \\ &= L_y[L_y,L_x] + [L_y,L_x]L_y + L_z[L_z,L_x] + [L_z,L_x]L_z \\ &= L_y(-i\hbar L_z) + (-i\hbar L_z)L_y + L_z(i\hbar L_y) + (i\hbar L_y)L_z \\ &= \end{split}$$

(I used (??)) to simplify the commutator; note also that any operator commutes with itself. It follows, of course, that L^4 also commute with L_y and L_z :

$$[L^2, L_x] = 0, \quad [L^2, L_y] = 0, \quad L^2, L_z = 0$$
 (4.8)

or, more compactly,

$$[L^2, \mathbf{L}] = 0 \tag{4.9}$$

So L^2 is compatible with each component of ${\bf L}$, and we can hope to find simultaneous eigenstates of L^2 and (say) L_z :

$$L^2 f = \lambda f \quad \text{and} \quad L_z f = \mu f \tag{4.10}$$

We'll use a "ladder operator" technique, very similar to the one we applied to the harmonic oscillator back in Section 2.3.1. Let

$$\boxed{L_{\pm} \equiv L_x \pm iL_y} \tag{4.11}$$

The commutator with L_z is

$$[L_z, L_{\pm}] = [L_z, L_x] \pm i[L_z, L_y] = i\hbar L_y \pm i(-i\hbar L_x) = \pm \hbar(L_x \pm iL_y)$$

SO

$$[L_z, L\pm] = \pm \hbar L_{\pm} \tag{4.12}$$

And. of course,

$$[L^2, L_{\pm}] = 0 \tag{4.13}$$

I claim that if f es an eigenfunction of L^2 and L_z , so also is $L_{\pm}f$: (4.13) says

$$L^{2}(L_{\pm}f) = L_{\pm}(L^{2}f) = L_{\pm}(\lambda f) = \lambda(L_{\pm}f)$$
(4.14)

so $L_{\pm}f$ is an eigenfunction of L^2 , with the same eigenvalue λ , and (4.12) says

$$L_z(L_{\pm}f) = (L_z L_{\pm} - L_{\pm} L_z)f + L_{\pm} L_z f = \pm \hbar L_{\pm} f + L_{\pm} (\mu f)$$

= $(\mu \pm \hbar)(L_{\pm}f)$ (4.15)

so $L_{\pm}f$ is an eigenfunction of L_z with the *new* eigenvalue $\mu \pm \hbar$. We call L_+ the "raising" operator, because is *increases* the eigenvalue of L_z by \hbar , and L_- the "lowering" operator, because it *lowers* the eigenvalue by \hbar .

For a given value of λ , then we obtain a "ladder" of states, with each "rung" separated from its neighbors by one unit of \hbar in the eigenvalue of L_z . To ascend the ladder we apply the raising operator, and to descend, the lowering operator. But this process cannot go on forever. Eventually we're going to reach a state gor which the z-component exceeds the total, and that cannot be. There must exist a "top rung", such that

$$L_{+}f_{t} = 0 (4.16)$$

Let $\hbar l$ be the eigenvalue of L_z at this top ring (the appropriateness of the letter "l" will appear in a moment):

$$L_z f_t = \hbar l f_t; \quad L^2 f_t = \lambda f_t \tag{4.17}$$

Now,

$$L_{\pm}L_{\mp} = (L_x \pm iL_y)(L_x \mp iL_y) = L_x^2 + L_y^2 \mp i(L_xL_y - L_yL_x)$$

= $L^2 - L_z^2 \mp i(i\hbar L_z)$

or, putting in the other way around,

$$L^2 = L_+ L_{\pm} + L_z^2 \mp \hbar L_z \tag{4.18}$$

It follows that

$$L^{2}f_{t} = (L_{-}L_{+} + L_{z}^{2} + \hbar L_{z})f_{t} = (0 + \hbar^{2}l^{2} + \hbar^{2}l)f_{t} = \hbar^{2}l(l+1)f_{t}$$

and hence

$$\lambda = \hbar^2 l(l+1) \tag{4.19}$$

This tells is the eigenvalue of L^2 in terms of the maximum eigenvalue of L_z .

Meanwhile, there is also (for the same reason) a bottom rung, f_b , such that

$$L_{-}f_{b} = 0 (4.20)$$

Let $\hbar \bar{l}$ be the eugenvalue if L_z at this bottom rung:

$$L_z f_b = \hbar \bar{l} f_b; \quad L^2 f_b = \lambda f_b \tag{4.21}$$

Using (4.18), we have

$$L^{2} f_{b} = (L_{+} L_{-} + L_{z}^{2} - \hbar L_{z}) f_{b} = (+\hbar^{2} \bar{l}^{2} - \hbar^{2} \bar{l}) f_{b} = \hbar^{2} \bar{l} (\bar{l} - 1) f_{b}$$

and therefore

$$\lambda = \hbar^2 \bar{l}(\bar{l} - 1) \tag{4.22}$$

Comparing (4.19) and (4.116), we see that $l(l+1) = \overline{l}(\overline{l}-1)$