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1 Review of Quantum Mechanics

Let us start by surveying some of the basic ideas that are necessary for us to have mastered.. We can describe any quantum mechanical system by a set of states (discrete or continuous) which are occupied with calculable probabilities. The state of a system changes under the influence of external forces and we represent these forces by operators that act on the states. The inner product of two states defines a quantum mechanical amplitude and the absolute square of the amplitude is interpreted as a probability. To perform calculations we use representations of the states that are vectors in a linear vector space. We expand on these ideas below.

1.1 Dirac Notation

Up to this point we have usually written down a wavefunction to represent the state of a system where the wavefunction was explicitly a complex function of position and time. Often these wavefunctions are abbreviated to a form such as $|u\rangle$. This has the advantage of generalising our notation to cases involving spin (see Chapter 11). With spin we cannot write down a simple wavefunction and have to expand simple wave mechanics to include matrices. However, this abbreviation masks an important reason for using the Dirac formalism, which is that it contains a very important physical insight. We have become accustomed to the idea that wavefunctions obey a linear superposition principle. Dirac recognised that it is not just the wavefunctions that satisfy the superposition principle, but the states

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themselves. He postulated that the linear superposition of states is a feature of nature. If $|u\rangle$ and $|v\rangle$ are states, Dirac called them *kets*, and if a and b are complex constants, then if we define $|w\rangle$ by

$$|w\rangle = a|u\rangle + b|v\rangle \qquad -1-1$$

then $|w\rangle$ is also a ket. In other words $|w\rangle$, which is made up of a superposition of $|u\rangle$ and $|v\rangle$, is also a state of the system. We may draw an analogy here with three dimensional Euclidean space (called by convention E_3). In E_3 we know that any point in space may represented by $ax_1 + bx_2 + cx_3$ where the x_i are the unit vectors in the x,y and z directions. However we should be careful when using this analogy. In E_3 a,b,c are real (not complex) and the numbers of dimensions is limited to 3. In our ket "space" the dimensionality reflects the numbers of linearly independent states necessary to describe the system and can easily be infinite. This "space" of linearly independent state vectors is called a *Hilbert Space*.

1.2 Linear Independence

A set of states is said to be linearly independent if there is no solution to

$$c_1 |u_1\rangle + c_2 |u_2\rangle + c_3 |u_3\rangle + \dots = \sum_{i=1,n} c_i |u_i\rangle = 0$$
 1-2

except $c_1 = c_2 = c_3 = c_i = 0$.

1.3 Completeness

A set of kets is said to be complete if we can construct any state $|u\rangle$ from a linear superposition of linearly independent kets, i.e.

$$|u\rangle = \sum_{i=1,n} c_i |u_i\rangle.$$
 1-3

Note that this requirement is not the same as that of linear independence (Eq. 1-2). For example, x and y are independent directions but we cannot describe all space points without using the z direction.

1.4 Orthonormality

Dirac also defined the inner product (or scalar product) of two kets, say $|a\rangle$ and $|b\rangle$, writing it as $\langle a|b\rangle$. The inner product has the following property

$$\langle b|a\rangle^* = \langle a|b\rangle$$
 1-4

The objects occurring on the left side of the inner product are called *bra* vectors and are an entirely equivalent set of states with which to describe a system. In our usual wavefunction notation this is identical to the following: we define the inner product as

$$\int \boldsymbol{\psi}_b^*(r) \boldsymbol{\psi}_a(r) d^3 r \qquad 1-5$$

and the equivalent of Eq.1.4 is

$$\left(\int \psi_{b}^{*}(\vec{r})\psi_{a}(\vec{r})d^{3}\vec{r}\right)^{*} = \int \psi_{a}^{*}(\vec{r})\psi_{b}(\vec{r})d^{3}\vec{r}.$$
 1-6

However Eq. 1-6 will not apply to systems that contain spin whereas our more general notation, Eq. 1-4 does. We can describe our system by the complex conjugate of the wavefunction just as well as by the wavefunctions themselves, i.e. the set of states ψ_i is equivalent to the set of states (ψ_i)^{*}. We can replace all wavefunctions by their complex conjugates and we will always get the same answer for the expectation values. We say that the bra space is an entirely *equivalent representation* of the system as the ket space.

The kets (or bras) may be normalised so that

$$\langle a | a \rangle = 1$$
 1-7

if two kets have the property

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$$\langle a | b \rangle = \langle b | a \rangle = 0$$
 1-8

then they are called orthogonal. Kets satisfying Eq. 1-7 and Eq. 1-8 are said to be orthonormal. The complete set (or *basis*) of kets that span our Hilbert Space is chosen so that

$$\langle u_i | u_j \rangle = \delta_{ij}$$
 1-9

where δ_{ij} is the Krönecker delta and equals *1* if i=j, and 0 otherwise.

We can determine the coefficients c_i in the general decomposition of a state (Eq. 1-3) by using the orthonormality of the basis kets. We take the inner product of the ket $|u\rangle$ and the bra $\langle u_j |$ to get c_j i.e.

$$\langle u_j | u \rangle = \sum_{n=1,m} c_n \langle u_j | u_n \rangle = \sum_n c_n \delta_{jn} = c_j$$
 1-10

We can use Eq. 1-10 to rewrite the state $|u\rangle$ as

$$|u\rangle = \sum_{i} c_{i} |u_{i}\rangle = \sum_{i} \langle u_{i} |u\rangle |u_{i}\rangle = \sum |u_{i}\rangle \langle u_{i} |u\rangle$$
1-11

1.5 Operators

We have already discussed that states describe quantum mechanical systems. The forces on the system, its interactions, and indeed the effects of any observation of the system are described by operators. We are familiar with the ways in which operators can be used to calculate quantities like the average position or momentum. In the Dirac notation the action of an operator is as follows. If A acts on a state $|u\rangle$ it will produce another state $|v\rangle$

$$A|u\rangle = |v\rangle. 1-12$$

The operator A is said to be a linear operator if

$$|w\rangle = c|u\rangle + d|v\rangle$$

$$A|w\rangle = cA|u\rangle + dA|v\rangle$$
1-13

where c and d are complex constants. We will usually be concerned with linear operators. A useful operator, that we have already implicitly introduced, is the projection operator I

$$I = \sum_{n} |u_n\rangle \langle u_n|.$$
 1-14

This has the useful property (see Eq. 1-11) that $I|u\rangle = |u\rangle$.

1.6 Hermitian Operators

An operator A is defined as Hermitian if it satisfies the condition that for any two kets

$$\langle v | Au \rangle = \langle Av | u \rangle$$
 1-15

Hermitian operators (also called *self adjoint* operators) have many useful properties. Perhaps the most useful is that the eigenvalues of a Hermitian operator are real. This can be proved as follows.

$$\langle u \| Au \rangle = a \langle u | u \rangle = a \langle u | Au \rangle = \langle Au | u \rangle = a * \langle u | u \rangle = a^* = a$$

$$I-16$$

where we have used Eq. 1-15. The condition that $a^*=a$ means that a is real. This is very important since all measurements we make yield real values.

1.7 Expectation Values and Probability Amplitude

The kets contain all the information about the state of the system. Let us assume that we can calculate the expectation value of some observable A in a state $|u\rangle$

$$\langle A \rangle = \langle u | A | u \rangle.$$
 1-17

Projecting $|u\rangle$ into its eigenstates (Eq. 1-11) we find

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$$\langle A \rangle = \langle u | A \sum_{i} | u_{i} \rangle \langle u_{i} | u \rangle = \sum_{i} a_{i} \langle u | u_{i} \rangle \langle u_{i} | u \rangle = \sum_{i} a_{i} | \langle u_{i} | u \rangle |^{2}.$$
1-18

The correct interpretation of Eq. 1-18 is vital. It gives the value of the expectation value of a measurement of A on the system. If we start in a mixed state $|u\rangle$ then $|\langle u_i | u \rangle|^2$ is the probability of finding that state in an eigenstate $|u_i\rangle$. Remember that the result of making a measurement on a mixed state with an operator is to put the system into a new state whose eigenket corresponds to the eigenvalue measured. The quantity $\langle u_i | u \rangle$ is known as the *probability amplitude*.

1.8 Problems

- **1.1** If |i>,i=1,2,3,...n compose a set of states, write down and explain the conditions they must satisfy so they be *orthonormal* and *complete*.
- **1.2** Integration is a vital part of quantum mechanics. Make sure that you can evaluate the $\tilde{}$

following integrals: a) $\int_{0}^{\infty} r^{n} e^{-r/a} dr$ b) $\int \cos^{2} \theta d\Omega$ over all the solid angle.

2 Time Independent Perturbation Theory

Solutions to Schrödinger's equation are the key to classical quantum mechanics. Unfortunately very few problems have an analytical solution and almost none of the cases that do permit an analytical approach bear detailed comparison with reality. To model and predict the behaviour of realistic quantum systems we need to develop a method of solving these complicated problems. One of the most important methods is called *perturbation theory*. For some problems the potential is very similar to the potential in a problem that we can solve analytically. In perturbation theory we start with these known solutions, and by making small changes attempt to solve more complicated problems.

2.1 First Order Perturbation Theory

The simplest example of Perturbation Theory solves problems that do not explicitly depend on time and in which there are no states that are degenerate.¹ Let us assume that an unperturbed system of which we know the eigenstates is described by the Hamiltonian H_0 . The eigenstates (labelled 1,2,...,n) that describe this system satisfy

$$H_0 \left| \phi_n^0 \right\rangle = E_n^0 \left| \phi_n^0 \right\rangle$$
 2-1

¹ Two states are said to be degenerate if, although described by two orthogonal eigenkets, their energy eigenvalues are identical.

and the perturbed system, described by the Hamiltonian, H is:

$$H|\boldsymbol{\varphi}\rangle = E_n |\boldsymbol{\varphi}_n\rangle \qquad 2-2$$

where the perturbed Hamiltonian is different from the unperturbed system by a small potential, λV :

$$H = H_0 + \lambda V \tag{2-3}$$

The crucial factor that enables us to perform perturbation theory, is the perturbation parameter λ . By setting $\lambda = 0$ we have the fully unperturbed system. By setting $\lambda = 1$ we have a fully perturbed system. With the unperturbed system we assume that we can find solutions to the wave equation. Therefore our method of solution for the perturbed system will be very similar to the power series methods used to solve differential equations. We are going expand our unknowns in a power series in the perturbation parameter:

$$E_{n} = E_{n}^{0} + \lambda E_{n}^{1} + \lambda^{2} E_{n}^{2} + \dots$$

$$\left| \varphi_{n} \right\rangle = \left| \phi_{n}^{0} \right\rangle + \lambda \left| \phi_{n}^{1} \right\rangle + \lambda^{2} \left| \phi_{n}^{2} \right\rangle + \dots$$
2-4

As in a power series solution we match the coefficients in different powers of λ to guarantee that the solutions holds for all arbitrary values of λ . Substituting Eq. 2-4 into Eq. 2-2 yields

$$(H_0 + \lambda V) (|\phi_n^0\rangle + \lambda |\phi_n^1\rangle + \lambda^2 |\phi_n^2\rangle + \dots) - (E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots) (|\phi_n^0\rangle + \lambda |\phi_n^1\rangle + \lambda^2 |\phi_n^2\rangle + \dots) = 0$$

$$2-5$$

Comparing the zeroeth order coefficients in the perturbation parameter yields the unperturbed equations and the first order terms yield

$$\left(H_0 - E_n^0\right) \left|\phi_n^1\right\rangle = -(V - E_n^1) \left|\phi_n^0\right\rangle$$
 2-6

taking the inner product with the nth unperturbed state gives:

$$\left\langle \phi_n^0 \left| H_0 - E_n^0 \right| \phi_n^1 \right\rangle = -\left\langle \phi_n^0 \left| V \right| \phi_n^0 \right\rangle + E_n^1 \left\langle \phi_n^0 \right| \phi_n^0 \right\rangle$$
2-7

The left hand side of Eq. 2-7 can be seen to be zero since H_0 is Hermitian

$$\left\langle \phi_{n}^{0} \left| H_{0} - E_{n}^{0} \right| \phi_{n}^{1} \right\rangle = \left\langle \phi_{n}^{0} \left| E_{n}^{1} - E_{n}^{0} \right| \phi_{n}^{1} \right\rangle = 0$$
 2-8

which gives the very important result:

$$E_n^1 = \left\langle \phi_n^0 \left| V \right| \phi_n^0 \right\rangle \tag{2-9}$$

Eq. 2-9 gives the first order energy correction to the n-th state due to a perturbation V. The calculation of the shifts to the states is a little more subtle. To evaluate these we take the expression for the first order coefficients Eq. 2-6 and take the inner product with an unperturbed state p:

$$\left\langle \phi_{p} \left| H_{0} - E_{n}^{0} \right| \phi_{n}^{1} \right\rangle = -\left\langle \phi_{p} \left| V - E_{n}^{1} \right| \phi_{n} \right\rangle$$
2-10

If we assume that there is no admixture of the original state into the perturbed state i.e.

$$\left|\phi_{n}^{1}\right\rangle = \sum_{j\neq n} a_{jn} \left|\phi_{j}\right\rangle$$
 2-11

Eq. 2-10 becomes

$$\left\langle \phi_{p} \left| \left(H_{0} - E_{n}^{0} \right) \sum_{j \neq n} a_{jn} \right| \phi_{j} \right\rangle = -\left\langle \phi_{p} \left| V \right| \phi_{n} \right\rangle = -V_{pn}$$
2-12

Using the Hermitian properties of H_0 and the orthonormality of the eigenkets yields

$$a_{np} = \frac{V_{pn}}{E_n^0 - E_p^0}$$
 2-13

and we can now substitute 2-13 into 2-11 to give the general form the modified states

$$\left|\phi_{n}^{1}\right\rangle = \sum_{p\neq n} \frac{V_{pn}}{E_{n}^{0} - E_{p}^{0}} \left|\phi_{p}\right\rangle$$
2-14

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Note that the changes to the states become large when the denominator becomes small or if V_{pn} is large.

2.2 Problems

- **2.1** Prove that the states in Eq. 2-14 remain normed.
- 2.2 A time independent system is represented by the Hamiltonian H_0 with eigenstate ϕ_0 . Show how if we introduce a small perturbing potential V we can calculate the **shift** in energy of this state and the change in the eigenstate. You may assume the eigenstate is not degenerate.

2.3 A simple harmonic oscillator has a Hamiltonian
$$H = \frac{p^2}{2m} + \frac{1}{2}Kx^2$$

The first two eigenstates are claimed to be of the form:

$$|0\rangle = \left(\frac{\alpha}{\pi^{1/2}}\right)^{1/2} e^{-\alpha^2 x^2/2}$$
$$|1\rangle = \left(\frac{\alpha}{2\pi^{1/2}}\right)^{1/2} 2\alpha x e^{-\alpha^2 x^2/2}$$

Find the condition that α has to satisfy for this to be true and show that if $\omega = (K/m)^{1/2}$ then the energies of these states are given by $E_0 = \hbar \omega / 2$, $E_1 = 3\hbar \omega / 2$.

2.4 Show that if we add a small perturbation to the harmonic oscillator in Qu. 2.3 of the form $bx^2/2$ then the change in energy of the ground state is approximately

$$\Delta E_0 \approx \frac{\hbar b}{4\sqrt{mK}}$$

Show that this is consistent with the analytical solution by replacing K with K+b in the solution to Qu 2.3.

.

You may use the following two integrals:

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$$\int_{-\infty}^{\infty} x^p e^{-ax^2} dx = \frac{(p-1)}{2a} \int_{-\infty}^{\infty} x^{p-2} e^{-ax^2} dx$$
$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$$

2.5 Use first order non-degenerate perturbation theory to calculate the change in binding energy of an ion consisting of a nucleus charge Ze and a single electron when the nuclear charge changes to +(Z+1)e.

3 Degenerate Perturbation Theory

In our last lecture we examined non-degenerate perturbation theory. Unfortunately the diversity of problems to which one can apply non-degenerate perturbation theory is limited by the fact that many physical systems exhibit degeneracy. A degenerate system is one where two or more states satisfy the same eigenvalue equation (Schrödinger's Equation) with the same eigenvalue (energy) but are distinct states. If there are n linearly independent that share the same eigenvalue then that set of states is said to be n-fold degenerate.

Degenerate systems do not lend themselves readily to the techniques we discussed in the last chapter. This should be evident from studying Eq. 2-14. When two states are degenerate the denominator is zero and the expression is meaningless. The only way one can attempt to rescue the technique is to require that the matrix element in Eq. 2-14 (V_{pn}) also vanishes for the degenerate states. This will not be possible unless we choose a different set of basis states. Let us assume that this is possible and that (to begin with) we have *s* linearly dependent eigenkets that belong to the eigenvalue *n* where

$$\langle u_{n\alpha} | u_{n\beta} \rangle = \delta_{\alpha\beta}$$

 $\alpha, \beta = 1, 2, \dots, s$ $3-1$

The first task is to find the correct states with which perform the perturbation theory. Let us write these states as

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$$\left|\phi_{ni}\right\rangle = \sum_{\alpha=1}^{s} c_{i\alpha} \left|u_{n\alpha}\right\rangle.$$
3-2

The condition that we can attempt our perturbation theory has to be that for states part of the same sfold degenerate eigenvalue (n) that

$$\langle \phi_{ni} | V | \phi_{nj} \rangle = \langle \phi_{ni} | V | \phi_{ni} \rangle \delta_{ij}.$$
 3-3

This condition is often loosely referred to as the states being *diagonalized* with respect to the perturbation.

The equations for the first order perturbation theory still hold so that (for example) Eq. 2-9 becomes

$$E_{ni}^{1} = \left\langle \phi_{ni} \left| V \right| \phi_{ni} \right\rangle.$$
3-4

If we know the right states to use we can easily calculate how the energy shifts. How do we pick the states? If we take the degenerate version of Eq. 2-6

$$(H_0 - E_n^0) |\phi_{ni}^1\rangle = -(V - E_n^1) |\phi_{ni}\rangle.$$
 3-5

Using Eq. 3-2 we can write this as:

$$\left(H_0 - E_n^0\right) \left|\phi_{ni}^1\right\rangle = -(V - E_n^1) \sum_{\alpha=1,s} c_{i\alpha} \left|u_{n\alpha}\right\rangle.$$
3-6

Taking the inner product of Eq. 3-6 with another (say β) eigenstate in the s-fold degenerate level gives:

$$\left\langle u_{n\beta} \left| \left(H_0 - E_n^0 \right) \right| \phi_{ni}^1 \right\rangle = - \left\langle u_{n\beta} \left| \left(V - E_n^1 \right) \sum_{\alpha = 1, s} c_{i\alpha} \right| u_{n\alpha} \right\rangle$$
3-7

In an identical fashion to our previous results the left-hand side of Eq. 3-7 is zero since the Hamiltonian is Hermitian and the state β has energy E_n . Thus equation 3-7 may be rewritten

$$\sum_{\alpha=1,s} \langle u_{n\beta} | V | u_{n\alpha} \rangle c_{i\alpha} = E_{ni}^{1} c_{i\beta}$$
3-8

which can also be written as

$$\sum_{\alpha=1,s} \left(V_{\beta\alpha} - E_{ni}^{1} \delta_{\alpha\beta} \right) c_{i\alpha} = 0.$$
3-9

This is a system of s homogenous equations for the unknowns (the c's). It possesses solutions (other than all the c's being zero) when

$$\det \left(V_{\beta\alpha} - E_{ni}^{1} \delta_{\alpha\beta} \right) = 0 \quad . \qquad 3-10$$

3.1 Examples

At first sight our degenerate perturbation theory seems rather complicated. Let us see how in practice the mathematics is sometimes a little less intimidating. First we will consider a system where we are given the normed eigenstates to use. In the second we will determine these states.

3.1.1 Threefold degenerate system in a magnetic field.

First let us see how simple calculating the changes to energies in a degenerate state can be when we know the appropriate eigenstates. Let us assume that we are working with a spin-1 particle bound in a radially symmetric potential. The degenerate states that describe the system are |+>, |0>, |-> corresponding to angular momentum orbital angular momentum components +1,0,-1 along the z-direction. Let us assume that we apply a perturbation given by

$$V = \frac{\mu}{\hbar} B_z \cdot L_z \qquad 3-11$$

We know that

$$\begin{array}{c} L_{z}|+\rangle = \mathbf{\hat{n}}|+\rangle \\ L_{z}|0\rangle = 0 \\ L_{z}|-\rangle = -\mathbf{\hat{n}}|-\rangle \end{array}$$

$$3-12$$

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and Eq. 3-3 is satisfied. As our conditions for doing perturbation theory are met (our states are diagonal with respect to the perturbation) we can right away write down the energy shifts from Eq. 3-4 to the states

$$\Delta E_{+} = \mu B$$

$$\Delta E_{0} = 0$$

$$\Delta E_{-} = -\mu B$$

$$3-13$$

3.1.2 Twofold degenerate system - the general solution

If we take a level with a two-fold degeneracy we can follow through the algebra we performed above and see exactly how the determination of the eigenstates works. Let us assume that there are two linearly independent eigenkets $|u_1\rangle$, $|u_2\rangle$ belonging to the n^{th} state. Let us assume that the two states with which we want to perform our perturbation theory are called $|v_1\rangle$ and $|v_2\rangle$ i.e.

$$|v_1\rangle = c_{11}|u_1\rangle + c_{12}|u_2\rangle$$

$$|v_2\rangle = c_{21}|u_1\rangle + c_{22}|u_2\rangle$$

$$3-14$$

Our sole aim here is to determine the constants c. From Eq. 3-9 we can then write

$$\begin{pmatrix} V_{11} - E_{ni}^{1} \end{pmatrix} c_{i1} + V_{12} c_{i2} = 0 V_{21} c_{i1} + \begin{pmatrix} V_{22} - E_{n1}^{1} \end{pmatrix} c_{i2} = 0$$
3-15

For the *i*'th degenerate state (either 1 or 2 here) we have two homogenous equations for c_{il} , c_{i2} . These only have a non-zero solution when the determinant of the coefficients of the *c*'s is zero, that is

$$\left(V_{11} - E_{ni}^{1}\right)\left(V_{22} - E_{ni}^{1}\right) - V_{21}V_{12} = 0$$
3-16

This is a quadratic equation for the energy shifts which yields two solutions, one for each degenerate state. If in addition one wants the normed states, Eq. 3-15 can be solved.

Finding these eigenkets is a cumbersome and laborious process. We will leave this subject here and move onto other approximate methods for stationary problems.

3.2 Problems

3.1 Show that the normed states which can be obtained from Eq. 3-15 are diagonal with respect

to the perturbing potential.

3.2

may

In time-independent perturbation theory the first order corrections to the wavefunctions are given by the expression

$$|\phi_{n}^{1}\rangle = \sum_{p \neq n} \frac{V_{pn}}{E_{n}^{(0)} - E_{p}^{(0)}} |\phi_{p}\rangle$$

- i) Explain carefully the meaning of the symbols in the equation above and discuss the significance of the inequality under the summation sign
- ii) Discuss briefly the problems of applying first order perturbation theory to a *degenerate* system .
- iii) Calculate the shift(s) in energy to a spinless particle in a spherically symmetric potential exposed to a weak uniform magnetic field B along the z direction. You assume that the interaction is of the form below and that the particle is in an L=1 state.

 $H = \alpha \mu B \cdot L$

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4 Variational Techniques

Before the arrival of fast computers it was often impossible to calculate the ground state of various systems. This was often due to the difficulty of realistically applying the perturbation techniques of the last chapters.

The Rayleigh-Ritz method was developed to address this problem. It does not assume that one has to find the eigenstates of the system but rather that we know some general features of the wavefunction. We will show here how it is used to calculate the ground state energy of a system.

4.1 Rayleigh-Ritz Technique

Let us assume that a system may be described by a Hamiltonian that possesses a number of energy eigenvalues which we can write in order of ascending energy, that is

$$E_1 \le E_2 \le E_3 \dots \qquad 4-1$$

Any state if the system can be expanded (at least in principle) in terms of the appropriate eigenstates

$$\left|\phi\right\rangle = \sum c_{n}\left|\phi_{n}\right\rangle.$$
4-2

The expectation value of the energy of the mixed state is given by:

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$$< E >= \frac{\langle \phi | H | \phi \rangle}{\langle \phi | \phi \rangle} = \frac{\sum |c_n|^2 E_n}{\sum c_n^2}.$$

4-3The smallest value that this can have is the lowest energy therefore

$$\frac{\left\langle \phi \middle| H \middle| \phi \right\rangle}{\left\langle \phi \middle| \phi \right\rangle} \ge E_1 \quad . \tag{4-4}$$

This means the expectation value of H with respect to any normalised state forms an upper bound to the energy of the ground state. To estimate this energy all we have to do is to find a sensible way to vary the wavefunctions sufficiently to get an estimate of this bound. We do this by assuming that we have a trial wavefunction that depends on several parameters and that we can calculate the expectation value:

$$|\psi_{T}\rangle = |\psi_{T}(\alpha_{1},\alpha_{2},\alpha_{3},...)\rangle$$

$$E(\alpha_{1},\alpha_{2},\alpha_{3},...) = \frac{\langle\psi_{T}|H|\psi_{T}\rangle}{\langle\psi_{T}|\psi_{T}\rangle}$$

$$4-5$$

We can then minimise the expectation value of the energy with respect to our parameters

$$\frac{\partial E(\alpha_1, \alpha_2, \dots)}{\partial \alpha_i} = 0.$$
4-6

The minimum corresponds to our estimate for the upper limit on the ground state wavefunction.

The entire success of the Rayleigh-Ritz method depends on choosing wavefunctions that are qualitatively similar to the "real" wavefunctions for which the integrals can be done. Although the variational method is very elegant and surprisingly accurate it has been superseded by numerical analysis techniques.

4.2 Problems

4.1 A particle of mass m is bound in the ground state of an exponential potential

$$V(r) = -\frac{4\pi}{3ma^2}e^{-r/a}$$

Use a simple trial function to obtain an upper bound for the ground state energy.

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5 Time-Dependent Perturbation Theory

Not all the problems with which we are confronted by in nature are of the type we have discussed above. In many cases, for example, there may be a potential applied to the system that is not constant. To predict the behaviour of such time-varying systems it is not possible to use the Time Independent Schrödinger Equation and instead we have to use the Time Dependent Schrödinger Equation.

5.1 Time-Dependent Schrödinger Equation

The Time Dependent Schrödinger Equation (TDSE) is given by

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle \qquad 5-1$$

where the energy (in the Time Independent Schrödinger Equation - TISE) has been replaced by the first derivative of the wavefunction with respect to time. If the Hamiltonian is time independent it is relatively easy to find a solution to the TDSE, namely:

$$\left|\psi(t)\right\rangle = \left|u_{n}\right\rangle e^{\frac{-iE_{n}t}{\hbar}}$$
5-2

where the u_n are solutions to the TISE. For stationary eigenstates this simply introduces an unobservable phase into the wavefunction.

5.2 Time Evolution of States

For a system composed of many stationary states we have already seen that we can in general construct a total wavefunction

$$\left|\psi\right\rangle = \sum_{n=1,m} c_n \left|u_n\right\rangle.$$
 5-3

If the Hamiltonian is time independent we expect this to evolve according to

$$\left|\psi(t)\right\rangle = \sum_{n=1,m} c_n \left|u_n\right\rangle e^{-\frac{iE_1t}{\hbar}}$$
5-4

Thus for any state $\psi(0)$ whose composition we know at time t=0 we can find the $\psi(t)$ by finding the values of *c* that are appropriate at t=0 and then letting the phases of each eigenstate evolve according to Eq. 5.2.

5.3 Perturbations

However useful we may find the formalism described by Eq. 5.4, it does not address the problem of how a system that starts off in a known state will react to a Hamiltonian that depends explicitly (or implicitly) on time.

Let us consider how to analyse such a problem. We begin by splitting the Hamiltonian into two parts, one that is time independent and one that depends on time

$$H(t) = H_0 + V(t)$$
. 5-5

This does not make the Schrödinger Equation any simpler to solve, but if we assume that V(t) is small we may try to solve the TDSE by using a form of perturbation theory. If we guess that the eigenstates at any time *t* will be close to the unperturbed eigenstates then we can still expand the wavefunction with the unperturbed eigenstates but with time varying coefficients:

$$\left|\psi(t)\right\rangle = \sum_{n=1,m} c_n(t) \left|u_n\right\rangle e^{-\frac{iE_1 t}{\hbar}}.$$
5-6

This should be contrasted with Eq. 5.4 where the coefficients c were constant with time. Simply substituting this into the TDSE gives:

$$i\hbar\sum_{n}c_{n}(t)|u_{n}\rangle e^{-iE_{n}t/\hbar} = \sum_{n}V(t)|u_{n}\rangle e^{-E_{n}t/\hbar}c_{n}(t)$$
5-7

and hence taking the inner product with an arbitrary eigenket $|u_p\rangle$ yields

$$i\hbar c_{p}(t) = \sum_{n} V_{pn}(t) e^{i\omega_{pn}t} c_{n}(t)$$
 5-8

where we have defined

$$V_{pn}(t) = \left\langle u_p \left| V(t) \right| u_n \right\rangle$$
 5-9

and

$$\boldsymbol{\omega}_{pn} = \left(\boldsymbol{E}_p - \boldsymbol{E}_n\right) / \boldsymbol{R}.$$
 5-10

The values of the coefficients c at t=0 may be determined from equation 5.6:

$$c_n(0) = \left\langle u_n \, \middle| \, \psi(0) \right\rangle$$

5-11

For the special case where the system is in a unique state i at t=0 i.e.

$$c_n(0) = \delta_{ni} \tag{5-12}$$

we see that Eq. 5.8 becomes

$$i\mathbf{h}\dot{c}_{p}(t) = V_{pi}(t)e^{i\omega_{pi}t}.$$
5-13

This is easily soluble for the case that p is the initial state i

$$c_{i}(\tau) = 1 + \frac{1}{i\hbar} \int_{0}^{\tau} V_{ii}(t)dt$$
 5-14

and where p is another state

$$c_p(\tau) = \frac{1}{i\hbar} \int_0^{\tau} V_{pi}(t) e^{i\omega_{pi}t} dt$$
5-15

5.4 Implicit Time Dependent Perturbation

In the special case that the perturbation does not depend explicitly on time but is applied to the system for some interval of time (say τ)



then Eq. 5.15 immediately yields the result

$$c_{p}(\tau) = \frac{V_{pi}}{\hbar\omega_{pi}} (1 - e^{i\omega_{pi}\tau}).$$
 5-16

The probability for the transition is from state *i* to *p* based on a potential *V* applied for period τ is

$$P_{i \to p}(\tau) = \left| c_{p}(\tau) \right|^{2} = \frac{4 \left| V_{pi} \right|^{2}}{\hbar^{2}} \frac{\sin^{2} \left(\frac{\omega_{pi} \tau}{2} \right)}{\omega_{pi}^{2}} = 4 \frac{\left| V_{pi} \right|^{2}}{\hbar^{2}} D(\omega_{pi}, \tau) \qquad 5-17$$

Where the function D is defined by

$$D(\omega_{pi},\tau) \approx \frac{\pi}{2} \hbar \tau \delta(E_p - E_i)$$
 5-18

so that the rate of change of probability i.e. the transition rate is given by

$$\dot{P}_{i\to p}(\tau) = \frac{2\pi}{\hbar} \left| V_{pi} \right|^2 \delta(E_p - E_i).$$
 5-19

If we have a distribution of final states (which is a realistic assumption) with density $\rho(E)$ then the rate of transition to these states (G) is obtained by integrating over Eq. 5.19

$$\dot{P}_{i\to G} = \int \frac{2\pi}{\hbar} |V_{pi}|^2 \,\delta(E_p - E_i) \rho(E_p) dE_p = \frac{2\pi}{\hbar} \Big[|V_{pi}|^2 \,\rho(E_p) \Big]_{E_p = E_i} \qquad 5-20$$

5.5 Problems

5.1 A system of hydrogen atoms in the ground state is contained between the plates of a parallel plate capacitor. A voltage pulse is applied to the capacitor so as to produce a homogenous electric field

$$E = 0$$
 $t < 0$, $E = E_0 \exp(-t / \tau)$ $t > 0$

Show that, after a long time, the fraction of atoms in the 2p (m=0) state is, to first order,

$$\frac{2^{15}}{3^{10}} \frac{a_0^2 e^2 E_0^2}{\hbar^2 (\omega^2 + 1/\tau^2)}$$

where a_0 is the Bohr radius and $\hbar \omega$ is energy difference between the 2p and the ground state. You may assume that the ground state of hydrogen is given by

$$|100\rangle = \frac{2}{\sqrt{4\pi}} \frac{1}{a_0^{3/2}} \exp(-r/a_0)$$

and the 2p state by

$$|210\rangle = \frac{1}{\sqrt{4\pi}} \frac{1}{(2a_0)^{3/2}} \frac{r}{a_0} \exp(-r/2a_0) \cos\theta$$

6 Interaction of Matter with Radiation

A system that is of particular importance to study is that of an atom exposed to electromagnetic radiation. Let us suppose that we apply an electric field given by:

$$\dot{E} = \dot{E}_0 \cos(kx - \omega t) \,. \tag{6-1}$$

If we assume that this field is applied in the *z* direction then the perturbing potential will be:

$$V(t) = eEz\cos\omega t \,. \tag{6-2}$$

Using the results in the last chapter if we start in a state i the probability of making a transition to a state p can be calculated by first evaluating the quantity:

$$c_{p}(t) = \frac{eE_{0}}{2i\hbar} \langle p|z|i \rangle_{o}^{\tau} \left(e^{i\omega t} + e^{-i\omega t}\right) e^{i\omega_{p}t} dt = -\frac{eE_{0}}{2\hbar} \langle p|z|i \rangle \left[\left(\frac{e^{i(\omega + \omega_{p}i)\tau} - 1}{\omega_{p}i + \omega}\right) + \left(\frac{e^{i(\omega_{p}i - \omega)\tau} - 1}{\omega_{p}i - \omega}\right) \right]$$

$$6-3$$

To calculate the probability of being in the state k we simply have to find the absolute magnitude (squared) of Eq. 6-3.

Note how in the presence of radiation the probability of making the transition becomes very large (and perturbation theory may break down) when the frequency of the radiation matches either +/- the

energy of the transition. In contrast, the transition probability is zero if the matrix element is zero. This is an example of a *selection rule* in quantum mechanics.

6.1 Emission and Absorption of Radiation

It should now be clear that the transition probabilities that can be calculated from Eq. 6.3 are large when the frequency of the driving oscillation matches that of the transition. The probabilities diverge when $\omega_{pi}=\pm\omega$. The positive frequencies are viewed as those where $E_p>E_i$. If the final state is of higher energy than the initial state then we have absorption of radiation. Negative frequencies where $E_p < E_i$ correspond to the emission of radiation.





To compute the probabilities for emission and absorption we can take the part of Eq. 6.3 that dominates. For absorption the term that contains ω_{pi} - ω in the denominator dominates; for emission the term that contains ω_{pi} + ω dominates.

The probability of absorption is then given by:

$$P_{i \to p}(\tau) = \frac{e^2}{\mathbf{h}^2} \left| \langle p | z | i \rangle \right|^2 E_0^2 \frac{\sin^2 \left[\frac{1}{2} \left(\omega_{pi} - \omega \right) \tau \right]}{\left(\omega_{pi} - \omega \right)^2}$$

$$6-4$$

and the probability of emission is given by:

$$P_{i\to p}(\tau) = \frac{e^2}{\mathbf{R}^2} \left| \left\langle p \left| z \right| i \right\rangle \right|^2 E_0^2 \frac{\sin^2 \left[\frac{1}{2} \left(\omega_{pi} + \omega \right) \tau \right]}{\left(\omega_{pi} + \omega \right)^2}.$$
6-5

We can repeat the above calculation in a more general fashion if we do not have a monochromatic source of radiation. We do this by first noting that the energy density of an electric field is given by:

$$\rho(E) = \frac{1}{2}\varepsilon_0 E_0^2. \qquad 6-6$$

The energy density in an incoherent wave - containing many frequencies - is of the form

$$\rho = \frac{1}{2} \varepsilon_0 \int_0^\infty E_0^2(\omega) d\omega. \qquad 6-7$$

Thus the transition probabilities in Eq. 6.4 and 6.5 become

$$P_{i \to p}(\tau) = \frac{e^2}{\mathbf{n}^2} \left| \left\langle p \left| z \right| i \right\rangle \right|^2 \int_0^\infty d\omega E_0^2(\omega) \frac{\sin^2 \left[\frac{1}{2} \left(\omega_{pi} \pm \omega \right) \tau \right]}{\left(\omega_{pi} \pm \omega \right)^2}.$$
6-8

Referring back to Eq. 5.18 we see that Eq. 6.8 becomes

$$P_{i\to p}(\tau) = \tau \frac{\pi}{2} \frac{e^2}{\mathbf{n}^2} \left| \left\langle p \left| z \right| i \right\rangle \right|^2 E_0^2 \left(\left| \boldsymbol{\omega}_{pi} \right| \right) \quad .$$
 6-9

We can convert Eq. 6-9 to an expression containing a photon flux. If $N(\omega)d\omega$ is the number of photons in the frequency range ω to ω +d ω normal to the direction of wave propagation per unit time then the energy density of the photons in this range is

$$\hbar\omega \frac{1}{c}N(\omega)d\omega. \qquad 6-10$$

Remembering that the energy density is given by Eq. 6.6 we can then put

$$E^{2}(\omega) = \frac{2}{\varepsilon_{0}c} \hbar \omega N(\omega)$$
 6-11

which means that the transition probability becomes:

$$P_{i \to p} = \tau \frac{\pi e^2}{\varepsilon_0 c \mathbf{h}} |\omega_{pi}| N(|\omega_{pi}|) |\langle p|z|i \rangle|^2.$$
6-12

Thus the transition rate is simply

$$\dot{P}_{i\to p} = \frac{\pi e^2}{\varepsilon_0 c \hbar} \left| \omega_{pi} \left| N(|\omega_{pi}|) \right| \left\langle p | z | i \right\rangle \right|^2 \quad .$$
6-13

6.2 Problems

6.1 Show that Eq. 6-13 may be extended to the case where the atoms (or the radiation) are randomly oriented and that this gives rise to the result (see Mandl Sec. 9.5)

$$\dot{P}_{i\to p} = \frac{4}{3} \pi^2 \alpha \left| \omega_{pi} \right| N(|\omega_{pi}|) \left| \left\langle p \left| \dot{R} \right| i \right\rangle \right|^2$$
7 Phase Space

To use Fermi's Golden Rule we need to be able to evaluate the density of states. In many cases the density may be approximated by the density of final states for a free particle (for example if the particle is weakly bound or weakly interacting) which can be calculated. The density of states refers to the number of available states in the space spanned by both momentum and position co-ordinates - and is known as *phase space*.

To make this more explicit let us consider a particle of momentum p inside a cubic volume with sides of length L. The allowed values of the momentum (in the *x*-direction) are given by:

$$p_x = \hbar k_x = \frac{2\pi \hbar n_x}{L}$$
 7-1

and likewise for p_y and p_z . The numbers n_x , n_y , n_z are all positive integers. Every combination of these integers represents a different state. The number of states in one dimension (x) in an interval dp_x is given by the differential of Eq. 7-1 namely

$$dp_x = \frac{2\pi\hbar}{L} dn_x.$$
 7-2

In three dimensions the total numbers of states dN is thus given by:

$$dN = dn_x dn_y dn_z = \left(\frac{L}{2\pi\hbar}\right)^3 dp_x dp_y dp_z$$
 7-3

where if we set the volume of the confining cube to be V then:

$$dN = dn_x dn_y dn_z = V \left(\frac{1}{2\pi\hbar}\right)^3 dp_x dp_y dp_z$$
 7-4

we can interpret the above equation as

$$dN = \frac{volume_{phase space}}{h^3}$$
 7-5

where Eq. 7.5 is read as stating that the number of states available equals the phase space volume scaled by Plank's constant.

In spherical co-ordinates (that we often use because of the spherical symmetry inherent in many problems in nature) we know that

$$d^{3}p = dp_{x}dp_{y}dp_{z} = p^{2}dpd\Omega = p^{2}dpd(\cos\theta)d\phi$$
 7-6

so that now we may rewrite Eq. 7.4 as:

$$dN = \frac{V}{h^3} p^2 dp d\Omega.$$
 7-7

We can convert this to an energy density by dividing through by dE:

$$\rho(E) = \frac{dN}{dE} = \frac{V}{h^3} p^2 \frac{dp}{dE} d\Omega.$$
 7-8

Remembering that classically $E=p^2/2m$ then if we let the velocity of the particle be *v*:

$$\frac{dp}{dE} = \frac{1}{v}$$
7-9

then equation 7.8 can simply be rewritten as

$$\rho(E) = \frac{V}{h^3} \frac{p^2}{v} d\Omega.$$
 7-10

This is an extremely useful formula, as we shall see in the next chapter. As it stands Eq. 7-10 contains an *arbitrary* quantization volume, V. We will see that the matrix element, when calculated for a real process, also contains a corresponding factor I/V. This leads to the cancellation of the arbitrary factor. It is vital that this volume does not appear in the final answer. We would like to use Fermi's Golden Rule to calculate real transition rates for real processes, and it would be inconsistent if the final answer depended on the artefact V. Sometimes Eq. 7-10 is written in the entirely equivalent form

$$\rho(E) = \frac{V}{\left(2\pi\hbar\right)^3} \, pmd\Omega \tag{7-11}$$

7.1 Problems

7.1 If an eigenstate of a system is given by

$$\psi(r) = const \times e^{\frac{p}{r}/\hbar}$$

then determine the constant of normalisation in a cubic box of side L.

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8 Scattering Theory

Our method for understanding Physics on the sub-macroscopic level is usually to collide a beam or particles (photons, electrons, protons, etc.) onto a target and study the products that are scattered into different directions.

In the next few chapters we will learn how a detailed study of these scattering processes can yield information about the nature of the scatter and hence the nature of the scattering potential. For example, if the target or the colliding particles, contain substructure we may observe a different distribution of collision products than we may have otherwise expected. The classic example of this is Rutherford's famous experiment where alpha particles were scattered off a gold foil. To develop our scattering theory we first need to define several terms that we are going to use when a measurement is made.

8.1 Cross-Section

Consider a beam of particles of mass *m* and momentum *p* scattering off an infinitely massive scattering centre located at the origin. Without the scattering potential the system is simply that of a plane wave with wave vector k=p/m and flux *I*. The *flux* specifies the number of particles crossing a unit area per unit time. If we assume that *n* is the number of particles scattered into a specific solid angle Ω per unit time (see Figure 8-1) then the differential cross-section is defined by the following equation

38 Scattering Theory Chap.8

$$\sigma(\theta, \varphi) d\Omega = \frac{n(\theta, \varphi)}{I} d\Omega$$
8-1

i.e. the differential cross-section is defined by the ratio of the scattered particles to the incoming flux. If we double the incoming flux then we expect to double the number of scattered products observed per unit time. In this way the cross-section is independent of the incoming intensity and reflects only the nature of the underlying scattering process.



Figure 8-1

The total cross-section (i.e. we look at all scatter products over all directions) is simply the integral of the differential cross-section i.e.

$$\sigma_{\text{total}} = \int \sigma(\theta, \phi) d\Omega$$
. 8-2



A typical cross-section that we shall calculate later (see Problem 8.5) is shown below:

Figure 8-2: Differential cross section for the scattering of an electron off a hard sphere.

Note how in Figure 8-2 the cross-section only varies with the outgoing polar angle. There is no dependence on the azimuthal angle due to spherical symmetry.

8.2 The Born Approximation

We can now use our time dependent perturbation theory to calculate the cross-sections. If we combine Fermi's Golden Rule (Eq. 5-20) with our expression for phase space (Eq. 7-11) we get for a state *i* scattering to a state *p* as in Figure 8-1 via a time independent potential S(r)

$$n(\theta,\varphi)d\Omega = \frac{2\pi}{\hbar} \left[\left\langle p \left| S(\vec{r}) \right| i \right\rangle \right]^2 \frac{V}{\left(2\pi\hbar\right)^3} \frac{p^2}{v} d\Omega \Big|_{E_p = E_i} \qquad 8-3$$

Note that in Eq. 8-3 V is the arbitrary quantization volume not the potential. The wavefunction for a single free particle travelling in a direction r with momentum p is given by

$$\left| p \right\rangle = \frac{e^{i\vec{p}\cdot\vec{r}/\hbar}}{V^{1/2}} \tag{8-4}$$

(see Problem 7.1) where this gives a density of one particle per volume V. Then Eq. 8-3 may be rewritten

$$n(\theta, \varphi) d\Omega = \frac{d\Omega}{\left(2\pi\hbar^2\right)^2} \frac{p^2}{vV} \left| \int d^3 r S(r) e^{i(p_i - p_p) \cdot r/\hbar} \right|_{p_p = p_i}^2.$$
 8-5

If the velocity of the particle is v=p/m a volume p/m of beam crosses unit area normal to p in unit time. Therefore the flux is

$$I = \frac{p/m}{V}.$$
 8-6

Substituting Eq. 8-6 into Eq. 8-5 we can extract the differential cross-section

$$\boldsymbol{\sigma}(\boldsymbol{\theta},\boldsymbol{\varphi}) = \frac{m^2}{\left(2\pi\hbar^2\right)^2} \left\| \int d^3 r S(r) e^{i(p_i - p_p) \cdot r/\hbar} \right\|_{p_p = p_i}^2.$$
8-7

Note that Eq. 8-7 is independent of the arbitrary normalisation volume - which is what we expect since a physical quantity cannot depend on the normalisation procedure. This equation was derived by Max Born and is known as the *Born Approximation*.

8.3 Matrix Element in The Born Approximation

The matrix element itself has an interesting feature. It may be written

$$\widetilde{S}(K) = \int d^3 r S(r) e^{iK \cdot r}$$
8-8

where we have put

$$\mathbf{h}\vec{K} = \vec{p}_i - \vec{p}_p \qquad 8-9$$

For a central potential we first write

$$K \cdot r = Kr \cos \theta \tag{8-10}$$

then

$$\widetilde{S}(\vec{K}) = \int r^2 dr d\Omega S(r) e^{iKr\cos\theta}$$
8-11

and thus integrating over $\cos\theta$ we have

$$\widetilde{S}(\dot{K}) = 2\pi \int \frac{r^2}{iKr} dr S(r) \Big[e^{iKr} - e^{-iKr} \Big] = \frac{4\pi}{K} \int S(r) \sin(Kr) r dr. \qquad 8-12$$

The scattering matrix element only depends on the modulus of K where we remind the reader that

$$\left(\hbar\vec{K}\right)^{2} = \left(\vec{p}_{p} - \vec{p}_{i}\right)^{2} = 2p^{2}(1 - \cos\theta) = 4p^{2}\sin^{2}\frac{\theta}{2}.$$
8-13

8.4 Time Independent Approach

Another very useful way to calculate the scattering of one particle is a time independent approach. In this method we assume that we have an infinite beam (rather than a single wavepacket) of particles. This is very like an experiment. The incoming wavefunction can be written

$$\psi_0(\vec{r}) = e^{ikz} \qquad 8-14$$

where the wavenumber k is given by

$$k = \left(2mE / \mathbf{R}^2\right)^{1/2}.$$
 8-15

This wavefunction represents a particle moving along the *z*-direction with uniform intensity and energy. Without any perturbing potential the Schrödinger equation reads (see problem 8.3)

$$\left(\nabla^2 + k^2\right)\psi_0 = 0 \tag{8-16}$$

and in the presence of a time independent potential we have

$$\left(\nabla^2 + k^2\right)\psi = \frac{2m}{\hbar^2}V\psi. \qquad 8-17$$

As we switch off the potential gradually we expect the solution of Eq. 8-17 to tend to Eq. 8-14 i.e.

$$\psi \to \psi_0 = e^{ikz} \tag{8-18}$$

To proceed we need to solve Schrödinger's Equation in Eq. 8-17.

8.5 Formal Solution of Schrödinger's Equation

Let us solve the Schrödinger equation by reference to a problem we understand well, that of an electrostatic potential from a distributed charge. The solutions to Poisson's Equation (which looks a little like Eq. 8-17)

$$\nabla^2 \psi = -\frac{1}{\varepsilon_0} \rho(\vec{r})$$
 8-19

are easy. They are obtained by considering the electrostatic potential from a point unit charge at s i.e.

$$\nabla^2 \psi = -\frac{1}{\varepsilon_0} \delta(\vec{r} - \vec{s}). \qquad 8-20$$

We know the solution to this is:

$$\psi = \frac{1}{4\pi\varepsilon_0 |\vec{r} - \vec{s}|}$$

as we know the potential due to a point charge! The potential due to a distributed charge is then given by the integral:

$$\Psi(r) = \int \frac{1}{4\pi\varepsilon_0 |r-s|} \rho(s) d^3 s \,. \tag{8-22}$$

Let us now consider the problem we are interested in, namely that of solving Schrödinger's Equation. Let us rewrite Eq. 8-17 as

$$\left(\nabla^2 + k^2\right)\psi(\vec{r}) = F(\vec{r}). \qquad 8-23$$

By analogy with our solution of Poisson's Equation we first solve:

$$\left(\nabla^2 + k^2\right)\psi(r) = \delta(r-s). \qquad 8-24$$

We can verify by direct substitution (see problem 8-4) that the solution is

$$\psi = -\frac{e \pm^{ikr}}{4\pi r}.$$
 8-25

This corresponds to spherical incoming and outgoing waves from a point "source". From an extended source:

$$\psi(r) = -\frac{1}{4\pi} \int \frac{e^{ik|r-s|}}{|r-s|} F(s) d^3s$$
8-26

where

$$F(\dot{s}) = \frac{2m}{\hbar^2} V(\dot{s}) \psi(\dot{s}) . \qquad 8-27$$

To get the general solution of the Schrödinger Equation (Eq. 8-17) we can add the solution to the unperturbed part (Eq. 8-18) to the "scattered" wavefunctions that arise from solutions to Eq. 8-26. In physical terms we are adding to the incoming wavefunction a component that represents the scattered wave

$$\Psi(r) = e^{ikz} - \frac{1}{4\pi} \int \frac{e^{ik|r-s|}}{|r-s|} F(s) d^3s \,.$$
8-28

8.6 Scattered Waves

Equation 8-28 is especially important. The second term on the right is very similar to Eq. 8-25 and represents an outgoing wave whose amplitude is modulated by some function $f(\theta, \phi)$.

$$\Psi(r) \approx e^{ikz} + \frac{e^{ikr}}{r} f(\theta, \phi).$$
8-29

The function $f(\theta, \phi)$ is known as the scattering amplitude and is related to the scattering cross-section by

$$\sigma(\vartheta, \phi) = \left| f(\theta, \phi) \right|^2$$
 8-30

Note that the scattering amplitude can be complex. The measured quantity (the cross-section) is determined by taking the square of the absolute magnitude. This means that when we have one or more scattering amplitudes contributing to a physical process that we will need to add the scattering amplitudes *before* computing the cross-section. This leads to interference effects.

In the case that we are observing the system a long way away from the scattering centre we note that if r>>s then:

$$|\dot{r} - \dot{s}| = r \left[1 - \frac{2}{r^2} \dot{r} \cdot \dot{s} + \frac{s^2}{r^2} \right]^{1/2} \approx r \left[1 - \frac{\dot{r} \cdot \dot{s}}{r^2} \right]$$
 8-31

The exponential term in the integral 8-28 can then be simplified

$$\frac{e^{ik|r-s|}}{|r-s|} \approx \frac{e^{ikr}}{r} e^{-ikr\cdot s/r}$$
8-32

which if we put

$$k' = kr / r \qquad 8-33$$

becomes

$$\frac{e^{ikr}}{r}e^{-ik\cdot s}.$$
8-34

Substituting the form Eq. 8-34 into Eq. 8-28 yields

$$\psi(r) = e^{ikz} + \frac{e^{ikr}}{r} \left[-\frac{2m}{4\pi\hbar^2} \int e^{-ik^2 \cdot s} V(s) \psi(s) d^3 s \right] = e^{ikz} + \frac{e^{ikr}}{r} f(\theta, \phi)$$
8-35

$$f(\theta,\phi) = -\frac{m}{2\pi\hbar^2} \int e^{-ik \cdot s} V(s)\psi(s) d^3s \qquad 8-36$$

8.7 Scattering Amplitude for Small Perturbations

We can take Eq. 8-36 and apply to the very important case where the potential is very weak. This means that the incident wave is only slightly distorted. We can put

$$\psi(s) \to e^{ik \cdot s}$$
 8-37

in Eq. 8-35 yielding

$$f(\theta,\phi) = -\frac{m}{2\pi\hbar^2} \int e^{-ik\cdot s} V(s) e^{ik\cdot s} d^3 s = -\frac{m}{2\pi\hbar^2} \int d^3 s e^{ik\cdot s} V(s)$$

$$K = k - k'$$
8-38

This is the Born Approximation for the scattering amplitude and yields our previous result for the cross-section when we take the absolute magnitude of the scattering amplitude (c.f. Eq. 8-7). The advantage of the form Eq. 8-36 is that if we have a number of different scattering amplitudes we can now sum then to obtain the correct cross-section.

8.8 Problems

8.1 Particles are incident on a spherically symmetric potential

$$V(r) = \frac{\beta}{r} \exp(-\gamma r)$$

where β and γ are constants. Show that in the Born approximation, the differential scattering cross-section for the scattering vector **K** is given by

i.e.

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$$\sigma(\theta,\phi) = \left\{\frac{2m\beta}{\mathbf{n}^2(K^2+\gamma^2)}\right\}^2$$

Use this result to derive the Rutherford formula for the scattering of alpha particles. Although this gives the right result, see if you can think of any reasons why this might not be a rigorous result.

8.2 Obtain in the Born approximation the differential cross-section for the scattering of the particles of mass m by the potential

$$V(r) = V_0 e^{-\alpha r}$$

- **8.3** Show that Eq. 8-16 is the Schrödinger Equation in 3 dimensions.
- **8.4** Prove that Eq. 8-25 is a solution of Eq. 8-24.
- 8.5 Calculate the differential cross-section for the scattering of a particle of energy E with mass
- *m* by a hard sphere of radius *a*.
- 8.6 A uniform beam of particles with momentum p are scattered by a potential V(r). The number scattered into a solid angle d Ω is given by

$$n(\theta,\phi)d\Omega = \frac{2\pi}{\hbar} \left[\left| \left\langle u_{p'} \left| V(r) \right| u_p \right\rangle \right|^2 \left(\frac{L}{2\pi\hbar} \right)^3 p' m d\Omega \right]_{p'=p}$$

- i) Explain very briefly the origin of the arbitrary length L and the meaning of p'
- ii) Assuming that the flux of incoming particles is given by $I = (p / m)L^3$ write down an expression for the differential cross section.
- iii) Defining $\mathbf{R}\vec{K} = \vec{p} \vec{p}'$ show that the cross-section only depends on the Fourier transform of the scattering potential
- iii) Calculate the differential cross-section for the elastic scattering of a charged particle off a Coulomb potential.[You may assume that

$$\int_{0}^{\infty} \sin bx dx = 1/b].$$

v) What are the limitations of this calculation?

9 Partial Waves

In the last chapter we saw that the scattering of a particle (or a beam of particles) off a scattering centre resulted in a solution of the Schrödinger Equation of the form

$$\Psi = e^{ikz} + f(\theta, \phi) \frac{e^{ikr}}{r}$$
9-1

where we separated the final wavefunction into two parts. The forwards going (unscattered part) of the amplitude and spherical waves. The spherical waves emanate from the scattering centre and are modulated by the scattering amplitude. We discovered we could calculate the scattering amplitude from the total cross-section. There is an extremely useful way of determining the scattering amplitude that attempts to resolve the scattering components of known angular momentum. This method of partial waves is what we shall discuss below.

Let us assume that we can expand the angular part of the incoming wave using as set of orthonormal solutions (spherical harmonics) to the Schrödinger Equation centred around the scattering centre i.e.

$$e^{ikz} = e^{ikr\cos\theta} = \sum_{l=0}^{l=\infty} u_l(kr)Y_l^0(\theta,\phi)$$
9-2

where the functions u_l can be determined by taking the inner product of Eq. 9-2 with another spherical harmonic

$$u_l(kr) = \int d\Omega Y_l^0(\theta, \phi) e^{ikr} \,. \qquad 9-3$$

Note that the expansion Eq. 9-2 has only been performed over the z=0 components of the spherical harmonics. If we assume the scattering potential is radially symmetric there can be no azimuthal dependence of the scattering.

At very low energies of the incident scattering particle we expect that only the lower angular momentum states will contribute to the expansion. In the limit let us consider the case of s-wave scattering where only the angular momentum zero state zero can contribute. Using the fact that

$$Y_0^0 = \frac{1}{\left(4\pi\right)^{1/2}} \qquad \qquad 9-4$$

we find

$$u_0(kr) = \frac{1}{(4\pi)^{1/2}} \int d(\cos\theta) e^{ikr\cos\theta} d\phi = (4\pi)^{1/2} \frac{\sin kr}{kr}$$
 9-5

i.e. at very low energies the incoming wave is given by

$$e^{ikz} \approx \frac{\sin kr}{kr}$$
. 9-6

If we compare this with our general form for the incident and scattered form of the wavefunction namely:

$$\Psi = e^{ikz} + \frac{e^{ikr}}{r} f(\theta, \phi)$$
 9-7

we can then write using our s-wave approximation

$$\psi = \frac{e^{ikr} - e^{-ikr}}{2ikr} + \frac{e^{ikr}}{r}f_0 = \frac{1}{2ik} \left[-\frac{e^{-ikr}}{r} + \frac{e^{ikr}}{r} (1 + 2ikf_0) \right]$$
9-8

We note that Eq. 9-8 has a total wavefunction made up of an incoming wave and an outgoing wave. As long as no particles are destroyed or created during the scatter the incoming flux must equal the outgoing flux i.e.

$$\left|1+2ikf_{0}\right|=1$$
9-9

or expressing this as an exponential may be written as

where the scattering amplitude is therefore

$$f_o = \frac{e^{2i\delta_0} - 1}{2ik} = e^{i\delta_0} \frac{\sin \delta_0}{k}$$
9-11

and (if we wish) we can write the total amplitude

$$\psi = \frac{1}{2ik} \left[\frac{-e^{-ikr}}{r} + \frac{e^{ikr}}{r} e^{2i\delta_0} \right] = e^{i\delta_0} \frac{\sin(kr + \delta_0)}{kr}.$$
9-12

Comparing this with Eq. 9-6 we see the effect of the scatter has been to change the phase of the scattered wave by δ_0 and the amplitude by an amount that depends on this phase shift. We can calculate the differential cross-section for the s-wave approximation by taking the square of the s-wave amplitude (Eq. 9-11)

$$\sigma(\theta, \phi) = \left(\frac{\sin \delta_0}{k}\right)^2 \qquad 9-13$$

9.1 Scattering off a hard sphere

A particularly simple and illuminating example is given by the problem of calculating the s-wave scattering off an impenetrable sphere. This is represented by an infinite potential at some radius a. The wavefunction must therefore be zero within, and on the boundary of, the sphere. Assuming we

can use the low energy s-wave approximation (Eq. 9-12) this can only be the case if $ka=-\delta_0$. Inserting this into Eq. 9-13 gives

$$\sigma(\theta,\phi) = \left(\frac{\sin ka}{k}\right)^2 \qquad 9-14$$

and the total cross-section is

$$\sigma_{tot} = \frac{4\pi \sin^2 ka}{k^2} \qquad 9-15$$

which in the limit that k becomes very small indeed becomes

$$\sigma_{tot} = 4\pi a^2 \qquad 9-16$$

This is very close to the classical result but demonstrates that quantum mechanics does not always predict what we might expect from classical arguments.

9.2 Problems

9.1 Find the s-wave phase shift for an attractive square wave potential $V=-V_0, r<a$, and V=0 for r>a. Show that the cross-section for s-wave scattering vanished if the scattering energy *E* is such that

$$\frac{\tan Ka}{Ka} = 1$$

where

$$K = \left[\frac{2m}{\mathbf{n}^2} \left(E + V_0\right)^2\right]^{1/2}$$

This is called the Ramsauer-Townsend effect and occurs in the scattering of electrons by rare gas atoms.

10 dentical Particles

To make any further progress in Quantum Mechanics beyond the calculational level we have to investigate, in a little more depth, some of the more "quantum" like features of the wavefunction. In particular we are going to be interested in the properties of the wavefunction that have no clearly defined classical analogue. We begin this with a short introduction to the idea of identical particles.

10.1 Classically Identical Particles

In classical mechanics the idea of identical particles does exist. One can imagine two objects, for example apples, which have exactly the same appearance, shape, weight etc. These apples would be labelled in normal usage "identical" insofar as if one were presented with one apple one could not say which one it was. This linguistic concept of "identical" is however *not* the same as our physics concept.

Consider two apples in a large space. One could, at a particular instant, label one (at least in one's mind) A and the other B. Even though there is no discernible difference between A and B one could then - for all subsequent times - be sure which apple was A and which was B. This could be achieved by very carefully following each apple. Since there is classically a unique and smooth trajectory in E^3 as a function of time all one would have to do is apply the Newton's laws at a particular instant t to predict (and label) the position of an apple at time t+dt. Thus one can differentiate between A and B for all time.

10.2 Quantum Mechanically Identical Particles

Quantum mechanically the differentiation between A and B is no longer possible. This is because at any instant the wavefunctions are non-localised. The spatial extent of a wavefunction in free space is normally infinite. Thus if we have two particles A and B that share identical properties (quantum numbers) we are not able to follow their wavefunctions unambiguously for all times. Suppose we were able to localise the wavefunction of A to some region of space x_A to $x_A + dx_A$ and B to x_B to $x_B + dx_B$. If at some small instant of time later on we calculate the probability, $P_A(y)$, that particle A is in another volume y to y+dy and the probability $P_B(y)$, that particle B may be observed at the same point we will general find that both $P_A(y)$, $P_A(y)$ are non-zero. Namely, if we do observe a particle at point y we cannot be sure whether it was the particle A or the particle B. One might argue that one could on the basis of probability assign a likelihood of one particle being A and the other B: for example an electron that started out in a cathode ray tube on Earth is more likely to be observed on earth than in Alpha Centauri. However likelihood is not the same as the absolute certainty that we had in the classical example above.

10.3 Wavefunction for Identical Particles

With state vectors we can examine indistinguishability a little more carefully. We assume that we have two particles which we can label^f (but not distinguish) as 1 and 2. Let us also assume that the particles can be in states $|\Psi_m\rangle$ and $|\Psi_n\rangle$ which are distinguishable because they have different quantum numbers. If our particles are indistinguishable then the state $|\Psi_m^1\rangle|\Psi_n^2\rangle$ must be entirely equivalent to $|\Psi_m^2\rangle|\Psi_n^1\rangle$ i.e. it won't affect the outcome of any measurement if we interchange labels 1 and 2 because we cannot tell experimentally which particle is in which state. Thus for the total wavefunction for two-particles we have a linear superposition of the two possibilities

$$\left|\Psi^{12}\right\rangle = c_{mn} \left|\psi_{m}^{1}\right\rangle \left|\psi_{n}^{2}\right\rangle + c_{nm} \left|\psi_{n}^{1}\right\rangle \left|\psi_{m}^{2}\right\rangle.$$
 10-1

This mixture contains equal proportions of each product state (since they are equally likely) thus

$$\left|c_{mn}\right| = \left|c_{nm}\right|. \tag{10-2}$$

In addition since the total wavefunction in Eq. 10-1 must be normalised we see that

$$\left|c_{mn}\right|^{2} + \left|c_{nm}\right|^{2} = 1$$
10-3

so that

$$|c_{mn}| = |c_{nm}| = \frac{1}{\sqrt{2}}.$$
 10-4

^f The reader may wonder how we can write down a state vector for a particle that we cannot distinguish for another. Does this not imply that we have somehow differentiated one particle from another by labelling one particle differently from another? This not an easy question to answer. Here on may simply assert that there is a *reality* associated with a particular particle, and this reality described by its wavefunction. Each wavefunction develops according the Schrödinger Equation. However we cannot directly access this wavefunction. We have to make an observation on the system as a whole and in making the observation the "information" about which wavefunction (or particle) was observed is lost.

10.4 Fermions and Bosons

There are two ways of enforcing Eq. 10-4. Either $c_{mn}=c_{nm}$ or $c_{mn}=-c_{nm}$. We can write down explicitly what Eq. 10-1 becomes in either case. For the case that $c_{mn}=c_{nm}$ we have

$$\left|\Psi^{12}\right\rangle = \frac{1}{\sqrt{2}} \left(\left|\psi_{m}^{1}\right\rangle\right|\psi_{n}^{2}\right) + \left|\psi_{n}^{1}\right\rangle\left|\psi_{m}^{2}\right\rangle\right). \qquad 10-5$$

In this case if we exchange particles 1 and 2 the wavefunction (Eq. 10-5) remains identical and is said to be symmetric on the exchange of particles. Particles whose two-particle state vectors possess this property are known as *bosons*. When c_{mn} =- c_{nm} we have

$$\left|\Psi^{12}\right\rangle = \frac{1}{\sqrt{2}} \left(\left|\psi_{m}^{1}\right\rangle\right|\psi_{n}^{2}\right) - \left|\psi_{n}^{1}\right\rangle\left|\psi_{m}^{2}\right\rangle\right).$$
 10-6

The reader will notice that if we now exchange particle 1 and 2 the wavefunction changes sign. It is said to be anti-symmetric on the exchange of particles. Particles whose two-particles state vectors possess this property are known as *fermions*.

10.5 Pauli Exclusion Principle

Perhaps one of the most important distinction between bosons and fermions is evident in the comparison of Eq. 10-5 and 10-6. In the case that the two particles are in an identical eigenstate the bosonic two particle wavefunction becomes

$$\left|\Psi^{12}\right\rangle = \left|\psi_{m}^{1}\right\rangle \left|\psi_{m}^{2}\right\rangle.$$
 10-7

This is evidently non-zero and is simply the product state of the two separate particles in state m. For fermions the product wavefunction is altogether more interesting:

$$\left|\Psi^{12}\right\rangle = \frac{1}{\sqrt{2}} \left(\left|\psi_{m}^{1}\right\rangle\right|\psi_{m}^{2}\right) - \left|\psi_{m}^{1}\right\rangle\left|\psi_{m}^{2}\right\rangle\right) = 0 \qquad 10-8$$

This means that the particles whose two particle wavefunctions are antisymmetric (i.e. fermions) are forbidden from occupying the same state, i.e. there is no probability that they can be found in the same state. This is often referred to as the Pauli Exclusion Principle. The exclusion - that two fermions are forbidden from being in the same state - should be thought of as consequence of our ideas about indistinguishability. In the next chapter we shall revisit bosons and fermions and see their relation to the spin of the particles.

10.6 Problems

10.1 Explain why Eq. 10-5 becomes Eq. 10-7 when the two states *m* and *n* are identical.

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11 Spin

One of the most puzzling features of the Quantum World is the phenomenon of "spin". The idea, as always, is motivated by experiment: if we put an electron into a magnetic field we will see that it will be in one of two distinct states. If we were performing a spectroscopic experiment we would see the line "split" from the field free value with one band moving down and the other moving up. Classically we could understand this if the electron were to have a magnetic moment (μ) which could interact with the magnetic field B giving an energy to the electron of $\Delta E \propto \mu^2 B$. For there to be only two levels it means that the magnetic moment must be aligned in just two directions antiparallel to one another. It is natural pick the B field direction as this axis of quantization. Thus in our semi-classical picture we envisage two cases - one with the electron moment aligned parallel and in the other with it aligned anti-parallel to the magnetic field.



Figure 11-1: Semi-Classical view of an "electron" interacting with a magnetic field.

In this simple picture we can easily understand how we arrive at the nomenclature spin. Classically a charged object that spins creates a magnetic moment (the small magnetic field produced by the

moving charge) which interacts with the externally applied magnetic field. From this we clearly expect spin to be related (somehow) to angular momentum and other rotational effects.

But there are problems with this semi-classical picture. First there is no evidence that the electron has any spatial dimension. Second there is the issue of why the "spin" is quantized. To tackle these problems we will first review the quantum mechanical view of angular momentum.

11.1 Angular Momentum Commutation Relations

Classically the angular momentum of a particle about a point is given by

$$\dot{L} = r \times \dot{p} \tag{11-1}$$

and in quantum mechanics we postulate that there will be an angular momentum operator L defined by

$$L = r \times p = -i\hbar r \times \nabla$$
 11-2

where we have replaced the momentum by its quantum mechanical operator. In Cartesian coordinates it is then easy to explicitly write down the form of the angular momentum operator

$$L = \begin{bmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_z & p_y & p_z \end{bmatrix} = -i\hbar \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \end{vmatrix}.$$
 11-3

which gives us the three forms for the angular momentum operators

$$L_{x} = -i\hbar \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$$

$$L_{y} = -i\hbar \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right)$$

$$L_{z} = -i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$$
11-4

These are our familiar forms for the angular momentum operators and, as we have done before, we can also define

$$L^2 = L_x^2 + L_y^2 + L_z^2. ag{11-5}$$

From these definitions (Eq. 11-4 and Eq. 11-5) it is easy to prove that

$$\begin{bmatrix} L_x, L_y \end{bmatrix} = i\mathbf{n}L_z$$

$$\begin{bmatrix} L_y, L_z \end{bmatrix} = i\mathbf{n}L_x$$

$$\begin{bmatrix} L_z, L_x \end{bmatrix} = i\mathbf{n}L_y$$
11-6

and that using these commutation relations that

$$[L^2, L_x] = [L^2, L_y] = [L^2, L_z] = 0.$$

11-7

These are very important commutation relations to which we will return later.

11.2 Angular Momentum in Spherical Co-ordinates

In spherical (rather than Cartesian) co-ordinates the angular momentum operators are easy to identify. First we define the relationship between the spherical co-ordinates and the Cartesian ones:

$$\dot{e}_r = i \cos\phi \sin\theta + j \sin\phi \sin\theta + k \cos\theta$$
$$\dot{e}_{\theta} = i \cos\phi \cos\theta + j \sin\phi \cos\theta - k \sin\theta$$
$$\dot{e}_{\phi} = -i \sin\phi + j \cos\phi$$

11-8

where the quantities $\vec{e}_r, \vec{e}_{\theta}, \vec{e}_{\phi}$ are unit vectors in the radial, polar and azimuthal directions respectively. The inverse can also be written down:

$$i = \dot{e}_r \sin \theta \cos \phi + \dot{e}_\theta \cos \theta \cos \phi - \dot{e}_\phi \sin \phi$$

$$j = \dot{e}_r \sin \theta \sin \phi + \dot{e}_\theta \cos \theta \sin \phi + \dot{e}_\phi \cos \phi.$$

$$i1-9$$

$$\dot{k} = \dot{e}_r \cos \theta - \dot{e}_\theta \sin \theta$$

In spherical co-ordinates

$$\dot{\nabla} = \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{e}_\phi \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi}$$
 11-10

so the components of the angular momentum may be written using

$$\begin{split} \dot{L} &= -ihr \times \dot{\nabla} = -i\hbar r \dot{e}_r \times \left(\dot{e}_r \frac{\partial}{\partial r} + \dot{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \dot{e}_\phi \frac{1}{r\sin\theta} \frac{\partial}{\partial \phi} \right) \\ &= -i\hbar \left(\dot{e}_\phi \frac{\partial}{\partial \theta} - \dot{e}_\theta \frac{1}{\sin\theta} \frac{\partial}{\partial \phi} \right) \end{split}$$

The components of the angular momentum may be written

$$L_{x} = i \cdot L = i \hbar \left(\sin \phi \frac{\partial}{\partial \theta} + \cot \theta \cos \phi \frac{\partial}{\partial \phi} \right)$$

$$L_{y} = j \cdot L = -i \hbar \left(\cos \phi \frac{\partial}{\partial \theta} - \cot \theta \sin \phi \frac{\partial}{\partial \phi} \right).$$

$$II-I2$$

$$L_{z} = k \cdot L = -i \hbar \frac{\partial}{\partial \phi}$$

It is important to note that we have done nothing except express the operators in spherical coordinates. An expression for L^2 may be found from Eq. 11-11 noting that from Eq. 11-9 the derivatives of the unit vectors with respect to the spherical co-ordinates are not constant. Fom Eq. 11-8

$$\frac{\partial \dot{e}_{\theta}}{\partial \theta} = -\dot{e}_{r}, \qquad \frac{\partial \dot{e}_{\phi}}{\partial \phi} = \dot{e}_{\phi} \cos \theta$$

$$\frac{\partial \dot{e}_{\phi}}{\partial \theta} = 0, \qquad \frac{\partial \dot{e}_{\phi}}{\partial \phi} = -\dot{e}_{r} \sin \theta - \dot{e}_{\theta} \cos \theta$$
11-13

Hence

$$L^{2} = -\mathbf{\hat{n}}^{2} \left(\hat{e}_{\phi} \frac{\partial}{\partial \theta} - \hat{e}_{\theta} \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \right) \cdot \left(\hat{e}_{\phi} \frac{\partial}{\partial \theta} - \hat{e}_{\theta} \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \right)$$
$$= -\mathbf{\hat{n}}^{2} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^{2} \theta} \frac{\partial^{2}}{\partial \phi^{2}} \right]$$
11-14

In the case that we have a central force (where classically the angular momentum is conserved) we can write down the time independent Schrödinger Equation

$$H\Psi(r,\theta,\phi) = E\Psi(r,\theta,\phi)$$
 11-15

where the Hamiltonian (H) is given by

$$H = -\frac{\mathbf{h}^{2}}{2m}\nabla^{2} + V(r)$$

= $-\frac{\mathbf{h}^{2}}{2m}\left[\frac{1}{r^{2}}\frac{\partial}{\partial r}r^{2}\frac{\partial}{\partial r} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^{2}\theta}\frac{\partial}{\partial\phi^{2}}\right] + V(r)$ ¹¹⁻¹⁶

It is very important to note that in Eq. 11-16 the operator ∇^2 has been expressed in spherical coordinates. The second part of ∇^2 is simply proportional to the angular momentum operator (Eq. 11-14) so we can write

$$H = -\frac{\hbar^2}{2mr^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{L^2}{2mr^2} + V(r). \qquad 11-17$$

From examination of Eq. 11-17 we can deduce the Hamiltonian will commute will commute with L^2 , L_x , L_y , and L_z . This is because all the terms (except L^2) contain terms in *r* only and L^2 commutes with

all the angular momentum operators. From Ehrenfest's theorem^f this automatically means that L^2 is a constant of motion as are L_x , L_y , L_z .

11.3 Simultaneous Determination of the Components of Angular Momentum

Ehrenfest's theorem tells us that L^2 is a constant of motion, as are L_x , L_y and L_z . However this does not mean that we can determine all of these components simultaneously. In fact the commutation relations Eq. 11-6 tell us that the x, y, z components of the angular momentum do not commute with each other. We know that in cases such as this (for example with x and p_x) we do not expect to be able to simultaneously observe both variables. This is a feature of quantum mechanics. We will show that we can simultaneously observe L^2 and one directional component (which by convention is usually L_z).

We will discuss simultaneous eigenfunctions in Chapter 12 but it is worthwhile here to prove that the commutation relations Eq. 11-6 do embody a very important feature of quantum mechanics. Let us assume we have two operators A and B that both commute with the Hamiltonian. The condition that either A or B commute with the Hamiltonian is that their eigenfunctions are also eigenfunctions of the Hamiltonian: this may be seen (non rigorously) from

. .

$$H|u\rangle = E_{u}|u\rangle$$

$$A|u\rangle = a|u\rangle$$

$$AH|u\rangle = HA|u\rangle$$
11-18

therefore

^f Ehrenfest's Theorem tells us that if an operator commutes with the Hamiltonian the observable which it represents is a constant of motion. This may be proved easily and is done so in Chapter 12.

$$[A, H] = 0 11-19$$

if Eq. 11-19 is zero it must be that the last line of Eq. 11-18 holds and that is only possible if H and A have simultaneous eigenfunctions. Now if A and B both commute with the Hamiltonian we have only two choices. If they commute with each other they have will both have the same eigenfunctions which are also eigenfunction of the Hamiltonian. If they do *not commute* then B will have another set of eigenfunctions /v> i.e.

$$H|v\rangle = E_{v}|v\rangle$$
$$B|v\rangle = b|v\rangle$$
$$BH|v\rangle = HB|v\rangle$$

such that [B,H]=0 but these will not be same as the same functions as the |u>.

Thus if we make a measurement in a particular direction (for example z) we select (put) the system into a simultaneous eigenfunction of both L^2 and L_z . The corresponding eigenfunction will not be an eigenfunction of both the Hamiltonian, L^2 and the component L_a (where a is any other direction).

11.4 Angular Momentum and Rotation

There is a very deep connection between angular momentum and rotation. This is most obvious from the form of the angular momentum operator L_z that we wrote down in Eq. 11-12. If there is no dependence of the state on the azimuthal angle(i.e. along some particular direction) the expectation value of the angular momentum along that particular direction will be zero i.e. $\langle L_z \rangle = 0$. However if the state has an eigenvalue $m \hbar$ with respect to L_z we know that

$$-i\mathbf{n}\frac{\partial}{\partial\phi}|u\rangle = m\mathbf{n}|u\rangle \qquad 11-20$$

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which of course is trivially solved by

$$|u\rangle = |u(r,\theta)\rangle e^{im\phi}$$
 11-21

Now Eq. 11-21 embodies a very interesting feature. Under the angular momentum L_z operator the state is only changing by a fixed factor (the eigenvalue) and the ϕ dependence is only a phase factor, albeit one that depends on the value of the angular momentum projection *m*.

Let us consider what happens to a vector \mathbf{r} when it is rotated about a small angle around the z direction

$$r \to r + dr$$
 11-22

where

$$dr = \frac{\partial \dot{r}}{\partial \phi} d\phi \qquad 11-23$$

which, if we wished, we could write in terms of components from Eq. 11-9. Comparing Eq. 11-20 and Eq. 11-23 we see that the angular momentum operator L_z is "responsible" for generating rotations about the z axis². To be more formal Eq. 11-22 can be expressed in terms of a rotation operator (which of course can be applied to states as well as vectors). For an infinitesimal rotation α ,

$$\vec{r} \to D_{\alpha}\vec{r} = (1 - \frac{i\alpha}{\hbar}L_z)\vec{r}$$

$$D_{\alpha} = (1 - \frac{i\alpha}{\hbar}L_z)$$
11-24

Repeated application of the operator D_a gives for a finite angle α ,

$$D_{\alpha} = \exp\left(-\frac{i\alpha}{\hbar}L_{z}\right)$$
 11-25

² In fact L_z is often call the generator of infinitesimal rotations.

i.e. the finite rotation operator in quantum mechanics is a simple function of the angular momentum operator.

11.5 Eigenvalues of Angular Momentum Operators

The eigenvalues corresponding to the operators L^2 and L_z are well known. They are given by

$$L^{2}|l,m\rangle = l(l+1)\hbar^{2}|l,m\rangle$$

$$L_{z}|l,m\rangle = m\hbar|l,m\rangle$$

$$m = -l,-l+1,...,l-1,l$$
11-26

where the values in 11-26 can be derived by an explicit solution to the differential equation 11-14 with the spherical harmonics $Y_{lm}(\theta, \phi)$. However here we will use a somewhat more elegant technique to obtain the eigenvalues of the angular momentum operators.

Let us define two operators

$$L_{+} = L_{x} + iL_{y}$$

$$L_{-} = L_{x} - iL_{y}$$
11-27

where L_{+} and L_{-} are known as the raising and lowering operators of the angular momentum. The commutation relations for these operators are:

$$L_{+}L_{-} = L_{x}^{2} + L_{y}^{2} - i[L_{x}, L_{y}] = L^{2} - L_{z}^{2} + \hbar L_{z}$$

$$L_{-}L_{+} = L_{x}^{2} + L_{y}^{2} - i[L_{y}, L_{x}] = L^{2} - L_{z}^{2} - \hbar L_{z}$$
11-28

which yields

$$[L_{+}, L_{-}] = 2\hbar L_{z}.$$
 11-29

We also have

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$$\begin{bmatrix} L_{z}, L_{+} \end{bmatrix} = \begin{bmatrix} L_{z}, L_{x} \end{bmatrix} + i \begin{bmatrix} L_{z}, L_{y} \end{bmatrix} = i \mathbf{h} (L_{y} - i L_{x}) = \mathbf{h} L_{+}$$
$$\begin{bmatrix} L_{z}, L_{-} \end{bmatrix} = \begin{bmatrix} L_{z}, L_{x} \end{bmatrix} - i \begin{bmatrix} L_{z}, L_{y} \end{bmatrix} = i \mathbf{h} (L_{y} + i L_{x}) = -\mathbf{h} L_{-}$$
11-30

The two sets of commutator relations Eq. 11-29 and Eq. 11-30 are all we need to extract the values of the eigenvalues of the angular momentum. Let us restate the problem. We have the equations

$$L^{2}|u\rangle = \alpha |u\rangle$$

$$L_{z}|u\rangle = \beta |u\rangle$$
11-31

and we need to find the simultaneous eigenvalues α, β . This is done as follows. First we take the second of the equation in Eq. 11-31 and multiply both sides by the raising operator L_+ :

$$L_{+}L_{z}|u\rangle = \beta L_{+}|u\rangle.$$

We note that from Eq. 11-30

$$L_+L_z = L_z L_+ - \mathbf{n} L_+$$

so

$$\left(L_{z}L_{+}-\hbar L_{+}\right)|u\rangle = \beta L_{+}|u\rangle \qquad 11-32$$

which may be rewritten as

$$L_z L_+ |u\rangle = (\beta + \hbar) L_+ |u\rangle.. \qquad 11-33$$

Similarly

$$L_z L_- |u\rangle = (\beta - \mathbf{h}) L_- |u\rangle. \qquad 11-34$$

Equations 11-33 and 11-34 are interpreted as telling us that if $|u\rangle$ is an eigenfunction of L_z with eigenvalue β then $L_+|u\rangle$ is also an eigenfunction of L_z with eigenvalue $\beta + \mathbf{n} \cdot L_-|u\rangle$ is an eigenfunction of L_z with eigenvalue $\beta - \mathbf{n}$. This is why L_+ and L_- are known as the raising and lowering operators.

We can also apply the same method to the total angular momentum. Starting with

$$L^2 |u\rangle = \alpha |u\rangle \qquad 11-35$$

we multiply by the raising operator

$$L_{+}L^{2}|u\rangle = \alpha L_{+}|u\rangle. \qquad 11-36$$

We have not explicitly calculated the commutator $[L^2, L_+]$ but we note that since L^2 commutes with both L_x and L_y it must also commute with the raising and lowering operators. Eq. 11-36 can then be written as

$$L^{2}L_{+}|u\rangle = \alpha L_{+}|u\rangle \qquad 11-37$$

and we can find a similar relation for the lowering operator

$$L^2 L_{-} |u\rangle = \alpha L_{-} |u\rangle. \qquad 11-38$$

This shows that the states $L_+|u\rangle$ and $L_-|u\rangle$ are also simultaneous eigenstates of the total angular momentum.

We can now calculate the eigenvalues α, β . The eigenvalues of L_z are limited by the condition $\beta^2 \leq \alpha$. There must then exist some maximum value of β (say β_{max}) and a minimum value β_{min} . If $|u_{min}\rangle$ and $|u_{max}\rangle$ are the corresponding eigenfunctions we must have

$$L_{+} | u_{\max} \rangle = 0$$

$$L_{-} | u_{\min} \rangle = 0$$
11-39

i.e. we cannot get any higher than the highest state or any lower than the lowest state. Thus operating on the first of Eq. 11-39 by the lowering operator and the second by the raising operator we see:

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$$L_{-}L_{+}|u_{\max}\rangle = 0$$

$$L_{+}L_{-}|u_{\min}\rangle = 0$$
11-40

Now we can use Eq. 11-28 that we derived before to give:

$$L_{-}L_{+}|u_{\max}\rangle = \left(L^{2} - L_{z}^{2} - \hbar L_{z}\right)|u_{\max}\rangle = 0$$

$$L_{+}L_{-}|u_{\min}\rangle = \left(L^{2} - L_{z}^{2} + \hbar L_{z}\right)|u_{\min}\rangle = 0$$
11-41

i.e.

$$\begin{aligned} \boldsymbol{\alpha} - \boldsymbol{\beta}_{\max}^2 - \hbar \boldsymbol{\beta}_{\max} &= 0 \\ \boldsymbol{\alpha} - \boldsymbol{\beta}_{\min}^2 + \hbar \boldsymbol{\beta}_{\min} &= 0 \end{aligned} \tag{11-42}$$

Eliminating α gives

$$\boldsymbol{\beta}_{\max}^2 + \boldsymbol{h}\boldsymbol{\beta}_{\max} = \boldsymbol{\beta}_{\min}^2 - \boldsymbol{h}\boldsymbol{\beta}_{\min}. \qquad 11-43$$

We can write down the solution

$$\beta_{\min} = -\beta_{\max}.$$
 11-44

Now from Eq. 11-34 we know values of β are separated by steps of **h** i.e.

$$\boldsymbol{\beta}_{\max} - \boldsymbol{\beta}_{\min} = n\boldsymbol{\lambda}$$
 11-45

so

$$\beta_{\max} = \frac{n\mathbf{h}}{2}.$$
 11-46

The value of α can be found from Eq. 11-42 and Eq. 11-46.

$$\alpha = \mathbf{R}^2 \left(\frac{n}{2}\right) \left(\frac{n}{2} + 1\right)$$
 11-47
Note that the minimum value of α (when n=0) is 0, then $3/4 \mathbf{h}^2 \left(\beta = -\frac{\mathbf{h}}{2}, \frac{\mathbf{h}}{2} \right)$, $2\mathbf{h}^2 \left(\beta = -\mathbf{h}, 0, \mathbf{h} \right)$

and so on. The solutions where n is even lead to our "normal" angular momentum states and we are left with the "unexpected" half integer solutions (spin 1/2) which we would like to connect to the intrinsic spin. It vital to note that while the integer solutions to spin have normal spatial wavefunctions, *no* such wavefunctions can be found that correspond to the half-integer case.

11.6 Intrinsic Angular Momentum

That we cannot find spatial wavefunctions that correspond to the half-integer spin eigenvalues does not necessarily mean that they do not exist. Remember that our problem was formulated in a way (using kets) that dictated the form of the ket. Rather than define angular momentum specifically with components, we generalise the operators and define angular momentum with the commutation relations Eq. 11-6 and 11-7. We will show how this can be done for spin-1/2 particles.

11.7 Matrix Representation

For particles that we would like to occur in two eigenstates (spin up and spin down) it is natural to write the eigenstates of the z-component as column vectors

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \left| \uparrow \right\rangle \text{spin up,} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \left| \downarrow \right\rangle \text{spin down.}$$

Any operator operation will have to be a 2x2 matrix. In order that this representation of spin yield the "right" eigenvalues we need to guarantee that

$$L_{z}|\uparrow\rangle = \frac{\mathbf{n}}{2}|\uparrow\rangle$$

$$L_{z}|\downarrow\rangle = -\frac{\mathbf{n}}{2}|\downarrow\rangle$$
11-48
11-48

In order to make it explicit that we are worried about the problem of intrinsic angular momentum and that the operators are distinct from the ones we have been dealing with before we will replace the L by an S *i.e.*

$$S_{z}|\uparrow\rangle = \frac{\hbar}{2}|\uparrow\rangle$$

$$S_{z}|\downarrow\rangle = -\frac{\hbar}{2}|\downarrow\rangle$$
11-49
11-49

This may be satisfied if S_z is given by

$$S_{z} = \frac{1}{2} \hbar \sigma_{z}$$

$$\sigma_{z} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$
11-50

If we wished to find a set of operators S^2 , S_x , S_y , S_z that satisfy Eq. 11-6 and 11-7 it is natural to do it from matrices similar to these in Eq. 11-50. Such a set of matrices does exist and they were first discovered by W. Pauli. They are named after him and are called the Pauli Spin Matrices. These are

$$\boldsymbol{\sigma}_{x} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \boldsymbol{\sigma}_{y} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \boldsymbol{\sigma}_{z} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$
 11-51

These three matrices form the x,y,z, components of a vector σ which is related to the spin operators by

$$\dot{S} = \frac{\hbar}{2}\dot{\sigma}.$$
 11-52

Using the definitions of the Pauli Spin Matrices it is easy to show that the matrix version of Eq. 11-6 and 11-7 does hold i.e.

$$\left[S_{x}, S_{y}\right] = i \hbar S_{z} \, etc. \qquad 11-53$$

and that

$$S^{2} = S_{x}^{2} + S_{y}^{2} + S_{z}^{2} = \frac{3}{4}\hbar^{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$
 11-54

Clearly the eigenstates $\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ have total angular momentum eigenvalue $3/4 \mathbf{n}^2$ and a spin

projection either $\pm h/2$ in the z direction. Note that the corresponding bra vectors are

$$\langle \uparrow | = (1 \quad 0), \langle \downarrow | = (0 \quad 1)$$

11.8 Spin and Angular Momentum

From the discussion above it should be clear that intrinsic angular momentum is a very different object than the spatial angular momentum. Being represented by the Pauli Matrices (for spin 1/2 particles) it does not contain any of the normal r, p operators or their components. The spatial degrees of freedom will commute with the intrinsic spin components.

$$[S,r] = [S,p] = [S,L] = 0,$$
 11-55

This means we can specify simultaneously the spatial and intrinsic components of a particles wavefunction and that the total wavefunction may be written as

$$|u\rangle = \Psi(r,\theta,\phi).|\lambda\rangle$$
 11-56

where $\left| \lambda \right
angle$ is the spin wavefunction.

Despite all this abstraction the intrinsic spin is a very real property of an electron. It does couple to a magnetic field and one can see this even with fairly simple experiment. Let us take a moment to see how we can write down the mathematics for an electron inside a magnetic field. Let us choose the applied magnetic field to be along the z-direction. We know that the spin part of the electron wavefunction will be composed of the spin up and spin down states $\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. In analogy to the

classical case the Hamiltonian will be perturbed by an amount proportional to the magnetic moment

$$\Delta H = -\dot{\mu}.\dot{B} = g \frac{e}{2m_e} \dot{S}.\dot{B} = g \frac{e}{2m_e} S_z B_z$$
11-57

We can then use perturbation theory to calculate energy shifts. All we need to be able to do to compute energy shifts is to calculate our usual matrix elements i.e.

$$\Delta E_{\uparrow} = g \frac{e}{2m_e} B\langle \uparrow | S_z | \uparrow \rangle = g \frac{e}{2m_e} B(1 \ 0) \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} =$$

$$g \frac{e}{2m_e} \frac{B\hbar}{2} (1 \ 0) \begin{pmatrix} 1 \\ 0 \end{pmatrix} = g \frac{e}{2m_e} \frac{B\hbar}{2}$$

$$\Delta E_{\downarrow} = g \frac{e}{2m_e} B\langle \downarrow | S_z | \downarrow \rangle = g \frac{e}{2m_e} B(0 \ 1) \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} =$$

$$-g \frac{e}{2m_e} \frac{B\hbar}{2} (0 \ 1) \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -g \frac{e}{2m_e} \frac{B\hbar}{2}$$
(1-58)

Eq. 11-58 gives the energy shifts. The factor of proportionality (g) between the spin and the magnetic moment g. This is the Landé g-factor for the electron - which is almost exactly 2.

11.9 Spin and Statistics

Finally we return to the question of spin and statistics. We saw that particles that have anti-symmetric wavefunctions obey the Pauli exclusion principle. We also stated that fermions (spin 1/2 particles)

have anti-symmetric wavefunctions and bosons (spin 0,1) have symmetric wavefunctions. Why should this be?

If we return to our generalised angular momentum discussion we see that the angular momentum operator is related to the rotation operator (Eq. 11-25). We might believe that the exchange properties arise trivially from the rotation operators. It is certainly true, for example, that if we take the generator of spin rotations to be S_z then, just as derived above, the generator of a finite rotation is

$$D_{\alpha} = e^{\frac{i\alpha}{\mathbf{k}}S_{z}} = e^{i\alpha\sigma_{z}/2}$$
 11-59

which if we expand the exponential in terms of σ_z becomes

$$D_{\alpha} = e^{i\alpha/2}$$
 11-60

and Eq. 11-60 shows that a fermion system is only identical to its original configuration after a rotation of 4π radians. It can be shown that spin 0 and spin 1 systems require only a rotation of 2π to return to their original configuration. Since exchanges of identical particles can be considered similar to rotations (in a classical two body system) we should not thus be surprised that the exchange properties of fermions and bosons are different.

However a "proof" of these properties lies beyond the scope of this course as it requires a detailed understanding of relativistic wave equations.

11.10 Problems

- **11.1** Prove the commutation relations 11-6. Prove Eq 11-7 by using the commutation relations 11-6.
- **11.2** Perform the calculation to show the final form of Eq. 11-14 is correct.
- **11.3** Prove the equation 11-34.

Prove by explicit matrix multiplication that the Pauli Spin Matrices give rise to Equations 11.4 11-53 and 11-54.

11.5 Show that the following matrices obey the appropriate commutation rules and have the correct eigenvalues to represent the three components of angular momentum of a spin-one particle

$$L_{x} = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, L_{y} = \frac{\hbar}{2} \begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix}, L_{z} = \hbar \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

Verify that the matrix representing the square of the total angular momentum also has the correct eigenvalues

The spin operators, \dot{s} , may be related to the Paul Spin Matrices by $\dot{s} = \frac{\hbar}{2} \dot{\sigma}$. Where 11.6 $\boldsymbol{\sigma}_{x} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \boldsymbol{\sigma}_{y} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \boldsymbol{\sigma}_{z} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

Show that the Pauli matrices have the correct commutation properties to be i) identified with spin ii)

Z.

A beam of spin 1/2 particles are placed in a single spin eigenstate aligned along the direction. Calculate the average value of the spin obtained by making repeated measurements of the spin along a direction θ to the z direction.

iii) What result would you expect from a single measurement.

12 Operators

Let us take a few moments to review what have learned about Quantum Mechanics and in particular about operators. We have used operators in Schrödinger's Equation and are quite familiar with most of their properties. However it is important to remember the following points that are really postulates. They embody what we know about nature as described by the Schrödinger Equation:

Postulate 1: Every dynamical variable may be represented by a Hermitian operator (see Chapter 1) whose eigenvalues represent the possible results of carrying out a measurement of the value of the dynamical variable. Immediately after such a measurement, the system will be in a state of the system identical to the eigenstate corresponding to the eigenvalue obtained as a result of the measurement.

Postulate 2: The operators representing the position and momentum of a particle are \vec{r} and $-i\vec{n}\nabla$ respectively. Operators representing other dynamical quantities bear the same functional relation to these as do the corresponding classical quantities to the classical position and momentum variables.

In Chapter 1 we already looked at many of the properties of operators under these assumptions and the reader is urged to remind themselves of how the expectation value of an observable is related to the probability amplitude. Here we will be concerned with the relationship between operators.

12.1 Compatible Observables

Two observables are said to be compatible if the operators representing them have a common set of eigenfunctions. This means that if one quantity is measured then the system will be left in an eigenfunction of that observable. Another measurement of the other observable will leave system in the *same* state. If one wished the system could be measured again with the first observable with the identical result as the first time, and so on. We interpret this as saying that the two observables are compatible, and that the system can have both measured unambiguously. This may be expressed mathematically as follows. Let us assume our two operators are Q and R. If a system is originally in a state

$$|u\rangle = \sum_{i} a_{i} |i\rangle$$
 12-1

then measurement with the operator Q will put the system into one of the eigenstates k with an eigenvalue q_k i.e.

$$Q|u\rangle = Q\sum_{i} a_{i}|i\rangle = \sum_{i} a_{i}q_{i}|i\rangle$$
12-2

and a subsequent operation with R yields

$$RQ|u\rangle = R\sum_{i} a_{i}q_{i}|i\rangle = \sum_{i} a_{i}r_{i}q_{i}|i\rangle$$
12-3

$$QR|u\rangle = Q\sum_{i} a_{i}r_{i}|i\rangle = \sum_{i} a_{i}q_{i}r_{i}|i\rangle$$
12-4

thus combining Eq. 12-3 and 12-4 by subtracting we arrive at

$$(QR - RQ)|u\rangle = [Q, R]|u\rangle = \sum a_i (q_i r_i - q_i r)|i\rangle = 0$$
12-5

which since $|u\rangle$ is not trivially zero implies

$$[Q,R] = 0 12-6$$

Thus in the case that the two operators are simultaneously measurable their commutator vanishes.

12.2 Commutation Relations and the Uncertainty Principle

Things are not quite as simple when the commutator does not vanish. We will examine this case in more detail. Let us take two Hermitian operators A, B. Let us also assume that their commutator can be calculated and is given by

$$[A,B] = iC 12-7$$

The first observation we make is that C is also a Hermitian operator(see Problem 12.1). As their commutator does not vanish they two variables will not have simultaneous eigenstates. To study their effect on a state u let us form an arbitrary mix of the two operators operating on this state:

$$|w\rangle = (A + i\lambda B)|u\rangle.$$
 12-8

Now by definition

$$\langle u | (A - i\lambda B) (A + i\lambda B) | u \rangle = \langle w | w \rangle \ge 0$$
 12-9

so expanding Eq. 12-9 gives

$$\langle u | A^2 + i\lambda [A, B] + \lambda^2 B^2 | u \rangle \ge 0$$
12-10

which can be rewritten in terms of expectation values

$$\langle A^2 \rangle + \lambda \langle C \rangle + \lambda^2 \langle B^2 \rangle \ge 0.$$
 12-11

For this to be true for all arbitrary values of λ it is necessarily the case that

$$\langle A^2 \rangle \langle B^2 \rangle \ge \langle C \rangle^2 / 4.$$
 12-12

The quantities on the left-hand side of Eq. 12-12 are the expectation values of the operators A and B squared. What do they represent? The interpretation of these is relatively straightforward. Take the

operator $A - \langle A \rangle$. This operator gives the deviation of the observable A from its expectation value and its expectation value is by definition zero. The observable $(A - \langle A \rangle)^2$ is the variable that gives the square of the deviation from the mean of A. Thus we state that its expectation value is the mean square i.e.

$$(\Delta A)^{2} = \left\langle \left(A - \langle A \rangle\right)^{2} \right\rangle = \left\langle A^{2} - 2A\langle A \rangle + \langle A \rangle^{2} \right\rangle = \left\langle A^{2} \right\rangle - \left\langle A \right\rangle^{2}$$
12-13

We can always define our co-ordinate systems such that the expectation value of A is zero and in such a case we can easily see that Eq. 12-12 becomes:

$$(\Delta A)^{2} (\Delta B)^{2} \geq \langle C \rangle^{2} / 4$$
 12-14

i.e.

$$\Delta A \Delta B \ge \langle C \rangle / 2. \qquad 12-15$$

For the case of position and momentum we note that Eq. 11-15 becomes the famous uncertainty relation

$$\Delta x \Delta p \ge \mathbf{n} / 2. \tag{12-16}$$

Let us summarise. We have argued that when two Hermitian operators commute their observables are simultaneously and precisely observable. When the operators do not commute a measurement of A we will leave the system in an eigenstate of A which is *not* an eigenstate of B. Operating on the system with A gives

$$A|u\rangle = \sum a_i |i\rangle_A.$$
 12-17

The system is will be left in a particular state $|i\rangle_A$. The state $|i\rangle_A$ is not an eigenstate of *B* but can of course be expanded in terms of the eigenstates of *B*:

$$|i\rangle_{A} = \sum b_{j} |j\rangle_{B}.$$
 12-18

A measurement of *B* will put the system into one of the eigenstates of *B* with probability b_j . The state $|j\rangle_B$ can be expanded in terms of the eigenstates of *A*

$$|j\rangle_{B} = \sum a_{i}^{jB} |i\rangle$$
 12-19

When we remeasure A we can measure anyone of its eigenstates and not just the original state that we measured in Eq. 12-14. From the point of view of the experimentalist a measurement of B spoils our knowledge of A and vice versa. There is no way we can predict from measurement of one variable what measurement we will make of the other variable if the operators do not commute.

12.3 Ehrenfest's Theorem

We include here a theorem that is very important. First we show that if an operator commutes with the Hamiltonian then it is associated with an observable that is a constant in time of the system.

This may be proved easily:

$$\frac{\partial}{\partial t} \langle Q \rangle = \frac{\partial}{\partial t} \langle \Psi | Q | \Psi \rangle = \left\langle \frac{\partial}{\partial t} \Psi | Q | \Psi \rangle + \left\langle \Psi | \frac{\partial}{\partial t} Q | \Psi \rangle + \left\langle \Psi | Q | \frac{\partial}{\partial t} \Psi \right\rangle$$
 12-20

Using the Schrödinger equation

$$H|\Psi\rangle = i\hbar\frac{\partial}{\partial t}|\Psi\rangle \qquad 12-21$$

and its Hermitian Conjugate

$$\left\langle \Psi \middle| H = -i\hbar \frac{\partial}{\partial t} \left\langle \Psi \right|$$
 12-22

yields

$$\frac{\partial}{\partial t} \langle Q \rangle = \frac{1}{i\hbar} \langle \Psi | - HQ | \Psi \rangle + \frac{1}{i\hbar} \langle \Psi | QH | \Psi \rangle + \langle \Psi | \frac{\partial}{\partial t} Q | \Psi \rangle$$

$$= \frac{1}{i\hbar} \langle \Psi [[Q, H]] \Psi \rangle + \langle \Psi | \frac{\partial}{\partial t} Q | \Psi \rangle$$
12-23

Thus the expectation value of any time independent operator is constant *if* the operator commutes with the Hamiltonian.

We next consider the commutator of the position operator with the Hamiltonian

$$[\mathbf{r}, H] = \left[\mathbf{r}, \frac{\mathbf{p}^2}{2m} + V\right] = -\frac{\hbar^2}{2m} [\mathbf{r}, \nabla^2] = -\frac{\hbar^2}{2m} (\mathbf{r} \nabla^2 - \nabla^2 \mathbf{r}) = -\frac{\hbar^2}{2m} (\mathbf{r} \nabla^2 - \nabla(1 + \mathbf{r} \nabla)) = -\frac{\hbar^2}{2m} (\mathbf{r} \nabla^2 - \nabla - \nabla \mathbf{r} \nabla) = -\frac{\hbar^2}{2m} (\mathbf{r} \nabla^2 - \nabla - \mathbf{r} \nabla^2 - \nabla) = -\frac{\hbar^2}{m} \nabla = \frac{\hbar^2}{m} \mathbf{p}$$

$$(\mathbf{r} \nabla^2 - \nabla - \nabla \mathbf{r} \nabla) = -\frac{\hbar^2}{2m} (\mathbf{r} \nabla^2 - \nabla - \mathbf{r} \nabla^2 - \nabla) = -\frac{\hbar^2}{m} \nabla = \frac{\hbar^2}{m} \mathbf{p}$$

$$(\mathbf{r} \nabla^2 - \nabla - \nabla \mathbf{r} \nabla) = -\frac{\hbar^2}{2m} (\mathbf{r} \nabla^2 - \nabla - \mathbf{r} \nabla^2 - \nabla) = -\frac{\hbar^2}{m} \nabla = \frac{\hbar^2}{m} \mathbf{p}$$

Thus the rate of change of the expectation value of the position is closely related to its classical form i.e.

$$\frac{d\langle \mathbf{r} \rangle}{dt} = \left\langle \frac{\partial \mathbf{r}}{\partial t} \right\rangle + \frac{1}{i\hbar} \left\langle [\mathbf{r}, H] \right\rangle = \left\langle \frac{\mathbf{p}}{m} \right\rangle$$
 12-25

Similarly we can show

$$\frac{d\langle \mathbf{p} \rangle}{dt} = \left\langle \frac{\partial \mathbf{p}}{\partial t} \right\rangle + \frac{1}{i\mathbf{h}} \left\langle [\mathbf{p}, H] \right\rangle = -\left\langle \nabla V \right\rangle$$
12-26

Equations
$$\frac{d\langle \mathbf{r} \rangle}{dt} = \left\langle \frac{\partial \mathbf{r}}{\partial t} \right\rangle + \frac{1}{i\mathbf{R}} \langle [\mathbf{r}, H] \rangle = \left\langle \frac{\mathbf{p}}{m} \right\rangle$$
 12-25

and
$$\frac{d\langle \mathbf{p} \rangle}{dt} = \left\langle \frac{\partial \mathbf{p}}{\partial t} \right\rangle + \frac{1}{i\hbar} \langle [\mathbf{p}, H] \rangle = -\langle \nabla V \rangle$$
 12-26

embody Ehrenfests theorem. They show that the expectation values in quantum mechanical systems obey the classical laws of motion.

12.4 Problems

12.1 Prove that the commutator of a pair of Hermitian operators is also a Hermitian Operator.

12.2 Show that if an operator commutes with the Hamiltonian then it is associated with an observable of the system that is constant in time.

Using the result derived above determine which of the following are constants of motion of the 1-dimensional Hamiltonian

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

- ii) momentum
- iii) position
- iv) energy
- **12.3** Prove 12-26
- **12.4** In the Library look up the *Correspondance Principle*. How does Ehrenefest's Theorem relate to this?

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12.5

13 Annihilation and Creation

In the last chapter we investigated the properties of raising and lowering operators for angular momentum. Operators that exhibit the "raising" and "lowering" feature are not limited to angular momentum. There is another very important example that we will look at now. This concerns the harmonic oscillator.

13.1 Harmonic Oscillator

Let us consider the harmonic oscillator in one dimension. The Hamiltonian of a particle in the oscillator potential is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$
 13-1

where ω is the classical oscillator frequency. Rather than solve the problem of determining the eigenvalues by explicitly determining the eigenstates let us use the following technique. Let us define two operators

$$a^{-} = \frac{1}{\sqrt{2m\hbar\omega}} (m\omega x + ip)$$

$$a^{+} = \frac{1}{\sqrt{2m\hbar\omega}} (m\omega x - ip)$$
13-2

Where a^+ and a^- are Hermitian conjugates. Let us also define the Hermitian operator

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$$N = a^+ a^-. 13-3$$

The definition of a^+ and a^- is such that

$$[a^-, a^+] = 1$$
 13-4

and

$$H = \hbar \omega \left(N + \frac{1}{2} \right). \tag{13-5}$$

Clearly if we know the eigenvalues of the operator N we will also know the eigenvalues of H. Therefore let us assume that $|\lambda\rangle$ is an eigenfunction of N with the eigenvalue λ , then

$$N|\lambda\rangle = \lambda|\lambda\rangle$$
 13-6.

Taking the inner product of Eq. 13-6 with $\langle \lambda |$ yields

$$\lambda = \langle \lambda | N | \lambda \rangle = \langle \lambda | a^{+}a^{-} | \lambda \rangle = \langle a\lambda | a\lambda \rangle \ge 0$$
13-7

where we have used the Hermitian properties of a^+ and a^- . According to Eq 13-7 there must exist a smallest eigenvalue λ_o . From Eq's 13-3, 13-4 and 13-6 we get

$$Na^{+}|\lambda\rangle = a^{+}a^{-}a^{+}|\lambda\rangle = a^{+}(a^{+}a^{-}+1)|\lambda\rangle = (\lambda+1)a^{+}|\lambda\rangle$$
13-8

and similarly

$$Na^{-}|\lambda\rangle = (\lambda - 1)|\lambda\rangle.$$
 13-9

In exactly the same way that we interpreted the raising and lowering operators acting on angular momentum states (Eq 11-34) we can understand Eq 13-8 and 13-9: if $|\lambda\rangle$ is an eigenstate of *N* with quantum number λ , then $a^+|\lambda\rangle$ and $a^-|\lambda\rangle$ are eigenstates of *N* with eigenvalues $\lambda+1$ and $\lambda-1$. Operating on the state with lowest eigenvalue λ_0 with a^- must give zero

$$a^{-}|\lambda_{0}\rangle = 0$$

thus

$$N|\lambda_0\rangle = a^+a^-|\lambda_0\rangle = 0.$$
 13-10

Equations 13-8 and 13-9 together with Eq 13-10 imply that the eigenvalues of N are given by

$$N|n\rangle = n|n\rangle, \quad n = 0,1,2,\dots$$
 13-11

The eigenvalues of the Hamiltonian are then given by

$$E_n = \hbar \omega (n + \frac{1}{2})$$

allowing us to place the following interpretation on the operator *N*. N is called the number operator because it counts the number of quanta of energy $\hbar\omega$ in our oscillator system. The operators a^+ and a^- acting on the states raise and lower the number of quanta in the system. They are called creation and annihilation operators.

13.2 The Vacuum

The lowest energy state $|\lambda_0\rangle = |0\rangle$ is termed the vacuum state and is the state with no quanta in it. Note that the vacuum is not "void" - the lowest energy state has a *vacuum energy* of $\frac{1}{2}\hbar\omega$.

13.3 Annihilation and Creation Operators

The annihilation and creation operators a^+ and a^- deserve a little more discussion. Since the effect of a+ is to create an extra quantum

$$a^+|n\rangle = c_n^+|n+1\rangle \qquad 13-12$$

and similarly

$$a^{-}|n\rangle = c_{n}^{-}|n-1\rangle \qquad 13-13$$

Taking the Hermitian conjugates of Eq 13-12 gives:

$$\langle n | a^- = c_n^+ \langle n+1 |$$

i.e.

$$\langle n | a^{-}a^{+} | n \rangle = \langle n | N + 1 | n \rangle = (c_{n}^{+})^{2} \langle n + 1 | n + 1 \rangle = (c_{n}^{+})^{2} = n + 1$$

$$\langle n | a^{+}a^{-} | n \rangle = (c_{n}^{-})^{2} \langle n - 1 | n - 1 \rangle = (c_{n}^{-})^{2} = n$$

$$13-14$$

which means that we can write formally

$$a^{+}|n\rangle = \sqrt{n+1}|n+1\rangle$$

$$a^{-}|n\rangle = \sqrt{n}|n\rangle$$
13-15

We have seen for the harmonic oscillator how we can create and destroy particles of a particular energy. This clearly lends itself to detailed calculations of nature in which the number of particles is not necessarily conserved. All fields are represented by a superposition of annihilation and creation operators for particles of particular energy and momentum.

13.4 Problems

13.1 Prove the commutation relation Eq 13-4.

13.2 If x and p are the position and momentum operators of a one dimensional harmonic oscillator the Hamiltonian may be written

$$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}.$$

If we define the operators

$$a = \sqrt{\frac{m\omega}{2n}} x + \frac{ip}{\sqrt{2mn\omega}}$$
$$a^{\dagger} = \sqrt{\frac{m\omega}{2n}} x - \frac{ip}{\sqrt{2mn\omega}}$$

i) show that
$$[a, a^{\dagger}] = 1$$

also show that if $N = a^{\dagger}a$ then

ii)
$$Na = a(N-1)$$

iii)
$$Na^{\dagger} = a^{\dagger}(N+1).$$

iv) $|n\rangle$ show

v)

If the eigenvalues of N are n and the corresponding normalized eigenstates that with an appropriate choice of phase

$$a|n\rangle = \sqrt{n}|n-1\rangle$$

 $a^{\dagger}|n\rangle = \sqrt{n+1}|n+1\rangle$

and

 $a^{\dagger}|n\rangle = \sqrt{n+1}|n+1\rangle$ Express x^2 in terms of *a* and a^{\dagger} and use first order perturbation theory to calculate expression for the shift in the n^{th} state energy due to an additional term αx^2 in the Hamiltonian.

88 Annihilation and Creation Chap. 13

14 Locality and Non-Locality in Quantum Mechanics

For the precursor to this lecture please see the following URL:

http://www.science-spirit.org/nonlocality/nonlocal.html

We now wish to investigate in a quantitative fashion the non-local features of the wavefunction. In order to do this we will show how specific predictions can be made that show a distinct difference between local and non-local theories. The method for doing this outlined below is due to John Bell and is one of the most important pieces of Classical Quantum Mechanics to have been discovered in the last 25 years.

14.1 Bell's Inequality

Let us suppose that we have two spin 1/2 particles produced in a singlet state. Further let us assume that these two particles move apart. At points A and B along the trajectory of these particles we can put two Stern-Gerlach magnets capable of measuring the spin-projection of the electrons along arbitrary directions **a**, **b** (see Fig. 15-1).



Figure 14-1

We know from the last chapter that when we measure spin at A this will affect our outcome at B. There are two possible interpretations. First that there is a non-local effect, that is, the measurement at A directly effects what is happening at B through a mysterious action-at-a-distance mechanism. Second the measurement of the particle at A reveals something about the particle at B - i.e. we are uncovering a hidden variable.

Let us work with the second assumption that there is a hidden variable, λ , which contains the information about the orientation of the spin. The probability of measuring spin up (+1) or spin down (-1) along any particular direction will given by a function of the orientation of the Stern-Gerlach Magnets and the variable λ i.e. the measurements of the spins are given by

$$A(a,\lambda) = \pm 1, B(b,\lambda) = \pm 1$$
 14-1

Now since we know that if we measure a spin up in one magnet (along a specific direction) if the other magnet is set to same direction we have to measure spin down this means that

$$A(a,\lambda) = -B(a,\lambda).$$
 14-2

The probability of measuring a particular pair of values for the spin is given by the product of the two probability functions integrated over the density of the hidden variable λ ,

$$P(a,b) = \int \rho(\lambda) d\lambda A(a,\lambda) B(b,\lambda) = -\int \rho(\lambda) d\lambda A(a,\lambda) A(b,\lambda)$$
14-3

where we have used Eq 15-1. The "trick: is to introduce a third direction c. If this is done we can compute the difference between two probabilities

$$P(a,b) - P(a,c) = -\int \rho(\lambda) d\lambda \Big[A(a,\lambda)A(b,\lambda) - A(a,\lambda)A(c,\lambda) \Big]$$
14-4

which may be written as

$$P(a,b) - P(a,c) = \int \rho(\lambda) d\lambda \Big[A(a,\lambda) A(b,\lambda) \Big(A(b,\lambda) A(c,\lambda) - 1 \Big) \Big]$$
14-5

Now since

$$A(\dot{a},\lambda)A(\dot{b},\lambda) \le 1$$
 14-6

Equation 15-4 becomes an inequality

$$P(a,b) - P(a,c) \ge \int \rho(\lambda) d\lambda \Big[A(b,\lambda) A(c,\lambda) - 1 \Big] \ge -P(b,c) - 1$$
14-7

i.e.

$$1 + P(b,c) \ge -P(a,b) + P(a,c)$$
 14-8

Now in classical quantum mechanics there exists a well tested prediction for P(a,b)

$$P(a,b) = -\cos\theta_{ab} = -\cos(\theta_a - \theta_b)$$
 14-9

So Equation 15-7 becomes

$$1 - \cos(\theta_b - \theta_c) \ge -\cos\theta_c + \cos\theta_b$$
 14-10

Where we have defined angles relative to *a*. Let us take the special case where both angles are small then

$$\frac{\left(\theta_{b}-\theta_{c}\right)^{2}}{2} \geq \frac{\theta_{c}^{2}}{2} - \frac{\theta_{b}^{2}}{2}$$
14-11

which on further expansion yields

$$\theta_b \ge \theta_c$$
 14-12

Clearly this is not true for all angles so there is a clash between a Hidden variable theory and the predications from Standard Quantum Mechanics.

14.2 Problems

- 15-1 Prove Equation 15-12.
- 15-2 Prove Equation 15-9

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