ON THE BEHAVIOUR OF THE SOLUTIONS OF CERTAIN SCHROEDINGER EQUATIONS FOR VANISHING POTENTIALS

by

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B.A., University of British Columbia, 1959

A THESIS SUBMITTED IN PARTIAL FULFILMENT OF
THE REQUIREMENTS FOR THE DEGREE OF
MASTER OF SCIENCE

in the Department of
PHYSICS

We accept this thesis as conforming to
the required standard

THE UNIVERSITY OF BRITISH COLUMBIA

September 1961

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Date June 27, 1961.

ABSTRACT

In studying the diamagnetism of free electrons in a uniform magnetic field it was found that reducing the field to zero in the wavefunction did not yield the experimentally indicated free particle plane wave wavefunction. However, solving the Schroedinger Equation resulting from setting the field equal to zero in the original equation did yield a plane wave wavefunction. This paradox was not found to be peculiar to the case of a charged particle in a uniform magnetic field but was found to occur in a number of other systems. In order to gain an understanding of this unexpected behaviour, the following systems were analyzed: the one-dimensional square well potential; a charged, spinless particle in a Coulomb field and in a uniform electric field; a one-dimensional harmonic oscillator; and a charged, spinless particle in a uniform magnetic field. From these studies the following were obtained: conditions for determining the result of reducing the potential in a wavefunction; the condition under which the potential of a system may be switched off while maintaining the energy of the system constant; the relationship between the result of physically switching off a potential, the result of reducing it in the wavefunction, and the solution of the Schroedinger Equation obtained by decreasing the potential to zero in the original wave equation; and a general property of any wavefunction with respect to reducing any parameter within this wavefunction.

ACKNOWLEDGEMENTS

I would like to thank Dr. Robert Barrie, who suggested the problem in this thesis, for his supervision and many interesting discussions.

I also wish to gratefully acknowledge the financial assistance given me by the National Research Council in the form of a bursary.

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CHAPTER I

INTRODUCTION

1. GENERAL DISCUSSION

One of the problems which arises in studying the magnetic properties of solids is that of the orbital diamagnetism of free electrons. This can be treated[1] by solving the Schroedinger Equation for an electron in a uniform magnetic field. Since the case of a weak field is of interest, the result of reducing the field to zero in the solution of this Schroedinger Equation was investigated.

The apparent experimental result of switching off the magnetic field is that the electron directly and continuously goes over to a free particle whose eigenfunction is a plane wave. The mathematical treatment of decreasing the field to zero is not so straightforward. If the field is decreased in the original wave equation for the electron in the field the result is an equation whose solution is a plane wave. However, if the field is reduced to zero in the solution of the original equation a plane wave is not obtained. Whereas the former case is consistent with what is expected the latter case is inconsistent with what appears to be experimental evidence. So the situation is that the result is consistent or inconsistent with the apparent experimental observations depending at which stage of the mathematics the field is decreased to zero. This paradox of not obtaining the experimentally indicated free particle plane wave solution by reducing the field, or potential, in the eigenfunction solution of the original equation is not peculiar to the case of an electron in a uniform magnetic field. It also occurs in other systems such as a one-dimensional harmonic oscillator, a particle in a square well potential and a charged, spinless particle in either a Coulomb or uniform electric field.

The preceding suggests the following questions regarding a particle experiencing an external field:

(a) Under what conditions, if any, is the same result obtained by

  (i) reducing the field to zero in the <u>solution</u> to the original wave equation and by

  (ii) solving the <u>equation</u> obtained from the original one by letting the field go to zero?

(b) What is the meaning or significance of those situations where the results are different depending on whether the field approaches zero in the original equation or in its solution?

The situation discussed above may be illustrated by the block diagram

$$\begin{tikzcd}
\text{corner 1} \arrow[rr, "\text{solution}"'] \arrow[d, "\text{field to 0}"] & & \text{corner 3} \arrow[d, dashed, "?"', "\text{field to 0}"] \\
\text{corner 2} \arrow[rr, "\text{solution}"'] & & \text{corner 4}
\end{tikzcd}$$

where the corners are occupied as follows: corner one by the original wave equation for the particle in the field; corner two by the free particle equation obtained from the equation in corner one by decreasing the potential to zero; corner three by the solution of the equation in corner one; and corner four by the solution of the equation in corner two. If the entry in corner four may also be obtained by reducing the potential in the wavefunction occupying corner three the block diagram is said to be closed or completed.

In terms of this block diagram the preceding questions may be simply stated as in the following.

(a) Under what conditions can the block diagram be completed?

(b) What is the significance of those situations in which the block diagram cannot be completed?

2. BOUNDARY CONDITIONS

To completely and uniquely describe a physical system in either quantum or classical mechanics boundary conditions must be introduced in addition to the differential equation. Since the Schroedinger Equation alone is insufficient to fully describe a physical situation the block diagram, as it stands, deals with incompletely specified systems. Unexpected results may therefore occur. If boundary conditions are introduced in conjunction with the wave equations, corners one and two of the block diagram will give a complete description of their respective physical situations and the problem will be formulated in terms of fully specified systems. Henceforth in this thesis the block diagram will be considered only in terms of fully specified systems, that is, where corners one and two are occupied by the boundary conditions corresponding to their respective systems in addition to the respective wave equation.

Since the transition from corner one to corner two is made by decreasing the potential to zero in some manner, it follows that the boundary conditions in corner two should be obtained by decreasing the potential in the boundary conditions of corner one. With the exception of the positive total energy Coulomb and uniform electric field cases, the above procedure results in the boundary conditions being the same in both corners one and two. These exceptions will be treated in section two of chapter three and in chapter four.

With regard to boundary conditions two categories of systems may be distinguished. These types of systems are those in which

(a) the only potential or field the particle experiences is that due to an external source; or

(b) in addition to the potential in (a) the particle is subject to geometric constraints.

The only type of geometric constraint considered in this thesis is that of a particle being contained in a physical container. In the latter case, as herein considered, the particle is always bound whereas in the former case it may or may not be bound. The original system of an electron in a uniform magnetic field can be made to illustrate either type of system. Corresponding to (a) the system simply consists of an otherwise unconstrained electron moving in a uniform magnetic field which fills all space. In this case the external source is that which produces the magnetic field. An example of (b) is an electron confined within a crystal and experiencing a constant magnetic field at all points within the crystal.

In the main body of this thesis only the first type of system will be analysed. In the appendix the second type of system will be discussed. The only type of geometric constraint to be treated in the appendix is that of a physical container which is mathematically described by an abrupt, infinite wall potential.

3. SINGULARITIES

Since a differential equation is characterized by the number and type of its singularities, the singularities of the differential equations in corners one and two of the block diagram will be studied. The situation the block diagram represents is that of comparing the result of applying a given procedure to the solution of an initial equation with the solution of a derived equation where the derived equation is obtained by applying the same procedure to the initial equation. In effect the solutions of two differential equations, an initial and a derived one, are being compared. If the initial and derived equations have different types of singularities these equations are from different classes and it may not be reasonable to a priori expect the initial solution to go over to the solution of the derived equation by application of the same procedure.

With the exception of the square well case, in all the cases herein considered the derived equation differs from the initial one with regard to a singularity classification as seen from the following table:

Differential Equation	Singularity at origin	Singularity at infinity	
		type	order
Free particle	none	irregular	fourth
Square well potential	none	irregular	fourth
Coulomb field	regular	irregular	fourth
Uniform electric field	none	irregular	fifth
Harmonic oscillator	none	irregular	sixth
Uniform magnetic field	none	irregular	sixth

Since the wave equation for both the free particle and the square well potential have the same singularity pattern the square well potential will be treated first. The Coulomb equation is treated next since in addition to its regular singularity at the origin it has the same type of singularity at infinity as does the free particle equation. The cases of negative and positive total energy are treated separately for both the square well and the Coulomb potentials. The uniform electric field, whose equation has a singularity at infinity one order greater than has the free particle equation, is treated next. Chapters six and seven are devoted to the harmonic oscillator and uniform magnetic field cases whose equations have singularities at infinity two orders larger then the free particle equation.

4. TERMINOLOGY

Before completing this introduction the terminology associated with the potential going to zero will be specified. The word "reduce" (and its derivations) refers only to the potential going to zero in the wavefunction. That is, "reduction" is associated with the step from corner three to corner four in the block diagram. This term refers to a purely mathematical procedure with no dependence on, or relation to, any parameter or variable; for example, no connection with time. An example of reduction is $\lim_{x \downarrow b} f(x)$; x is said to be "reduced" to b.

The step from corner one to corner two, that is, the potential going to zero in the wave equation, will not at present have any definite term ascribed to it. Non-committal terms such as "the potential is decreased" or the "potential goes to zero" will be used.

The expression "switch off" and its derivatives refers only to the physical process of the potential being diminished to zero. The physical process of "switching off" a potential is a time dependent process in which the potential is a function of the time. For example, the switch off may be exponential with a time constant, a step function with respect to time or linear over a time interval. To incorporate the time dependence of the switch off in the wave equation requires a time dependent Hamiltonian. However the point of interest in this thesis is to describe the result of switching off rather than to describe the behaviour of the system while the potential is being switched off. Hence the precise time dependence of the switch off is not of interest and all the Hamiltonians will be independent of time regardless of whether the time dependent or independent wave equation is used. In chapter five a distinction will be drawn between two different types of switch off.

5. AIM OF THESIS

In this thesis the various aforementioned systems are analyzed with the following intentions:

(a) to obtain general criteria for determining the wavefunction obtained by reducing the potential to zero in the initial wavefunction;

(b) to determine under what conditions the block diagram is completed and the meaning of such a completion;

(c) to determine the meaning of those situations in which the block diagram is not closed; and

(d) to determine the relationship between reducing the potential in the wavefunction, decreasing the potential in the wave equation and the method of switching off the potential.

CHAPTER II

ONE DIMENSIONAL SQUARE WELL POTENTIAL

1. NEGATIVE ENERGY SOLUTIONS

A particle having negative total energy in a square well potential, whose potential is zero at infinity, corresponds to the physical situation of a particle whose kinetic energy is less than the absolute value of its negative potential energy in the region where the potential is non-zero. In the region where the potential is non-zero the criteria for the above system are:

(2.1) $E - V \geq 0$

(2.2) $0 \leq |E| \leq V_0$ and $0 \leq T \leq V_0$

where E denotes the total energy, V the potential energy and T the kinetic energy. Both conditions follow from the conservation of energy and the fact that the kinetic energy is positive while both the total and potential energies are negative. The particle's negative total energy, caused by the potential energy dominating over the kinetic energy, implies that the particle is confined within the region of the potential. In classical mechanics there is no possibility of the particle leaving the region of the well. In quantum mechanics the probability of the particle being outside the region of the potential is small and decreases exponentially as the distance from the region of potential increases.

The square well potential, V, may be described as follows:

$$V = \begin{cases} -V_0 & -a < x < a \\ 0 & |x| > a \end{cases}$$

where V_0 is positive. The wave equation is then

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E+V_0)\psi = 0 \quad , \quad a > |x| > 0 \tag{2.3}$$

$$\frac{d^2\varphi}{dx^2} + \frac{2mE}{\hbar^2}\varphi = 0 \quad , \quad a < |x| \tag{2.4}$$

To maintain continuity at $x = \pm a$ the boundary conditions $\varphi(a) = \psi(a)$, $\varphi(-a) = \psi(-a)$, $\varphi'(a) = \psi'(a)$ and $\varphi'(-a) = \psi'(-a)$ are imposed. The solution of (2.3) is $\psi = A \sin \alpha x + B \sin \alpha x$ where $\alpha = +\sqrt{\frac{2m(E+V_0)}{\hbar^2}}$ and is real by (2.1).

To avoid an unbounded solution and to permit normalization the boundary conditions that φ tends to zero as $|x|$ tends to infinity are imposed. The solution of (2.4) is then

$$\varphi = \begin{cases} C\,e^{-\beta x} & x > a \\ D\,e^{\beta x} & x < -a \end{cases} \qquad \text{where} \qquad \beta = +\sqrt{\frac{-2mE}{\hbar^2}}$$

and is real and positive. By matching the solutions at $x = \pm a$ [2] two conditions and their corresponding solutions are obtained. These continuity conditions on the wavefunction determine the allowed values for the total energy E.

(a) The solution corresponding to the condition

$$\alpha \tan \alpha a = \beta$$

(2.5)
$$\begin{cases} C e^{-\beta x} & x > a \\ B \cos \alpha x & -a < x < a \\ C e^{\beta x} & x < -a . \end{cases}$$

By matching at either boundary the relation between the coefficients is $C = B e^{\beta a} \cos \alpha a.$

$B = \sqrt{\dfrac{\alpha \beta}{\alpha \cos^2 \alpha a + \beta \sin \alpha a \cos \alpha a + a \alpha \beta}}$ is

obtained from the normalization condition $\int_{-\infty}^{+\infty} |\psi|^2 dx = 1.$

(b) The solution associated with the condition

$\alpha \cot \alpha a = -\beta$ is

(2.5')
$$\begin{cases} C e^{-\beta x} & x > a \\ A \sin \alpha x & -a < x < a \\ -C e^{\beta x} & x < -a . \end{cases}$$

$C = -\frac{\alpha}{\beta} A e^{\beta a} \cos \alpha a$ and $A = \sqrt{\dfrac{\alpha \beta^3}{\alpha^3 \cos^2 \alpha a + a \beta^3 \alpha - \beta^2 \sin \alpha a \cos \alpha a}}$ are obtained as before by matching at a boundary and from normalization.

As V_0 is reduced to zero, β goes to $i\alpha$. In order that the wavefunction be well behaved the energy, β and α must be determined from the appropriate continuity condition. The first condition is $\alpha \tan \alpha a = \beta$. An obvious solution when α becomes $-i\beta$ is $\alpha = \beta = E = 0$. The other permissible values of E are determined by substituting $-i\beta$

for α in the above condition and solving the obtained $\tan(-i\beta a) = i$. This is equivalent to $\tanh \beta a = -1$. The solution of this for finite, positive a is $\beta = -\infty$. Since β is defined as being positive this is an unacceptable solution. Hence the only acceptable value for E is zero. The condition $\alpha \cot \alpha a = -\beta$ yields the identical result when V_0 is reduced to zero. Hence as V_0 is reduced to zero α and β go to zero. Thus A, B, and C go to zero as the potential does. Hence for either condition the wave-function goes to zero as the potential does. It should also be noted that the continuity conditions implying that E being zero is its only acceptable value is in accord with the potential going to zero consistent with criteria (2.2).

The result of decreasing the potential in the wave equation will now be studied in order to determine what happens when the potential goes to zero in the wave equation and the ensuing wave equation is solved. If the potential is decreased such that for all intermediate values of the potential the criteria (2.2) of the system are satisfied it is apparent that the final result of decreasing the potential to zero is a (free) particle with neither kinetic nor potential energy, that is, the total energy, E, is zero. Hence as the potential goes to zero all the energy levels collapse to zero. Since E goes to zero as V does

$$\frac{d^2\Psi}{dx^2} = 0 \tag{2.6}$$

is the equation describing the result of decreasing potential in the above manner. That is, it is (2.6) [rather than the apparent $\frac{d^2\Psi}{dx^2} + \frac{2mE}{\hbar^2}\Psi = 0$, $(E \neq 0)$] which describes the system when the potential is decreased as above. By a well known theorem[3] regarding the solution of Laplace's Equation with boundary conditions, the solution of (2.6) with the boundary conditions that Ψ goes to zero as $|x|$ tends to infinity is $\Psi = 0$. If, however, the potential is decreased without explicitly requiring that the criteria of the system be satisfied for all intermediate values of the potential the resulting equation is

$$\frac{d^2\Psi}{dx^2} + \frac{2mE}{\hbar^2}\Psi = 0. \tag{2.7}$$

This is the equation obtained if the potential is mathematically set equal to zero in (2.3). The general solution of (2.7) is $\Psi = Ae^{\sigma x} + Be^{-\sigma x}$ where σ is in general complex with the real part non-negative. The condition that $\Psi = 0$ at $x = +\infty$ implies A is zero and $\Psi = 0$ at $x = -\infty$ implies B is zero. Hence the only solution consistent with the boundary conditions is $\Psi = 0$ regardless whether the criteria (2.2) are explicitly introduced or not. The reason for obtaining $\Psi = 0$ both times is that the boundary conditions are the same. That is, even though in the latter treatment (2.2) was not explicitly applied to E it was implicitly applied since the boundary conditions for a bound system were maintained.

The block diagram can now be considered. The block diagram for the negative energy solutions for the square well potential is occupied as follows: corner one by equations (2.3) and (2.4) and the boundary conditions that the wavefunction be zero at $x = \pm \infty$; corner two by the same boundary conditions and by equation (2.6) or (2.7) depending on what is stipulated regarding decreasing the potential; corner three by wavefunction (2.5) or (2.5^1); and corner four by $\Psi = 0$. As has been demonstrated the result of reducing the potential in the wavefunction (2.5) or (2.5^1) is $\Psi = 0$. Hence the result of reducing the potential in corner three is the same as solving corner two and the block diagram is closed.

2. POSITIVE ENERGY SOLUTIONS

The physical situation which the mathematics of this section describes is that of a particle feeling the effect of a square well potential whose value is such that the particle's total energy is positive. If the potential is assumed negative the kinetic energy is then greater than the absolute value of the potential energy. This is the case of scattering by a square well potential.

The procedure for treating this case is similar to the negative energy case. However the result of reducing the potential is different. The potential is as in section one since it is assumed to be negative. For the region $|x| > a$ the equation is again (2.4) but with the boundary conditions that φ behaves as a sinusoidally oscillating function at $x = \pm\infty$. Hence φ is $C \sin \beta x + D \cos \beta x$ where $\beta = +\sqrt{\frac{2mE}{\hbar^2}}$. For $|x| < a$ the equation is again (2.3) with the solution $\Psi = A \sin \alpha x + B \cos \alpha x$ where $\alpha = +\sqrt{\frac{2m(E+V_0)}{\hbar^2}}$. The functions φ and Ψ and their first derivatives are again matched at $x = \pm a$ to produce two sets of solutions each corresponding to a different relation between α and β.

(a) Associated with the condition $\alpha \tan \alpha a = \beta \tan \beta a$ is the solution

$$(2.8) \qquad \begin{cases} B \cos \alpha x & |x| < a \\ D \cos \beta x & |x| > a \end{cases} .$$

To maintain continuity of the wavefunction at $|x| = a$ the relation between B and D is $B \cos \alpha a = D \cos \beta a$.

As V_0 is reduced to zero, α approaches β and, in order that the wavefunction be well-behaved, D approaches B. Hence $B \cos \beta x$ is the solution everywhere when the potential is zero. Since this solution is applicable in all space the normalization condition $\int_{-\infty}^{+\infty} |\Psi|^2 dx = 1$ is not applicable and B is arbitrary. B is usually chosen to be unity as this normalizes the function to unit flux.

(b) Corresponding to the condition $\alpha \cot \alpha a = \beta \cot \beta a$ is the solution

(2.8')
$$\begin{array}{ll} A \sin \alpha x & |x| < a \\ C \sin \beta x & |x| > a \, . \end{array}$$

By the same argument as in the preceding the solution $\sin \beta x$ is found to apply at all points when the potential is reduced to zero.

As the potential is reduced to zero α goes to β and the continuity conditions at $x = \pm a$ which determine the allowed values of E become identities. Hence the end result is a free particle with an arbitrary total energy E and a trigonometric wavefunction.

The result of the potential going to zero in the wave equation will now be investigated. Unlike the negative energy case, E is not bounded by the potential. Hence decreasing the potential to zero does not influence E and the resulting wave equation is (2.7). When the boundary conditions that Ψ oscillates sinusoidally at $x = \pm\infty$ are imposed the solution normalized to unit flux is

(2.9)
$$\cos \sqrt{\frac{2mE}{\hbar^2}}\, x$$

(2.9')
$$\sin \sqrt{\frac{2mE}{\hbar^2}}\, x$$

or a linear combination of the two.

The physical significance of decreasing the potential is that the particle in question is acted upon by a diminishing force. When the potential reaches zero there is no force acting on the particle and it is then a free one. This is consistent with the above results.

The block diagram for the positive energy square well case is occupied as follows: corner one by equations (2.3) and (2.4) and the boundary conditions that φ sinusoidally oscillates at $x = \pm\infty$; corner two by equation (2.7) with the above boundary conditions on Ψ ; corner three by wavefunction (2.8) or (2.8'); and corner four by wavefunction (2.9) or (2.9'). As has been demonstrated (2.8) reduces to (2.9), or (2.8') to (2.9'), when the potential is reduced in the wavefunction (2.8) or (2.8'). Hence the block diagram is closed.

CHAPTER III

COULOMB POTENTIAL

1. NEGATIVE ENERGY CASE

A particle with negative total energy in a Coulomb field corresponds to an attractive potential binding the particle to the source of the potential as in the example of the hydrogen atom.

In this Coulomb case the potential is $-\frac{A}{r}$ where A is a non-negative constant and r is the distance from the source of the potential to the particle. Corresponding to the criteria (2.2) in chapter two the total energy in this case is bounded as follows:

$$-\frac{mA^2}{2\hbar^2} \leq E < 0. \tag{3.1}$$

In fact the exact allowed energy values for the negative energy case are

$$E_n = -\frac{mA^2}{2n^2\hbar^2} \qquad n = 1, 2, 3, \ldots \tag{3.2}$$

The allowed energies being negative corresponds to the particle being bound within a finite region of space. Hence the wavefunction satisfies the normalization condition

$\int_{\text{all space}} |\Psi|^2 \, d\tau = 1.$ This normalization condition in turn implies that Ψ goes to zero as any spatial coordinate approaches infinity.

The wave equation for this system is

$$\nabla^2 \Psi + \frac{2m}{\hbar^2}\left(E + \frac{A}{r}\right)\Psi = 0 \tag{3.3}$$

and is expressed in spherical coordinates. By introducing the quantum numbers ℓ and m the equation is separated in the usual manner into angular and radial equations. The solution for a given ℓ and m is the product $R_\ell(r)\, Y_{\ell m}(\theta,\varphi)$ where $Y_{\ell m}(\theta,\varphi)$ is a spherical harmonic. The radial equation for the Coulomb field is

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2mR}{\hbar^2}\left(E + \frac{A}{r} - \frac{\hbar^2 \ell(\ell+1)}{2mr^2}\right) = 0.$$

The independent variable r is replaced by $\rho = +\sqrt{\frac{8m|E|}{\hbar^2}}\, r$.

In terms of ρ the solution is[4]

$$R_{n\ell}(\rho) = C_{n\ell}\, e^{-\rho/2} \rho^\ell L^{2\ell+1}_{\ell+n}(\rho)$$

where L is an associated Laguerre polynomial and $C_{n\ell}$ is a normalizing coefficient to be determined from

$$\int_0^\infty R_{n\ell}(r)\, r^2\, dr = 1$$

and the relation

$$\int_0^\infty e^{-z} z^{2\ell}\left[L^{2\ell+1}_{n+\ell}(z)\right]^2 z^2\, dz = \frac{2n\left[(n+\ell)!\right]^3}{(n-\ell-1)!}\ .$$

The normalized total wavefunction is

$$\Psi_{\ell mn}(r,\theta,\varphi) = -\left[\left(\frac{2mA}{n\hbar^2}\right)^3 \frac{(2\ell+1)(\ell-|m|)!\,(n-\ell-1)!}{8\pi n\,[(n+\ell)!]^3(\ell+|m|)!}\right]^{1/2} e^{-\rho/2} \rho^\ell L^{2\ell+1}_{\ell+n}(\rho)\, P^m_\ell(\cos\theta)\, e^{im\varphi} \tag{3.4}$$

where $\rho = \frac{2mAr}{n\hbar^2}$ is used as it is equivalent to the original definition when (3.2) is used.

If the potential is reduced to zero through A going to zero then the wavefunction (3.4) also goes to zero. Furthermore by (3.2) all the energy eigenvalues collapse to zero. As the energy goes to zero the linear and angular momentum, and therefore ℓ, go to zero. Hence the wavefunction goes to zero as $A^{3/2}$.

The treatment of decreasing the potential in the wave equation is similar to that used in the negative energy square well case. If the potential is decreased such that the criteria (3.1) and (3.2) are satisfied, E goes to zero as the potential does and the wave equation describing the result of decreasing the potential to zero in this manner is

$$\nabla^2 \Psi = 0 \tag{3.5}$$

in analogy to (2.6). The solution is $\Psi = 0$ by the same theorem[3] since the boundary condition is Ψ goes to zero as r goes to infinity. If the potential is decreased without explicitly stipulating that E goes to zero the wave equation becomes

$$\nabla^2 \Psi + \frac{2mE}{\hbar^2} \Psi = 0 \tag{3.6}$$

in analogy to (2.7). Since the same boundary condition is maintained the solution is $\Psi = 0$ by an argument essentially the same as the one following equation (2.7) in chapter two.

Again $\Psi = 0$ is the solution when the potential is decreased to zero in the wave equation regardless of the explicit conditions on E. This is because the boundary condition (that Ψ goes to zero as r goes to infinity such that $\int_{all\ space} |\Psi|^2 d\tau = 1$) implies the particle is bound, the energy is negative and (3.1) is satisfied.

The block diagram for the negative energy case of the Coulomb potential is populated as follows: corner one by equation (3.3) and the boundary condition that Ψ goes to zero as r goes to infinity; corner two by either equation (3.5) or (3.6)(depending on the conditions explicitly imposed on decreasing the potential) and the above boundary condition; corner three by wavefunction (3.4); and corner four by $\Psi = 0.$ Since the result of reducing the potential in (3.4) is $\Psi = 0$ the block diagram is closed.

The classical switching off of this potential in a manner such that the criteria of the system are satisfied for intermediate values of the potential will now be considered. The classical criteria for the negative total energy Coulomb case are the force equation

(3.7) $$mv^2 r = A$$

and the inequality

(3.8) $$\frac{mv^2}{2} - \frac{A}{r} < 0.$$

The latter follows from the conservation of energy for a bound system with zero potential at infinity. By an analysis based on (3.7) it will now be shown that the velocity goes to zero as the potential is switched off. As the potential is switched off, A goes to zero and hence v^2r goes to zero. Since A being decreased implies the force, $-\frac{A}{r^2}$, is decreased in magnitude, the result in view of the finite tangential velocity, v, is that r will tend to increase. Hence for v^2r to go to zero v must go to zero with the result that as the potential is switched off the kinetic energy goes to zero. Hence the result of switching off in the above manner is a particle without kinetic or potential energy, that is with zero total energy.

Before concluding the classical switching off of this Coulomb potential some results, which will be useful further on in this thesis, will be presented. Of the various ways of discretely switching off the potential consistent with the criteria (3.7) and (3.8) the least favorable one is if a given decrease occurs instantaneously. It is assumed that the potential parameter instantaneously goes from A to A_1 where $A_1 < A$. At the instant of decrease (3.7) is satisfied by A and (3.8) must be satisfied by both A and A_1. Combining (3.7) and (3.8) at this instant yields

$$\frac{1}{2}mv^2r = \frac{A}{2} < A_1 . \tag{3.9}$$

This inequality implies that the potential cannot be switched off to zero in a finite number of steps if the criteria of the system are to be satisfied for intermediate values of the potential. Since all that was required of A_1 was that it be less than A and in view of the fact that a continuous switching off may be approximated with arbitrary accuracy by a discrete method of switching off, one may therefore conclude that in a continuous switching off, satisfying the criteria for intermediate values of the potential, the potential must take an infinite time to reach zero. The final total energy resulting from such a switch off is again zero.

2. POSITIVE ENERGY SOLUTIONS

The physical situation which this case describes is that of the scattering of a spinless, charged particle by a Coulomb force. In this case the total energy is positive and constant for all points of the particle's path.

It is convenient to consider the incident particle as being described by a plane wave in the z-direction and to work in parabolic coordinates.[5] Hence a solution of the form $\Psi = e^{ikz} F$ is sought for the equation

$$\nabla^2 \Psi + \left(k^2 - \frac{A}{r}\right)\Psi = 0 \tag{3.10}$$

where $A = \frac{2mZe^2}{\hbar^2}$, $k^2 = \frac{2mE}{\hbar^2}$, $\frac{\hbar^2 A}{2mr}$ is the potential and e is the charge on the incident particle. The equation satisfied by F is $\nabla^2 F + 2ik\frac{\partial F}{\partial z} - \frac{AF}{r} = 0$.

At this stage the transformation to parabolic coordinates is made. Due to the axial symmetry of the system and the separating out of the incident plane wave, the solution will depend on $\zeta = r - z$ only. Hence $F(r-z)$ is substituted for F. After multiplying through by r the resulting equation in terms of ζ becomes $\zeta\frac{d^2F}{d\zeta^2} + (1-ik\zeta)\frac{dF}{d\zeta} - \frac{AF}{2} = 0$.

By introducing $x = ik\zeta$ a confluent hypergeometric equation in x is obtained. Hence $F = {}_1F_1\left(\frac{-iA}{2k}, 1, ik\zeta\right)$.

When normalized to unit flux the total wavefunction is

(3.11) $$\Psi(r,\theta) = e^{-\frac{\pi A}{4k}}\,\Gamma\left(1+\frac{iA}{2k}\right) e^{ikz}\,{}_1F_1\left(\frac{-iA}{2k}, 1, ik\zeta\right).$$

If the potential is reduced to zero in the above wavefunction, that is A reduced to zero, all the terms involving A go to unity and the wavefunction becomes the plane wave e^{ikz}.

Since the Coulomb potential is a long range one with the same value at $z = +\infty$ and $z = -\infty$ the boundary condition at infinity behaves in a different manner for this potential than for the square well potential. In this case the parameter A explicitly appears in the asymptotic expression for the wavefunction. This and the uniform electric field are the only cases in this thesis in which the potential parameter is explicitly involved in the boundary condition. The boundary condition accompanying the equation in which the potential is zero will differ from the condition with the initial equation to the extent that A is set equal to zero in the initial boundary expression. The boundary condition at infinity for the positive energy solutions of the Coulomb potential is[6]

$$(3.12)\quad \Psi \sim \left(1+\frac{iA^2}{4k^3(r-z)}\right)\exp\left(ikz+\frac{iA}{2k}\log k(r-z)\right) +$$
$$\frac{A\hbar^2}{4rm^2v^2}\csc^2\frac{\theta}{2}\exp\left(ikr-\frac{iA}{2k}\log kr-\frac{iA}{2k}\log(1-\cos\theta)+i\pi+2i\eta_0\right).$$

When A is decreased to zero in (3.12) this boundary condition becomes

$$(3.13)\qquad \Psi \sim e^{ikz}$$

The result of decreasing the potential to zero in the wave equation can now be studied. As in the positive energy case of the square well potential, decreasing the potential does not place any restrictions on E. The equation resulting from decreasing the potential to zero in (3.10) is

$$(3.14)\qquad \nabla^2\Psi + k^2\Psi = 0.$$

The general solution of (3.14) normalized to unit flux is $e^{i\underline{k}\cdot\underline{r}}$. By imposing the boundary condition (3.13) for r going to infinity the general solution becomes e^{ikz}. The same result may be obtained by recalling that the incident wave vector was $\vec{k} = (0, 0, k)$. In the absence of any potential, as is the case in (3.14), $\vec{k}$ remains unaltered. Hence the general solution $e^{i\mathbf{k}\cdot\mathbf{r}}$ again becomes e^{ikz}. If in a given problem the incident wave vector is not parallel to an axis a rotation of the coordinate system is first carried out such that the wave vector is parallel to an axis in the new coordinate system. The problem is then treated as above in the new coordinate system.

The block diagram for the positive energy Coulomb case is occupied as follows: corner one by equation (3.10) and boundary condition (3.12); corner two by equation (3.14) and boundary condition (3.13); corner three by wave-function (3.11); and corner four by e^{ikz}. As has been demonstrated, the result of reducing the potential in the third corner is the entry in the fourth corner. Hence the block diagram is closed.

The physical situation is straight-forward. The system consists of a particle with total energy, E, experiencing a Coulomb force. The result of switching off this force to zero is a free particle with the same total energy. This total energy is now all kinetic energy.

CHAPTER IV

UNIFORM ELECTRIC FIELD

1. DESCRIPTION OF SYSTEM

The system under consideration in this chapter is that of a charged, spinless particle, incident from $z = +\infty$ travelling towards $z = -\infty$, being repelled by a uniform electric field. This field, $\vec{F}$, is chosen to be parallel to the z-axis and the charge on the particle is denoted by e. In this chapter e is assumed to be positive. However the arguments and results are equally applicable to a negatively charged particle when the directions are reversed. In this system the particle experiences a potential $-eFz + C$. Since C is arbitrary it is chosen to be zero thus making the zero of potential at the origin. The particle's total energy is denoted by $\mathcal{E}$. E is the total energy associated with the motion parallel to the z-axis and is a positive or negative constant.

2. WAVEFUNCTION BEHAVIOUR AND BLOCK DIAGRAM

The Schroedinger Equation for this system is

$$\nabla^2 \Psi + \frac{2m}{\hbar^2}(\mathcal{E} + eFz)\Psi = 0. \tag{4.1}$$

Ψ is expressed as $\Psi(x,y,z) = X(x)Y(y)Z(z)$ and three ordinary differential equations are obtained which involve the constants k_x, k_y and k_z where $k_x^2 + k_y^2 + k_z^2 = \frac{2m\varepsilon}{\hbar^2}$. k_x^2 and k_y^2 are $\frac{2m}{\hbar^2}$ times the energy associated with the motion in the x and y directions respectively and as such are positive. k_z^2 is $\frac{2mE}{\hbar^2}$ and is positive or negative as E is. The equations for X and Y yield the free particle plane wave solutions $X(x) = e^{ik_x x}$ and $Y(y) = e^{ik_y y}$. The equation for $Z(z)$ is

$$\frac{d^2 Z}{dz^2} + \left(\frac{2meF z}{\hbar^2} + k_z^2\right) Z = 0. \tag{4.2}$$

If the changes in variables $Z = \sqrt{\frac{2meF z}{\hbar^2} + k_z^2}\, W$,

$v = \frac{2}{3}\left(\frac{2meF z}{\hbar^2} + k_z^2\right)^{3/2}$ and then $u = \frac{\hbar^2 v}{2meF}$ are made in (4.2) the resulting equation for W is

$$u^2 \frac{d^2 W}{du^2} + u \frac{dW}{du} + \left(u^2 - \frac{1}{9}\right) W = 0.$$

This is a Bessel Equation and its general solution is

$W = A\, J_{1/3}(u) + B\, J_{-1/3}(u).$ The general expression for $Z(z)$ is therefore

$$Z(z) = \sqrt{\frac{2meF z}{\hbar^2} + k_z^2}\left[A\, J_{\frac{1}{3}}\left(\frac{\hbar^2}{3meF}\left(\frac{2meF z}{\hbar^2} + k_z^2\right)^{3/2}\right) + B\, J_{-\frac{1}{3}}\left(\frac{\hbar^2}{3meF}\left(\frac{2meF z}{\hbar^2} + k_z^2\right)^{3/2}\right)\right]$$

where A and B will be

chosen to satisfy the boundary conditions.

As was seen in the positive energy Coulomb case, the asymptotic behaviour of the wavefunction for a long range potential is not simply a trigonometric or an imaginary exponential type of function. Since this uniform electric field potential is a long range one, all that will be specified regarding the boundary conditions is that the wavefunction goes to zero exponentially as z approaches $-\infty$ and that it oscillates as z approaches $+\infty$. The boundary conditions to be satisfied by $Z(z)$ may be more quantitatively stated as follows:

(4.3) $\quad z << -\frac{E}{eF}$ implies $Z(z)$ tends to zero exponentially with decreasing z ;

(4.4) $\quad z >> -\frac{E}{eF}$ implies $Z(z)$ oscillates with z .

To satisfy the boundary condition for z tending to $-\infty$ A is equal to $-Be^{i\pi/3}$. This relation is obtained by applying the following procedure:

$$\frac{\hbar^2}{3meF}\left(\frac{2meF}{\hbar^2}z + \frac{2mE}{\hbar^2}\right)^{3/2} \approx -i\left(\frac{2meF|z|}{\hbar^2}\right)^{3/2}$$

for z tending to $-\infty$ is used and $2meF/z/\hbar^{-2}$ is recognized as being positive; the relations[7]

$$I_{\pm\nu}(x) = e^{\pm i\nu\pi/2}\, J_{\pm\nu}\left(x\, e^{-i\pi/2}\right) \qquad \text{are used;}$$

and A is expressed in terms of B such that, for z tending to $-\infty$, $Z(z)$ is proportional to the K_ν function where[8] $K_\nu(x) = \pi\frac{\left(I_{-\nu}(x) - I_\nu(x)\right)}{2\sin\nu\pi}$. B is determined by using the asymptotic forms[9]

$$(4.5) \qquad J_{\pm\nu}(x) \sim \sqrt{\frac{2}{\pi x}}\cos\left(x \mp \frac{\nu\pi}{2} - \frac{\pi}{4}\right)$$

and the normalization condition $v|\psi|^2 = \frac{1}{2\pi\hbar}$ for z tending to $+\infty$ where v is the magnitude of the velocity parallel to the z-axis. B is then found to be $\frac{1}{\sqrt{3eF}}$.

With A and B thus specified the asymptotic forms of $Z(z)$ for $|z|$ tending to infinity can be written down. By use of[10] $K_\nu(x) \sim \sqrt{\frac{\pi}{2x}}\, e^{-x}$ it is seen that for z tending to $-\infty$

$$(4.6) \qquad Z(z) \sim \sqrt{\frac{3}{\pi\hbar}}\left(\frac{m}{8eF|z|}\right)^{1/4} e^{2\pi i/3} \exp\left[-\frac{(2meF|z|)^{3/2}}{3meF\hbar}\right].$$

(4.6) goes to zero exponentially as z goes to $-\infty$. By use of (4.5) the asymptotic form of $Z(z)$ as z tends to $+\infty$ is seen to be

$$(4.7) \qquad Z(z) \sim \left(\frac{2m}{\pi^2\hbar^2 eFz}\right)^{1/4}\left\{\exp\left[-i\left(\frac{(2meFz)^{3/2}}{3meF\hbar} - \frac{\pi}{12}\right)\right] - \exp\left[-i\left(\frac{(2meFz)^{3/2}}{3meF\hbar} - \frac{3\pi}{4}\right)\right]\right\}.$$

(4.7) oscillates with varying z. Hence with the above choices for A and B the boundary conditions are satisfied.

The solution of (4.2) which is normalized to unit flux at $z = +\infty$ and which satisfies the boundary conditions (4.3) and (4.4) is therefore

$$(4.8) \qquad Z(z) \sim \frac{1}{\hbar}\sqrt{\frac{2m}{3eF}(eFz+E)}\left\{ J_{-\frac{1}{3}}\left[\frac{(2meFz+2mE)^{3/2}}{3meF\hbar}\right] - e^{i\pi/3} J_{\frac{1}{3}}\left[\frac{(2meFz+2mE)^{3/2}}{3meF\hbar}\right]\right\}.$$

The result of reducing the potential in the wavefunction (4.8) will be studied in conjunction with the effect of decreasing the potential to zero in the boundary conditions. This is done in order to determine whether the result of reducing the potential in the wavefunction satisfies the conditions on the wavefunction obtained by decreasing the potential in the boundary conditions. The cases of positive and negative E must be distinguished.

In reducing the potential in the wavefunction (4.8) for the case of positive E, equations (4.5) and the small F approximations $\sqrt{\frac{2meF}{\hbar^2}z + \frac{2mE}{\hbar^2}} \approx \sqrt{\frac{2mE}{\hbar^2}} = k_z$

and $\frac{\hbar^2}{3meF}\left(\frac{2meF}{\hbar^2}z + k_z^2\right)^{3/2} = k_z z + \frac{k_z^3\hbar^2}{3meF}$

are employed. As F is reduced to zero the wavefunction (4.8) becomes

$$(4.9) \quad Z(z) \approx \sqrt{\frac{2m}{\pi\hbar^2 k_z}}\left\{\exp\left[-i\left(k_z z + \frac{k_z^3\hbar^2}{3meF} - \frac{\pi}{12}\right)\right] - \exp\left[-i\left(k_z z + \frac{\hbar^2 k_z^3}{3meF} - \frac{3\pi}{4}\right)\right]\right\}.$$

With E positive F will be decreased to zero in the boundary conditions (4.3) and (4.4). As F is decreased to zero (4.3) becomes the condition that for $\zeta << -\infty$ $Z(\zeta)$ goes to zero exponentially with decreasing ζ. (4.4) becomes the condition that for $\zeta >> -\infty$ $Z(\zeta)$ oscillates with ζ. As the former is meaningless the latter is the only condition imposed on the wavefunction by the boundary conditions when F is decreased to zero. Since (4.9) oscillates for all ζ it is consistent with the above condition on the wavefunction. Hence reducing the potential in (4.8) when E is positive yields an acceptable and consistent result.

When the preceding approximations for small F and the previous formulas[7, 8, 10] for $I_{\pm\frac{1}{3}}$ and $K_{\frac{1}{3}}$ are used, the wavefunction (4.8) for negative E becomes

$$(4.10) \qquad Z(\zeta) \approx e^{i\pi/6} \sqrt{\frac{3}{2\pi\hbar}} \left(\frac{m}{2E}\right)^{1/4} \exp\left[|k_\zeta|\zeta - \frac{|k_\zeta|^3 \hbar^2}{3meF} \right]$$

as F is reduced. F will now be decreased to zero in the boundary conditions with E negative. (4.3) becomes the condition that for $\zeta << \infty$ $Z(\zeta)$ is zero and (4.4) becomes the condition that for $\zeta >> \infty$ $Z(\zeta)$ is oscillatory with respect to ζ. Since the latter is meaningless the former is the only condition imposed on the wavefunction by the boundary conditions when F is zero and

E is negative. The result of reducing F to zero in (4.10) is a zero wavefunction for all z less than infinity in accord with the above condition. Hence reducing the potential to zero for E either positive or negative produces a satisfactory result in that the condition on the wavefunction is satisfied in both cases.

For both positive and negative E the result of decreasing the potential in the wave equation (4.2) is

$$\frac{d^2 Z}{dz^2} + \frac{2mE}{\hbar^2} Z = 0 . \tag{4.11}$$

If E is positive the condition on the wavefunction that it be oscillatory with z for $z >> -\infty$ implies that the solution of (4.11) corresponding to a particle incident from $z = +\infty$ is

$$Z(z) = e^{-ik_z z} . \tag{4.12}$$

If E is negative and F is zero the condition on Z is that it be zero for $z << \infty$. In this case the solution of (4.11) is $Z = 0$.

Since the potential is a function of z only, only functions of, or concerned with, z need be considered in the block diagram.

As it has been explained in chapter one, the potential in the boundary conditions must be decreased to zero in going from corner one to corner two. Since the boundary condition in corner two is therefore different for positive E from what it is for negative E , the two cases of positive and negative E must be distinguished. Hence a separate block diagram will be used for each of the two energy cases.

In the case of positive E the block diagram is populated as follows: corner one by equation (4.2) and boundary conditions (4.3) and (4.4); corner two by equation (4.11) and the condition that the wavefunction oscillates with z for $z >> -\infty$; corner three by the wavefunction (4.8); and corner four by wavefunction (4.12). The entry in corner four and the equation (4.9) with F reduced to zero, which is the result of reducing the potential in the wavefunction occupying corner three, differ by a phase factor but describe the same physical situation. Hence to the extent that the entry in corner four and the result of reducing the potential in the wavefunction in corner three are physically indistinguishable, the block diagram is closed.

In the case of negative E the block diagram is occupied as follows: corners one and three as in the positive E case; corner two by equation (4.11) and the condition that for $z << \infty$ the wavefunction is zero; and corner four by $Z = 0$. The result of reducing the potential to zero in corner three, that is, (4.10) with $F = 0$, and the entry in corner four are the same. The block diagram is therefore completed.

3. PHYSICAL ANALYSIS

In the equation (4.9) resulting from reducing the field to zero in the positive E case, the plane wave momentum-distance expression, that is, $k_3 \zeta$, is found in the argument of the exponential thus indicating the desired plane wave result. However the term $\frac{k_3^3 \hbar^2}{3meF}$ introduces an infinite phase factor as F is reduced to zero. Since only $|\Psi|^2$ corresponds to a physical observable and phase factors are not physically observable, the presence or absence of such an infinite phase factor would not be detectable. Hence no physical explanation of this infinite phase factor is possible. Furthermore, since at $\zeta = +\infty$ an infinite kinetic energy is required to maintain the total energy constant this system does not precisely correspond to an actual physical situation. Hence an unusual and physically inexplicable item such as an infinite phase factor should not be surprising or disturbing. It is however satisfying that all the physically observable features are well behaved.

The classical motion of the particle in this field will now be analyzed. The classical process which this case represents is that of a charged, spinless particle incident from $\zeta = +\infty$ being reflected back at some point ζ_0. This is supported in the preceding mathematics by the fact that as

z approaches $+\infty$ the wavefunction becomes (4.7) which describes a free particle travelling in the $-z$ direction. The fact that the particle is reflected back is supported by (4.6) which, for all finite E, indicates zero probability for the particle being at z for z tending to $-\infty$.

The two cases of positive and negative E have been distinguished and have given different results. The physical significance of the value of the total energy, E, is to indicate at what point in space, once the zero of potential is fixed, the particle is classically reflected back by the potential barrier. This point of course corresponds to the position where the particle has zero kinetic energy. With the zero of potential at the origin, as is herein chosen, positive E corresponds to reflection at a position with negative z coordinate and negative E corresponds to reflection back at a position with positive z coordinate. The exact coordinate at which the particle is reflected back is given by $z_0 = -\frac{E}{eF}$. z_0 is the value of z for which the argument of the Bessel Functions $J_{\pm\frac{1}{3}}$ in (4.8) is zero. $z > z_0$ implies this argument is real; $z < z_0$ implies this argument is imaginary. $z < z_0$ corresponds to the region of space which, in classical mechanics, the particle may never enter.

The effect of the potential being switched off on the point of reflection will now be studied. For positive

E, the point of reflection, z_0 , goes to $-\infty$ as F is switched off. That is, for F = 0 the result is a particle travelling from $z = +\infty$ to $z = -\infty$ without being reflected at an intermediate position. Hence for F = 0 and E positive the wavefunction for $z > -\infty$, that is, at all points, should be a plane wave describing a free particle travelling from $z = +\infty$ to $z = -\infty$. As can be seen from (4.9) reducing the potential in the initial wavefunction with positive E gives this result. If E is negative z_0 goes to $+\infty$ as F is switched off and the point of reflection is at $z = +\infty$. If a particle entering from $z = +\infty$ is reflected back at $z = +\infty$ the result is that the particle is never in any finite region of space. This situation is described by a zero wavefunction for $z < +\infty$. As F is reduced to zero in the initial wavefunction and E is negative, (4.8) becomes (4.10) which is zero for all $z < +\infty$ when F is zero. Hence for both positive and negative total energy reducing the potential in the wavefunction yields a result in accord with the physical situation arising from switching off the potential.

CHAPTER V

THE HARMONIC OSCILLATOR

1. TIME INDEPENDENT TREATMENT

The time independent harmonic oscillator wave equation and its solution are well known.[11] The wave equation is

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2} m\omega_c^2 x^2\right)\Psi = 0 \tag{5.1}$$

where $\omega_c = \sqrt{\frac{\text{elastic constant}, K}{\text{mass}, m}}$ is the classical frequency associated with this oscillator. The energy E takes values given by

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega_c \tag{5.2}$$

where n is a non-negative integer. The normalization condition on the wavefunction is $\int_{-\infty}^{+\infty} |\Psi|^2\, dx = 1.$ This implies the boundary conditions that Ψ goes to zero as x goes to $\pm\infty$. For a given n the normalized solution of (5.1) is

$$\Psi_n(x) = \sqrt[4]{\frac{m\omega_c}{\pi\hbar(n!)^2 2^{2n}}}\; e^{-m\omega_c x^2/2\hbar}\, H_n\left(x\sqrt{\frac{m\omega_c}{\hbar}}\right). \tag{5.3}$$

Since the potential energy is $\frac{1}{2} m\omega_c^2 x^2$ reducing the potential to zero is equivalent to reducing K or ω_c to zero. Reducing ω_c to zero reduces the wavefunction to zero for all values of n. The wavefunction goes to zero as $\omega_c^{1/4}$ or $K^{1/8}$.

The effect of decreasing the potential to zero in the wave equation will now be determined. If the potential goes to zero such that the energy values explicitly satisfy (5.2) for intermediate values of the potential the resulting wave equation is

$$(5.4) \qquad \frac{d^2\psi}{dx^2} = 0.$$

If the potential goes to zero without explicitly requiring that (5.2) be satisfied the wave equation becomes

$$(5.5) \qquad \frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0.$$

Since the boundary conditions that ψ is zero at $x = \pm\infty$ are associated with both (5.4) and (5.5) $\psi = 0$ is the solution of both (5.4) and (5.5) with these boundary conditions. This is the same as in the negative energy cases of the square well and Coulomb potentials.

The block diagram for the time independent harmonic oscillator is occupied as follows: corner one by equation (5.1) and boundary conditions that ψ goes to zero as x goes to $\pm\infty$; corner two by the same boundary conditions and equation (5.4) or (5.5) depending on the explicit assumptions regarding decreasing the potential; corner three by wave-function (5.3); and corner four by $\psi = 0$. The result of reducing the potential to zero in corner three yields the entry in corner four. Hence the block diagram is completed.

2. TIME DEPENDENT TREATMENT

The time dependent wave equation for a harmonic oscillator is

$$(5.6) \qquad i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}Kx^2\right)\Psi(x,t)$$

where $V = \frac{1}{2}Kx^2$ is the potential energy at position x. Since the potential is independent of the time the solution of the time dependent equation may be expressed as an infinite sum of the solutions of the time independent wave equation with the coefficient depending on the time. Using this technique, the normalized solution to (5.6) is[12]

$$(5.7) \quad \Psi(x,t) = \left(\frac{\alpha^2}{\pi}\right)^{1/4} \exp\left(-\frac{\omega_c t}{2} - \frac{\alpha^2 x_0^2}{4} - \frac{\alpha^2 x^2}{2}\right) \sum_{n=0}^{\infty} \left(\frac{\alpha x_0}{2}\right)^n \frac{H_n(\alpha x)}{n!} e^{-in\omega_c t}$$

where $\alpha^4 = \frac{mK}{\hbar^2}$ and x_0 is the initial position of the centre of the wave packet. When K is reduced to zero ω_c and α also go to zero and $\Psi(x,t)$ becomes zero. Therefore the result of reducing the potential to zero is the same for the solutions of both the time dependent and time independent wave equations.

The result of decreasing the potential to zero in the time dependent wave equation will now be analyzed. Since E does not appear in (5.6) the result of decreasing the potential to zero in (5.6) is

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} \tag{5.8}$$

regardless of whether or not (5.2) is satisfied for intermediate values of the potential. The solution of (5.8) is

$Ae^{\pm ikx}e^{\pm iEt/\hbar}$. For the wavefunction to vanish at both $x=\pm\infty$ A must be zero and hence the solution of (5.8) consistent with the boundary conditions is $\Psi = 0$. If the system satisfies (5.2) for intermediate values of the potential the solution of (5.8), before the boundary conditions are applied, is Ψ is a constant since E and $k=\sqrt{\frac{2mE}{\hbar^2}}$ go to zero as the potential does. To satisfy the boundary conditions this constant is then zero.

The block diagram for the time dependent harmonic oscillator is populated as follows: corner one by equation (5.6) and boundary conditions that Ψ goes to zero as $|x|$ goes to infinity; corner two by the same boundary conditions and the equation (5.8); corner three by the wavefunction (5.7); and corner four by $\Psi=0$. Since reducing the potential in (5.7) yields zero the block diagram is closed.

It should be noted that for both the time dependent and time independent treatments of the harmonic oscillator the energy eigenvalues are given by $E_n = (n+\frac{1}{2})\hbar\omega_c$ with n a non-negative integer. Hence in both treatments it is apparent, from this eigenvalue equation, that all the energy eigenvalues go to zero as the potential does if the potential is decreased in such a manner that (5.2) is satisfied for all intermediate values of the potential.

The procedure used to solve the above time dependent wave equation may be equally well applied to solving the time dependent equations corresponding to the other potentials. However, as the preceding has shown, the result of reducing the potential to zero is the same for the solutions to both the time dependent and time independent equations. Hence in studying the result of reducing the potential it is sufficient to deal with the solution of either the time dependent or time independent wave equation.

3. CLASSICAL ANALYSIS OF SWITCHING OFF

Before discussing the switching off processes the classical description of, and criteria for, a harmonic oscillator will be given. The physical system considered as a harmonic oscillator consists of a particle oscillating about an equilibrium position under the influence of a force directed towards the equilibrium position and of magnitude proportional to the particle's distance from this equilibrium position. The equation of motion is $x = a \cos \omega_c t$. The magnitude of the velocity at position x is $\sqrt{\frac{K(a^2-x^2)}{m}}$ where a is the amplitude.

The kinetic energy, T, potential energy, V, and total energy, E, of a harmonic oscillator with amplitude "a" obey the following criteria:

$$(5.9)\quad \begin{cases} T + V = E = \text{constant with respect to position and time} \\ E = \text{maximum } T = \text{maximum } V = \frac{1}{2}Ka^2 \\ 0 \le T \le \text{maximum } T \;;\quad 0 \le V \le \text{maximum } V. \end{cases}$$

The first criterion states that conservation of energy holds for all positions and time. The second criterion indicates that the total energy, E, depends only on the elastic constant, K, and amplitude a.

In this section a detailed classical analysis will be given of the two basic ways of switching off a potential in a physical system. The harmonic oscillator has been chosen for this detailed analysis since this system is common, useful and relatively simple. However this distinction in methods of switching off the potential is applicable to all other systems. The aim of this analysis is to illustrate the two types of switch off and to make clear the distinction between them.

These two methods of switching off will be referred to as type I and type II. A type I switch off is where the criteria of the particular system are satisfied for all intermediate values of the potential. For example, in a type I switch off a harmonic oscillator with amplitude "a" remains a harmonic oscillator with amplitude "a" for all intermediate values of the potential, that is, (5.9) is satisfied for all intermediate values of the potential. A type II switch off is one in which the potential is switched off without the criteria of the system being satisfied for all intermediate values of the potential. That is, the characteristic relationships between the various parameters are not satisfied during the switching off process.

Before examining the switching off processes it should be noted that for a harmonic oscillator the only way the potential may be switched off without imposing geometric constraints, decreased in the wave equation or reduced in the wavefunction is by the elastic constant, K, becoming zero.

The type I switch off of the harmonic oscillator will be studied first. The conditions on the switching off process in order that the process be of type I may be formulated in the form of the following theorem.

THEOREM: To satisfy the condition that for all nonzero values of the potential the system is a harmonic oscillator with amplitude a, the switch off must be done in the following manner:

(a) The potential may be switched off only in discrete decrements and these may occur only while the particle is at an extremity.

(b) The particle ends up at one of the extremities with neither kinetic nor potential energy relative to the equilibrium position, that is, the final total energy is zero.

Proof: First it will be shown that the final situation is a particle with neither kinetic nor potential energy relative to the equilibrium position. Let the potential be physically lowered by some arbitrary amount. By (5.9) the total energy is lowered by the same amount as is the maximum potential energy. This is repeated with the result that the maximum potential energy and the total energy are again lowered by identical amounts. This procedure is continued until the potential reaches zero. It is obvious, upon reference to (5.9), that as the potential is thus switched off the velocity, kinetic and total energies all go to zero. So the result is a particle with neither motion nor potential energy with respect to the equilibrium position.

Now consider the particle at any position ξ other than at an extremity. It then has a potential energy of $\frac{1}{2}K\xi^2$, a kinetic energy of $\frac{1}{2}mv^2 = \frac{1}{2}Ka^2 - \frac{1}{2}K\xi^2$ with corresponding velocity of $v = \sqrt{\frac{K(a^2-\xi^2)}{m}}$ and experiences a force of magnitude $K\xi$ towards the equilibrium position. When the particle is at ξ let the potential be lowered by an arbitrary amount. If $\xi = 0$ the particle will have a velocity such that its kinetic energy at this position is greater than the new, lower maximum potential energy and the condition for a harmonic oscillator is not satisfied. If $\xi \neq 0$ the particle will have a greater velocity at this position than would be the case if it were undergoing a harmonic motion with a maximum potential equal to the lower potential energy. If the particle is approaching $x=o$ then at $x=o$ the particle will have a velocity due to its velocity at ξ plus the velocity acquired in going from ξ to zero under the influence of the lower potential. Since the velocity at ξ is greater than that which would be the case if the lower potential were operative during the entire journey from $x=a$ to $x=o$, the velocity at $x=o$ corresponds to a kinetic energy at $x=o$ greater than the maximum of the lower potential. Thus the particle again disobeys (5.9). If the particle is moving away from $x=o$ a similar argument shows that it would overshoot $|x| = a$ and would then no longer be a harmonic oscillator with amplitude a. Hence the potential may not be lowered at any position such that $\xi \neq \pm a$. Furthermore, switching off the potential in a continuous manner while the particle executes its motion is also inconsistent with the stipulation that the system be a harmonic oscillator since it involves lowering the potential at points other than $\pm a$. Therefore the only remaining method, and an obviously acceptable one, is to lower the potential in finite steps when the particle is at $\pm a$. That this method complies with the stipulations of this type of switch off may be seen from the following argument. While the particle is at $\pm a$ the potential is lowered. The result of this is the following: the total energy and maximum potential energy are correspondingly lowered; the maximum kinetic energy is correspondingly lowered because the force and acceleration are less over the whole distance from $x=a$ to $x=o$; and the system remains a harmonic oscillator with amplitude a but with a lower total energy and greater period.

Whether the particle eventually ends up at $x=a$ or $x= -a$ depends solely on the technique used to switch off the potential. For example, if it is wished that the particle end up at $x=a$ this can be achieved by any type I switch off wherein the last step (to zero) occurs when the particle is at $x=a$. It should also be noted that the particle cannot end up at the equilibrium position. q.e.d.

A type II switch off of the harmonic oscillator potential will now be illustrated. There are numerous ways in which a system may undergo a type II switch off. However the following particular example will illustrate the principles and the result of such a switch off.

It will be assumed that the potential is switched off during a time interval very short compared to the period. The potential is switched off over a time interval Δt centred on a time, t_s , the latter being called the "time of switch off." During this time interval the particle travels a distance Δx . Δx is much less than the amplitude "a" since Δt is much less than the period. Let x_o be the centre of Δx . In this type II switch off the result is a free particle with speed within the range

$$\sqrt{\frac{K}{m}\left(a^2-(x_0-\Delta x)^2\right)} \qquad \text{to} \qquad \sqrt{\frac{K}{m}\left(a^2-(x_0+\Delta x)^2\right)}$$

unless x_0 is within Δx of the equilibrium or the extreme position. If $|x_0| \leq \Delta x$ then the free particle's speed is in the range $\ell\sqrt{\frac{K}{m}}$ to $\alpha\sqrt{\frac{K}{m}}$ where ℓ is the lesser of

$$\sqrt{a^2-(x_0-\Delta x)^2} \qquad \text{or} \qquad \sqrt{a^2-(x_0+\Delta x)^2} \qquad \text{and } \alpha$$

is greater than ℓ but less than a. If $\big|\,|x_0| - a\,\big| \leq \Delta x$ then the free particle's speed is greater than zero but less than $\sqrt{\frac{K}{m}\left(a^2-(|x_0|-\Delta x)^2\right)}$.

Hence when such a type II switch off is carried out the result is a particle with a speed greater than zero and less than $a\sqrt{\frac{K}{m}}$. This speed depends on the particle's position at the time of switch off and on the distance covered during the switching off process. The significant point to notice in this example of a type II switch off is that nothing is stipulated, discussed or assumed regarding the behaviour of the system during the time interval Δt.

The two preceding examples have dealt with a system and process treated in classical terms. It is now of interest to describe the system <u>resulting</u> from the classical switch off in quantum mechanical terms. The result of the type I switch off was a particle with zero total energy.

In quantum mechanics this particle would be described by a constant wavefunction. If this wavefunction also had to satisfy the normalization condition $\int_{-\infty}^{+\infty} |\Psi|^2 dx = 1$ then this constant would be zero. As will be recalled from sections one and two, the result of reducing the potential in the wavefunction for the harmonic oscillator was also zero. The system resulting from the type II switch off is described by a plane wave $e^{\pm ikx}$ where $|k|$ has a value greater than zero and less than $\sqrt{\frac{Km}{\hbar}}\, a$. It should be pointed out that the "a" in $\sqrt{\frac{Km}{\hbar}}\, a$ is not a quantum mechanical quantity but enters from the restriction of the velocity of the free particle being described. This plane wave was not obtained by reducing the potential in the harmonic oscillator wave-function.

CHAPTER VI

UNIFORM MAGNETIC FIELD

The system under consideration in this chapter consists of a spinless particle with charge e moving in a uniform magnetic field $\vec{H}$ which fills all space. The velocity perpendicular to the field will be denoted by $\vec{v}$. The z-axis is chosen in the direction of the field.

1. QUANTUM MECHANICAL TREATMENT

When $(-Hy, 0, 0)$ is chosen as the vector potential and when $\psi = e^{i(k_x x + k_z z)} \chi(y)$ is chosen as the form of the wavefunction the equation determining χ is[13]

$$(6.1) \qquad \chi'' + \frac{2m}{\hbar^2}\left[E - \frac{p_z^2}{2m} - \frac{1}{2}m\left(\frac{eH}{mc}\right)^2\left(y + \frac{cp_x}{eH}\right)^2\right]\chi = 0.$$

If $y_0 = -\frac{cp_x}{eH}$ and $\omega = \frac{eH}{mc}$ are substituted in (6.1) an equation formally identical to the Schroedinger Equation for a harmonic oscillator is obtained.

To normalize a wavefunction of the above form it is sufficient to integrate from $-\infty$ to $+\infty$ with respect to y only. This is the case since the parts of the wavefunction depending on x and z are already in the form of plane waves and in unbounded space no further normalization is possible or necessary. The normalization condition is therefore $\int_{-\infty}^{+\infty} |\Psi|^2 dy = 1$. This imposes the boundary conditions that Ψ goes to zero as $|y|$ goes to infinity.

Using the same techniques as in the harmonic oscillator case the normalized wavefunction is

$$(6.2) \quad \Psi = e^{i(k_x x + k_z z)} \sqrt[4]{\frac{m\omega}{2^{2n}(n!)^2 \pi \hbar}}\, e^{-m\omega(y-y_0)^2/2\hbar}\, H_n\left(\sqrt{\frac{m\omega}{\hbar}}\,(y-y_0)\right).$$

If the field $\vec{H}$ is reduced to zero Ψ goes to zero. The rate of Ψ approaching zero is $e^{-\alpha/H}$ as H goes to zero. This is an essential singularity as H goes to zero and will be studied in section three.

By again using the analogy between (6.1) and the wave equation for a harmonic oscillator the allowed energy values are seen to be[14]

$$(6.3) \qquad E_n = (n+\tfrac{1}{2})\hbar\omega + \frac{p_z^2}{2m}$$

where n is a non-negative integer. As the field is decreased to zero ω goes to zero and the only energy is $\frac{p_z^2}{2m}$. That is, as H goes to zero the energy values associated with the transverse motion all become zero leaving only the energy associated with the unaffected motion parallel to the field.

The result of decreasing H to zero in (6.1) is

$$\chi'' + \frac{p_y^2}{2m}\chi = 0 \qquad (6.4)$$

where $\frac{p_y^2}{2m}$ is $E - \frac{p_z^2}{2m} - \frac{p_x^2}{2m}$

since there is no field. When (6.4) is combined with the boundary conditions that χ goes to zero as $|y|$ goes to infinity, the only acceptable solution (as in the previous cases) is $\chi = \psi = 0$.

The block diagram for this system is occupied as follows: corner one by equation (6.1) and the boundary conditions that ψ goes to zero as y goes to $\pm\infty$; corner two by the same boundary conditions and equation (6.4); corner three by wavefunction (6.2); and corner four by $\psi = 0$. As has been shown, reducing the field in the wavefunction (6.2) results in $\psi = 0$. Hence the block diagram is completed.

2. CLASSICAL ANALYSIS OF SWITCHING OFF

In classical terms the force equation for a stable orbit in a uniform magnetic field is

$$\frac{e}{mc} H = \frac{v}{r}. \qquad (6.5)$$

Stating that a system behaves as a charged particle moving in a uniform magnetic field implies that the particle is moving in a stable orbit in the plane perpendicular to the field. (6.5) is the necessary and sufficient condition for such a stable orbit. Hence (6.5) may be considered as the classical criterion of this system.

Before considering the actual switching off processes the following point should be emphasized. The particle's speed, v , remains constant independent of the field's behaviour because the force is always perpendicular to the field and no further constraints may be introduced.

In discussing the switching off of the magnetic field the two types must again be distinguished. Type I will again be studied first.

The type I switch off was defined as being the type in which the system satisfies the defining criteria for all intermediate values of the potential. Stating that the criterion of this system is satisfied for all intermediate field values means that the equation (6.5) is satisfied for these intermediate field values. Therefore, the field must be switched off in a manner such that at all intermediate stages the particle, travelling with finite velocity, $\vec{v}$, has sufficient time to reach the distance, r , which satisfies (6.5) for the various intermediate field values. Since a continuous switch off may be approximated with arbitrary accuracy by a discrete switch off, only the latter need be considered even though the results will apply to both methods. The details of a discrete type I switch off will now be analyzed.

If in a given step the field is lowered from H to H_1 then the radius, r_1, associated with H_1 is greater than r associated with H. For (6.5) to be satisfied the radius must therefore be r_1 when the field is H_1. Hence a time greater than τ, where τ is $\frac{r_1 - r}{v}$, must elapse before the step from H to H_1 can be considered completed. This requirement regarding the time is necessary to enable the particle, with its finite velocity, to reach the position required by (6.5). Before undertaking any given decrement the previous step must of course be completed. In the final step the field goes from some H^1 to zero and the radius goes from some finite r' to r_0 where r_0 is infinite. As above a time greater than $\frac{r_0 - r}{v}$ is required in order that this step be completed in a type I manner. Since the final step must be completed before the field can be considered as switched off, this infinite time for the last step shows that a type I switch off of this uniform magnetic field cannot be done in a finite time.

The stipulations for a type I switch off also imply that any result or effect due to any given step must be identical to the result or effect obtained by carrying out this same step in an arbitrarily large number of arbitrarily small, consecutive type I steps. From this point of view an arbitrary step from H_i to H_f and then the step from H_a to zero will be studied. In lowering the field from H_i to H_f the radius increases from r_i to r_f. If a very large number of steps are employed the radius increases as

in the monotonic sequence: $r_i, r_1, r_2, \ldots, r_f - \Delta r, r_f$.
For (6.5) to be satisfied for all intermediate values a time greater than $\frac{r_{K+1} - r_K}{V}$ must elapse before the corresponding decrease in the field can be considered as completed and the next decrease can be undertaken. Hence the total time which must elapse in going from H_i to H_f is greater than

$$\frac{r_1 - r_i}{V} + \frac{r_2 - r_1}{V} + \frac{r_3 - r_2}{V} + \ldots + \frac{r_f - (r_f - \Delta r)}{V} = \frac{r_f - r_i}{V}.$$

This agrees with the previous result. The field going from H_a to zero will now be studied. If this switching off is done in an arbitrarily large number of small steps the field goes through the values of the following monotonically decreasing sequence: $H_a, H_1, H_2, \ldots, \Delta H, 0$.
As previously explained, a time greater than $\frac{r_{K+1} - r_K}{V}$ must elapse before the step from H_K to H_{K+1} can be considered as completed. Hence for the switch off from H_a to zero to be completed in a type I fashion, the required time is greater than $\frac{r_1 - r_a}{V} + \frac{r_2 - r_1}{V} + \ldots + \frac{r_0 - r_{\Delta H}}{V} = \frac{r_0 - r_a}{V}$.
Since r_0, corresponding to zero field, is infinite and r_a is finite, this time is infinite. Hence, as before, an infinite time is required for a type I switch off of the magnetic field. The point of view that the result of any step must be equivalent to the result of an arbitrarily large number of steps between the same initial and final field values emphasizes the fact that the switching off process cannot be considered completed until sufficient time has

elapsed for the final step to be completed.

Since a type I switch off requires an infinite time as demonstrated above, any switch off completed in a finite time is of type II. A switch off in which the field goes to zero in a time comparable to the period of the orbiting particle is of type II and may be used as an example. The result of this switch off is a free particle with speed V . The direction of the free particle's velocity depends upon the details of the switch off. In fact the result of any type II switch off is as above. Since a type II switch off is done in a finite time and in view of the particle's finite velocity, the particle may be localized within a given finite volume for any particular type II switch off.

Although the discussion in this section has been in classical terms only, it is of interest to describe in quantum mechanical terminology the systems <u>resulting</u> from these two types of switch off. The result of the type I switch off was a particle, with velocity, $\vec{V}$, at infinity. Since the particle is at infinity its probability of being in any finite elementary volume is zero. Hence $|\psi|^2$ is zero and ψ is also zero. This is also the result obtained by reducing the field in the wavefunction. The result of a type II switch off has $e^{\pm i \underline{k} \cdot \underline{r}}$ as its wavefunction where $k = \frac{mv}{\hbar}$ and the direction of $\vec{k}$ is determined by the details of the switching off process. This plane wave was not obtained by reducing the field in the wavefunction.

Before completing this section an apparent inconsistency between the quantum mechanical and classical values for the transverse energy, when the field is zero, will be pointed out. As shown in the previous section, the quantum mechanical expression for the transverse energy becomes zero as the field is decreased to zero. However in both types of classical switch off the transverse velocity, and hence transverse kinetic energy, remains constant for all values of the field including zero field.

3. WAVEFUNCTION ESSENTIAL SINGULARITY FOR ZERO FIELD

In this system the dominating factor in the wavefunction as the field is reduced to zero is $e^{-\alpha/H}$, that is, the wavefunction goes to zero exponentially as $\frac{1}{H}$ goes to infinity. Since this is an essential singularity an expansion about $H = 0$ is impossible and therefore perturbation techniques will not give the wavefunction for a charged particle in a uniform magnetic field for small fields.

Although the harmonic oscillator and magnetic field wave equations and wavefunctions are formally the same there is one fundamental difference and it is this difference which corresponds to the vastly different physical behaviour between the two systems with regard to the potential being switched off. In the harmonic oscillator case the independent variable is simply x--independent of all parameters or anything else. However in the magnetic field case the "independent variable" is ($y-y_0$). Since H is a parameter independent of position $dy = d(y-y_0)$ and ($y-y_0$) is then the independent variable of an equation formally identical to the one for a harmonic oscillator. In the harmonic oscillator case the potential going to zero does not in any way influence the independent variable x whereas when the magnetic field goes to zero the "independent variable" ($y-y_0$) goes to infinity. Now it shall be shown how the behaviour of the magnetic field "independent variable" mathematically expresses the behaviour of the particle in the field. $y_0 = -\frac{cp_x}{eH}$ can be identified as the y coordinate of the centre of the circular path in the plane perpendicular to the field. Substituting $p_x = mv_x + \frac{eA_x}{c}$ and $A_x = -Hy$ in the expression for y_0 gives $y - y_0 = \frac{cm}{eH} v_x$. Similarly[14] $x - x_0 = \frac{cm}{eH} v_y$ can be introduced where x_0 is identified as the x coordinate of the centre of the above circular path. Squaring and adding produces the familiar result $r^2 = (x-x_0)^2 + (y-y_0)^2 = \frac{m^2c^2v^2}{e^2H^2}$. As the field goes to zero the radius r goes to infinity in agreement with the result of a type I switch off. These differences between the magnetic field and the harmonic oscillator cases, namely the behaviour of the independent variables and the essential singularity in the former, correspond to the physical difference that in the magnetic field case the velocity is undiminished and the particle must go off to infinity in a type I switch off whereas in the harmonic oscillator case the velocity becomes zero and the particle is contained within a finite region of space in a type I switch off.

CHAPTER VII

CONCLUSION

1. DISCUSSION OF SWITCHING OFF PROCESSES

In this thesis two types of switching off have been distinguished; namely, type I in which the criteria relating the parameters of the system are satisfied for all intermediate values of the potential and type II in which these criteria are not satisfied for intermediate values of the potential. In all the bound systems considered there was at least one classical relation or equation which characterized the system. In all the unbound systems there was no such criterion. Hence it follows that distinguishing between the two types of switching off is meaningful only in the case of a bound system.

Criteria determining the type of switch off a bound system undergoes will now be given. Since the switching off processes have been discussed in classical terms the criteria will be given in classical terms. Due to the uncertainty principle these criteria cannot be directly extended to quantum mechanics and therefore no specific quantum mechanical criteria for distinguishing the two switching off methods will be given. Even though the characteristics distinguishing the two types of switch off are not given in quantum mechanical terms the actual distinction in methods is applicable to a quantum mechanical description of a system. Furthermore, since the actual experimental procedures used in switching off potentials are usually of a classical nature, this classical differentiation between the types of switching off is applicable in determining the type of switch off used experimentally. Since a switch off is either of type I or type II, it is sufficient to give the criteria for a type I switch off since a switch off in which these criteria are not met is necessarily of type II.

In any bound system the maximum kinetic energy ever attained must be less than or equal to the maximum of the absolute values of the potential energy. It is therefore apparent that unless the velocity is somewhere zero the potential energy cannot go to zero in a finite number of steps without violating this energy criterion for sufficiently small potential. This may be easily seen in a case where the total energy is negative. For example, in the negative energy Coulomb case (see inequality (3.8)) where the velocity is nowhere zero, the potential cannot be zero for non-zero velocity without this inequality being disobeyed. By use of (3.9) it was explicitly shown that the potential cannot go to zero in a finite number of steps. The harmonic oscillator illustrates the case in which the potential can go to zero since there is a position at which the velocity is zero and the potential can there be lowered. If a criterion of a system stipulates that the particle must be at infinity in order to satisfy this criterion when the potential is zero, then the potential in this system cannot be switched off in a type I manner in a finite time. This was demonstrated in chapter six section two. Hence, the two requirements of a system in order that a type I switch off to zero may be done in a finite time are: first, the particle need not necessarily go to infinity in order to satisfy the criteria of the system for zero potential; and secondly, there be a position at which the particle's kinetic energy is zero. In a system which meets these requirements the potential may, in principle, be switched off to zero in a finite time in a type I manner by lowering the potential while the particle is at a position of zero velocity. This however requires a finite lowering of the potential in a zero time interval. Since this cannot be achieved a type I switch off to zero in a bound system is not experimentally feasible. Hence any experimental switch off to zero in a bound system is of type II.

The preceding discussion is concerned with a type I switch off in which the potential is switched off to zero. However, to an arbitrary degree of accuracy, a type I lowering of the potential from an initial value to a lower, nonzero final value may be experimentally carried out in those cases where the potential may be lowered during a finite, non-zero time interval and still be in accord with the conditions for a type I switch off during this lowering. For example, in the uniform magnetic field and bound Coulomb cases the potential or field may be experimentally lowered from some initial value to a non-zero final one in a type I manner. The details of the procedure may vary from case to case but the point is that such a type I lowering is experimentally feasible.

Since in an unbound system there is no distinction between the two methods of switching off, the two types are identical and both correspond to any given experimental switch off.

2. REDUCTION OF THE POTENTIAL IN WAVEFUNCTION

In all of the systems studied the result of reducing the potential in the wavefunction was one of the following two:

(a) a zero wavefunction;

(b) an oscillatory wavefunction -- either a trigonometric or imaginary exponential function.

Each of the results (b) corresponded to an unbound system. Each of the results (a), with the exception of the negative total energy uniform electric field case, corresponded to a bound system. This exception will be treated in section five. The reasons for this correspondence between a zero final wavefunction and a bound system will be seen in the succeeding paragraphs.

A significant and satisfying common feature of those wavefunctions which went to zero, excepting the above exception, will now be presented. As was previously stated, the wavefunction went to zero only if it described a bound system. The fundamental characteristic of a bound system is the normalization condition $\int_{\text{all space}} |\Psi|^2 \, d\tau = 1$. For all bound systems this condition determines a normalization coefficient which causes the wavefunction to obey this condition. In all the wavefunctions under consideration (see (2.5), (2.5'), (3.4), (5.3), (6.2)) it is this normalization coefficient which goes to zero. Except for the magnetic field wavefunction, these wavefunctions go to zero only on account of their normalization coefficient. If the normalization coefficient would have been absent in these systems the wavefunction resulting from reducing the potential would have been a constant but not, in general, zero. The physical significance of this will now be given. In all the bound systems considered, except for the magnetic field case, the total energy goes to zero as the potential does in a type I switch off. (The significance of specifying type I switch off will be seen further on in this section.) Hence the end result is a particle with zero total energy. Having zero total energy, this particle has an equal probability of being anywhere, that is, a constant wavefunction to within a phase factor. In general, it is only upon application of the normalization condition, with its associated boundary conditions, that this constant must be zero. In the magnetic field case the normalization coefficient also goes to zero. However, the wavefunction goes to zero more rapidly due to a dominating exponential factor. As shown in chapter six, this exponential decrease to zero corresponds to the particle going to infinity. The preceding considerations suggest the following general statements:

(a) In all bound systems in which it is not imperative that the particle go to infinity in a type I switch off, the wavefunction, in general, goes to zero due to the normalization coefficient.

(b) If the particle must go to infinity in a type I switch off then the normalization coefficient again goes to zero but is dominated by an exponentially decreasing factor which describes the particle going to infinity.

The preceding has shown how the characteristic property of a bound system directly determines the result of reducing the potential in the wavefunction of such a system.

In an unbound system the boundary conditions at $\pm\infty$ are that the wavefunction oscillates since $\int_{\text{all space}} |\psi|^2 d\tau = 1$ need not be satisfied. Furthermore, there are no conditions by which the potential restricts the total energy. Hence reducing the potential in the wavefunction for an unbound system yields a free particle wavefunction which satisfies the boundary conditions. Thus for an unbound system the result of reducing the potential in the wavefunction is that expected from experimental observations.

The relation between the result of reducing the potential in the wavefunction and the results of the two types of switching off will now be discussed. Bound systems will again be discussed first.

As demonstrated in the examples of switching off in the previous chapters, the system resulting from a type I switch off is quantum mechanically described by the result of reducing the potential in the wavefunction of the original system, that is, by a zero wavefunction for a bound system. The reason for this correspondence between the results of a type I switch off, and reducing the potential in the wavefunction, will become apparent when the properties of a type I switch off and of a wavefunction are compared.

In addition to other parameters and variables, the wavefunction is a function of the potential of a system and fully describes the system in terms of the potential and these other parameters and variables. For any specific system there is a one to one correspondence between the system with a specific set of parameters and a particular wavefunction.

Consider a wavefunction describing any particular system. If the potential parameter within the wavefunction is changed, the result is a wavefunction describing a system with the same characteristics and criteria but with a different potential energy. That is, the wavefunction now describes the same kind of system which has adjusted itself such as to satisfy its characteristic criteria when the potential is equal to its new value. Now consider a particular system described by a particular wavefunction. Let the potential of this system be switched off and consider the system as the potential is being lowered. Since the switching off process is not being described, it is unnecessary to stipulate whether the process is classical or quantum. As long as the system satisfies the criteria of the original system, the switch off is of type I and the original wavefunction, with the potential reduced, may be used to describe the system at any particular stage. However, as soon as the criteria of the original system are no longer satisfied, the potential is no longer being switched off in the original system but in another, different system. At this stage, where the switch off is no longer of type I and the potential is being switched off in a different system, reducing the potential in the original wavefunction no longer corresponds to the physical process and a different wavefunction describing this different system must now be introduced and the potential reduced in this latter wavefunction. Hence it is seen that the identification of the result of a type I switch off with the result of reduction in the wavefunction follows from the primary property of a wavefunction and a type I switch off.

As shown in section one, any experimental switch off to zero in a bound system is necessarily of type II. It has just been demonstrated that the result of reducing the potential to zero in a wavefunction describes the result of a type I switch off. Hence reducing the potential to zero in a wavefunction describing a bound system does not correspond to an experimentally feasible method of switching off the potential in this system. This is the reason the result of reducing the potential to zero in the wavefunction of a bound system does not yield the plane wave wavefunction indicated by experimental observations. However a type I switch off to a non-zero value is possible in some bound systems. In these systems the result of such a lowering to a non-zero value is described by the result of reducing the potential to this non-zero, final value in the original wavefunction.

In quantum mechanical terminology, reducing the potential in the wavefunction of a bound system describes a process whereby the system proceeds through successive stationary states of this same system, where each stationary state corresponds to a lower potential than the previous one, until the stationary state corresponding to zero potential is reached. The wavefunction resulting from reducing the potential to any value, including zero, is the wavefunction describing the stationary state corresponding to this reduced value of the potential.

Since in an unbound system the two types of switching off are equivalent and reducing the potential in the wavefunction describes the result of a type I process, it follows that the result of reducing the potential to zero in the wavefunction describes the result of physically switching off the potential in an arbitrary manner. This is supported by the examples of unbound systems which have been analyzed in chapters two, three, and four. Hence in all unbound systems, the result of reducing the potential to zero in the wavefunction is a free particle wavefunction as is expected from experimental observations.

3. DECREASING THE POTENTIAL IN THE WAVE EQUATION

The result of decreasing the potential in the wave equation will now be discussed. The case of a bound system will be treated first.

If in the wave equation for a bound system the potential is decreased to zero and the other parameters are varied in accord with the criteria of the system, this method of decreasing the potential obviously corresponds to a type I switch off. When the resulting equation is solved in conjunction with the boundary conditions obtained from the original ones by decreasing the potential to zero the result is a zero wavefunction which describes the result of a type I switch off. If however the potential is mathematically set equal to zero in the equation without influencing any of the other parameters this then corresponds to the potential being decreased without imposing the criteria of the system. If the resulting equation is solved in conjunction with the boundary conditions derived from the original ones by decreasing the potential to zero, the solution is again a zero wavefunction which again describes the result of a type I switch off. This at first appears surprising since the potential in the equation was decreased in a manner analogous to a type II switch off. If, however, this latter resulting equation is solved in conjunction with different boundary conditions the solution will be a different, non-zero wavefunction. If these different boundary conditions are chosen to be those for a free particle the solution is a plane wave which is the wavefunction describing the result of a type II switch off.

The preceding paragraph has demonstrated that the boundary conditions, associated with the wave equation resulting from decreasing the potential in the original equation, determine the type of switch off to which decreasing the potential in the wave equation corresponds. This is reasonable if the following is considered. Maintaining the boundary conditions of a bound system implies that the system remains the same and that therefore the criteria of the bound system are satisfied. Hence if the boundary conditions are maintained for all values of the potential it is apparent that the conditions for a type I switch off are satisfied. If, however, the boundary conditions are altered while the potential is being decreased then the resulting equation in conjunction with these different boundary conditions describes a system whose characteristics differ from those of the initial system. This corresponds to a type II switch off.

If in the wave equation for an unbound system the potential is set equal to zero, no other parameters may be affected since for such systems the potential places no restrictions on the other parameters. If the resulting equation is solved in conjunction with boundary conditions obtained from the original ones by decreasing the potential to zero the solution is an oscillating free particle wave-function. Since the boundary conditions are not altered, with the exception of decreasing the potential if it explicitly appears in them, the system remains the same and the above process corresponds to a type I switch off which for unbound systems is identical to a type II switch off. Hence the solution of the wave equation for an unbound system, with the potential decreased to zero, in conjunction with the above boundary conditions corresponds to the experimentally observed result.

4. DISCUSSION OF THE ORIGINAL PROBLEM AND PARADOX OF AN ELECTRON IN A UNIFORM MAGNETIC FIELD

The original problem in section one of chapter one will now be analyzed. In this problem of an electron in a uniform magnetic field the system is a bound one and the field is switched off in a finite time. This switch off is therefore of type II. It therefore follows that the experimental result cannot be described by the result of reducing the field in the wavefunction.

The paradox arose in the original treatment because reducing the potential in the wavefunction gave zero whereas a plane wave solution, which agreed with experimental observation, was obtained by solving the equation resulting from decreasing the potential to zero in the original equation. This plane wave solution was obtained because no boundary conditions were associated with the wave equation. That it was this absence of accompanying boundary conditions which led to the plane wave solution will be shown in the following paragraph.

Since boundary conditions did not accompany the wave equation the type of switch off used was not specified. Neglecting the boundary conditions that the wavefunction goes to zero at $\pm\infty$ is the same as imposing different ones. If the general solution which oscillates at $\pm\infty$ is taken as the solution to the wave equation with zero potential, the effect is equivalent to specifying these different boundary conditions as being done for a free particle. This is what was in fact done. As shown in the previous section, this change in boundary conditions results in a wavefunction describing a type II switch off. Hence the solution obtained in this way describes the experimental result of a free particle since in actuality a type II switch off is experimentally carried out. However, since reducing the potential to zero in the wavefunction corresponds to a type I switch off, these two mathematical descriptions of the final system do not agree. Hence the original paradox arose because one wavefunction was obtained by dealing with an incompletely specified bound system, and it described the result of a type II switch off, whereas the other wavefunction was obtained by dealing with a fully specified system and it described the result of a type I switch off.

If, however, the original boundary conditions had been associated with the wave equation in which the potential was decreased the solution of this equation would have been in agreement with the result of reducing the potential in the wavefunction. These identical results would not have described the physical situation with the potential switched off since all the mathematics would describe the result of a type I switch off.

5. A COMMENT ON THE UNIFORM ELECTRIC FIELD CASE

The uniform electric field system is an unbound one for both positive and negative values of the total energy, E. As was shown in chapter four, the significance of the value of E is to indicate the position at which a particle incident from $z=+\infty$ is classically reflected. Hence in this case negative E does not indicate a bound system. Negative E corresponds to reflection at $z=+\infty$ when the field is zero. Hence negative E corresponds to a zero probability of the particle being in any finite region of space when the field is zero. Rather than a normalizing coefficient, it is this impossibility of a particle with negative E being in a finite region of space when the potential is zero which accounts for the zero wavefunction when the potential is reduced to zero.

6. SUMMARY OF THESIS CONCLUSIONS

(a) For an unbound system.

(i) The result of reducing the potential to zero in the wavefunction of the system is an oscillating function describing a free particle whose kinetic energy is equal to the original total energy.

(ii) The system resulting from experimentally switching off the potential in any manner is described by both the result of reducing the potential to zero in the wavefunction and the solution of the wave equation with accompanying boundary conditions which are obtained by decreasing the potential to zero in the original wave equation and boundary conditions respectively.

(iii) Only in an unbound system can the potential be reduced in the wavefunction or be experimentally switched off such that the total energy remains constant.

(b) For a bound system.

(i) The result of reducing the potential to zero in the wavefunction is a zero wavefunction.

(ii) Two methods of switching off must be distinguished. They are defined in section three of chapter five.

(iii) A type I switch off to zero is not experimentally feasible. The system resulting from this type of switch off is mathematically described by the result of reducing the potential to zero in the wavefunction or by the solution of the equation with accompanying boundary conditions which are obtained by decreasing the potential to zero in the original equation and boundary conditions respectively. Hence, the result of reducing the potential to zero in the wavefunction does not describe a system resulting from any feasible experimental switch off.

(iv) In some bound systems the potential may be experimentally lowered to a non-zero value in a type I manner. The result of such a lowering is described by the wavefunction obtained by reducing the potential in the initial wavefunction to this lower value.

(v) The potential in a bound system can be switched off to zero only in a type II fashion. The result of a type II switch off cannot be described by the result of altering in any manner the potential in the wavefunction. The result of a type II switch off can be described by the solution of the equation obtained from the original by decreasing the potential to zero only if the accompanying boundary conditions are changed to those for a free particle.

(c) Block diagram.

(i) For any system the block diagram is always completed if the corners are occupied by a complete description of their respective systems and if the steps from corner one to corner two and from corner three to corner four correspond to the same type of physical switch off.

(ii) In order to be closed a block diagram must deal only with a type I switch off since the step from corner three to corner four can correspond only to this process.

(iii) For an unbound system a closed block diagram is concerned with the actual physical process and its fourth corner describes the result of an experimental switch off.

(iv) In a bound system in which the potential goes to zero, a closed block diagram must deal with an experimentally impossible process and the entry in the fourth corner does not describe the result of an experimentally feasible procedure.

(v) An actual physical switch off to zero cannot be expressed as a closed block diagram for the case of a bound system.

(vi) For some bound systems a partial switch off to a non-zero value can be expressed in the form of a completed block diagram.

(d) General properties of a wavefunction.

(i) Since a given wavefunction describes a system with particular criteria, the wavefunction resulting from altering the value of any parameter in the initial wavefunction describes the initial system modified such that it has the new value for the parameter and still satisfies all the original criteria.

(ii) Changing the value of any parameter in the wave-function corresponds to the result of physically changing this parameter by the same amount in a manner such that the characteristic criteria of the system are satisfied for the initial, final and all intermediate values of this parameter. For any given system this manner of changing the value of the parameter may or may not be experimentally feasible.

APPENDIX

SYSTEMS CONTAINED WITHIN A PHYSICAL CONTAINER

A system contained by a physical container will now be discussed in order to see the effect of reducing the potential to zero in the wavefunction describing such a system. In discussing reducing the potential in the wavefunction of such a system one can properly discuss only a system whose dimensions do not need to exceed the dimensions of the container in order to satisfy the criteria of the system for sufficiently small potentials. If for sufficiently small values of the potential the radius must exceed the linear dimensions of any given container, then for these small potentials the system is not the one which the wavefunction describes. For these small potentials the system has an altered motion due to the superimposed rebound motion. Hence the renormalized wavefunction of the unconstrained system no longer describes the actual behaviour of the system at these small potentials. Therefore, reducing the potential in this wavefunction does not correspond to switching off the actual system. To describe such a constrained system for these small potentials a distribution function may be used. The potential would therefore have to be reduced in this distribution function. Hence this appendix applies only to a system whose dimensions need not exceed those of the container for very small potentials.

The constraint imposed by the walls of this container is expressed by a potential which abruptly goes to infinity. Let this constraining potential be R where $R = 0$ for $|x| < a$ and $R = \infty$ for $|x| > a$. This potential imposes two significant changes: the boundary conditions become $\Psi(+a) = \Psi(-a) = 0$ and the normalization condition in one dimension becomes

$$\int_{-a}^{+a} |\Psi|^2 \, d\xi = 1.$$

Two cases must be distinguished. The first is where the spatially restricting potential is imposed on an already bound system and the second is where this potential is imposed on an otherwise unbound system. Both these cases can be illustrated by the harmonic oscillator. The first will be considered first.

In the first case the total energy is that for a harmonic oscillator, that is[15] $E = (s + \frac{1}{2})\hbar\omega_c$ where s is not in general an integer. As the potential is reduced ω_c goes to zero and the result is again a particle with zero total energy. Hence a constant wave-function results. There would appear to be two choices for this constant; namely, $\frac{1}{2a}$ to satisfy the normalization condition or zero to satisfy the boundary conditions. Chandrasekhar[16] obtains $\alpha e^{-\rho^2/2} \rho(1 - \varepsilon\chi)$ as the solution of the first excited state of a bounded linear oscillator where α and ε are constants, χ is a power series in ρ^2 and $\rho = x\sqrt{\frac{m\omega_c}{\hbar^2}}$. Since ρ goes to zero as the potential does this wavefunction becomes zero. Hence the boundary conditions, rather than normalization condition, are satisfied.

The second case will now be considered. The treatment of this case will be in classical terms but the quantum mechanical description of the end result will be given. The situation is that of a particle constrained within a region $[-a, a]$ by perfectly rigid and elastic walls. Within this region the particle is subject to a force of magnitude Kx towards the centre, However the total energy of the particle is such that it still has a finite velocity when it reaches the walls. Its energy may therefore be written as $\frac{1}{2}Ka^2 + E_0$ where $\frac{1}{2}Ka^2$ is the total energy associated with the motion under the harmonic force and E_0 is the kinetic energy the particle has when it reaches a wall. If the potential is now switched off in a type I manner (which corresponds to reduction in the wavefunction) as in section three of chapter four, the result is a particle with energy E_0 bouncing between the walls. In quantum mechanics this resulting system is described by the wavefunction for a free particle constrained to the region $[-a, a]$.

The preceding examples suggest the following statements:

(a) If the external source potential is reduced to zero in the wavefunction describing a bound system which is further constrained by an abrupt, infinite potential, the result is a zero as was the case in the absence of the constraint potential.

(b) If the external source potential is reduced to zero in the wavefunction describing an unbound system which has an infinite constraining potential superimposed, the result is a free particle wavefunction within the box formed by this infinite potential.

(c) The boundary conditions, rather than the normalization condition, are the fundamental characteristics of a system.

These statements are consistent with the conclusions in chapter seven.

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