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CORRESPONDENCE IDENTITIES

by

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ABSTRACT

Bohr's correspondence principle relates quantum phenomena to classical mechanics in the limit $\hbar / S \to 0$, as the dynamical action variables S become large in comparison with Planck's constant. Relations between quantum and classical mechanics which hold even for low quantum numbers and relatively small values of the classical action are called correspondence identities. For the Coulomb potential the following three correspondence identities are known:

(1) The Rutherford Scattering identity The quantum-mechanical and classical angular differential cross sections for the scattering of a charged particle by a fixed charge are the same.

(2) The Bohr-Sommerfeld identity The old quantum theory, which postulated that only those orbits occur for which the action around the classical path of a periodic system is a multiple of $2\pi\hbar$, gives the correct energy levels of the hydrogen atom and hydrogenic ions.

(3) The Fock identity The classical and quantal microcanonical distributions in momentum of the electron in the hydrogen atom are equal for all values of the classical energy equal to the levels E_n.

These correspondence identities concern the system of electron and proton and in this thesis it is shown how each of the identities follows from a complete correspondence identity whereby the non-relativistic quantum dynamics of the system is obtained from the solution of the corresponding classical problem. A complete correspondence identity is provided by expressing the kernel of the spectral operator $I_E = \delta(E - H)$ in momentum representation for all real non-zero energies E, as a sum over paths of terms containing the classical action. For the bound states the paths are the classical paths. For positive energies they are the generalised classical paths which arise from the analytic continuation in energy of the bound state paths. The generalised classical paths are built up from the paths of scattering of both electrons and positrons and are needed to obtain the quantal barrier penetration in momentum space.

Because of the similarities between the techniques used in this thesis to provide a complete correspondence identity and those of the phase-integral approximation the results are compared wherever possible with those of Gutzwiller (1967).

Finally, a general derivation of a scattering cross section from the spectral operator is presented which does not require an explicit treatment of the long-range distortion in the case of the Coulomb potential.

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CONTENTS

CHAPTER 1

THE CORRESPONDENCE IDENTITIES

1) The Purpose of This Thesis

The present day theory of quantum mechanics is used widely in all fields of atomic physics. Its origins may be traced back to the beginning of the twentieth century and were due mainly to the failures of classical physics to account for the properties of black-body radiation and line spectra. The development of the subject from the very early theories to the unified and consistent theory of quantum mechanics took about twenty-five years and an extremely full and detailed account of this development is to be found in Jammer (1966).

For many years the theories of classical physics had remained unchallenged, and perhaps it is not surprising that quantum mechanics, being based on assumptions which clearly contradict some of the basic principles of classical mechanics and electrodynamics, took so long in its development. However, some of the delay must be attributed to the remarkable success enjoyed by certain theories of atomic structure which were, in fact, based on classical mechanics. So striking was the success of these classical theories that the results predicted, later, by quantum mechanics were identical. Such identities we have called correspondence identities, and the purpose of this thesis is to explain the correspondence identities that exist for the hydrogen atom and hydrogenic ions.

It is quite fair to say that the correspondence identities associated with the hydrogen atom are the ones which have had most effect in the development of quantum mechanics, and bearing this in mind it is necessary that they be understood. Not all of the correspondence identities, however, have had parts to play in the development of the subject, and as we shall see one of the identities was first discovered in 1935 - well after the birth of quantum mechanics.

Because of the historical importance of the correspondence identities and their relevance in the development of quantum mechanics it will be necessary in the opening sections of this chapter to consider in more detail than is usual for theses on quantum mechanics some of the early quantum theories and theories of atomic structure. The chapter will be concluded with a discussion of the correspondence identities with particular reference to both the early quantum theory and also to their present day application in atomic physics.

2) The Nuclear Atom

Regularities in the lines of the hydrogen spectrum were well known by spectroscopists and empirical formulae had been produced to describe them. No theoretical interpretation of the regularities could be given however because of the inconsistencies met with in each of the existing models of the atom. The two most notable models were the 'plum-cake' model of Thomson and the nuclear model due to Rutherford. The nuclear model of the atom ran into the serious problem of instability: the electrons revolving around the nucleus would constantly be emitting radiation, losing energy, and would fall towards the centre. The size of the atom would continually be decreasing, which was in direct contradiction to the predictions of the Kinetic Theory, and also continuous radiation and not line radiation would be observed. The Thomson model, on the other hand, could not explain the results of scattering experiments with α-particles that were being carried out by Geiger, Marsden and Rutherford.

It was observed that α-particles mostly passed without deviation through air and thin layers of foil, but occasionally they were scattered through large angles, often by as much as 150°. These large angles of scattering were also due to single collisions and this was confirmed by observing the collisions in a Wilson cloud chamber. The large forces necessary to produce this type of collision could only arise in the nuclear model and did not arise in the Thomson model.

Rutherford produced firm evidence in favour of the nuclear model by evaluating the angular differential cross section (by means of classical mechanics) for the scattering of α-particles by heavy nuclei. The well known formula for the angular differential cross section $\sigma(\Theta)$ is given by:

$$\sigma(\Theta) = \left(\frac{Ze^2}{mV^2}\right)^2 \operatorname{cosec}^4 \frac{\Theta}{2} \tag{1.1}$$

where the α-particle is assumed to carry a charge $2e$, have mass m and an incident velocity V. This formula was verified experimentally by Geiger and Marsden, and by making absolute measurements for fixed values of Θ and V, Rutherford was then able to infer successfully the nuclear structure of some of the elements. It was well known at the time that quantal corrections had to be made to certain classical formulae of atomic physics. No such corrections were needed in the Rutherford formula.

3) The Bohr-Sommerfeld Theory of Atomic Structure

The nuclear model of the atom was chosen by Bohr as a basis for his theory of atomic structure. He overcame the problem of instability by postulating the existence of stable orbits in which the electrons could rotate without the emission of radiation. When an electron jumped from one stable orbit to another of lower energy it would radiate a photon of energy $h\nu$ and the size of the atom would be maintained by the existence of a ground state from which the electron could not decay.

In 1913 Bohr applied these concepts to the hydrogen atom, assuming the electron to move around the proton in a planetary fashion according to the laws of classical mechanics. He considered only circular motion and obtained the stable orbits by imposing a quantum condition on the value of the classical angular momentum. By requiring that the angular momentum be equal to a whole number n of units of $h/2\pi$ he obtained for the energy levels of these orbits the values :

$$E_n = -\frac{e^4 m 2\pi^2}{h^2 n^2} \quad , \quad n = 1, 2, \ldots . \qquad (1.2)$$

With this model Bohr was able to explain the Balmer series formula and confirm the predictions of the Ritz combination principle. His expression for the Rydberg constant in terms of well known constants was also in excellent agreement with the experimentally observed value and the radius of the smallest Bohr orbit was of the order of 10^{-8} cm as predicted by the Kinetic Theory.

Bohr's successful theory of the hydrogen atom was put on a much more general and sophisticated basis by Sommerfeld. He postulated that the stationary states of any periodic system with f degrees of freedom would be determined by the quantum conditions :

$$\oint p_k dq_k = n_k h \quad , \; k = 1, 2, \ldots f \tag{1.3}$$

where p and q are the usual canonical variables in phase space. For the hydrogen atom he considered the general elliptic motion of the electron and by taking polar coordinates (r , θ) in the plane of the orbit he obtained for the energy levels

$$E_n = \frac{-2\pi^2 e^4 \mu}{h^2 (n_r + n_\theta)^2} \tag{1.4}$$

where $n_r + n_\theta = n$ and μ is the reduced mass of the electron and proton. The energy levels, however, were the same as these obtained by Bohr, who had only considered circular motion.

Sommerfeld was searching for some explanation of the fine structure of the lines in the hydrogen spectrum and considered the solution of the problem in three dimensions. Again no new energy levels could be found, but by considering the relativistic change in the mass of the electron, Sommerfeld was able to show that the orbits were then no longer closed, but precessed about the nucleus. In this way he was able to account for the fine structure of the hydrogen lines.

4) The Correspondence Principle

An important development in the understanding of the quantum theory was Bohr's correspondence principle. The Bohr-Sommerfeld theory could be used effectively (in the case of hydrogen) to obtain the atom's stationary states. A description of the processes resulting from transitions between these stationary states was the subject of the correspondence principle.

It had its foundation in the assumption that quantum theory contains classical mechanics as a limiting case.

Planck had noted that as $h \to 0$ his radiation formula goes over into the Rayleigh-Jeans formula. Bohr noticed the same was true as the frequency ν becomes small for fixed h. For a periodic system the concept of $\nu \to 0$ may be interpreted in the following way. In terms of the change in energy, ΔE, the frequency of the emitted radiation is given by

$$\Delta E = h\nu \; . \tag{1.5}$$

As $\nu \to 0$, then ΔE must also tend to zero. This situation arises when the energy levels almost form a continuum. In terms of quantum numbers, n, this suggests that the change in n must be small compared with n. In the case of the hydrogen atom this occurs in transitions between highly excited states. From purely classical considerations Bohr could conclude that an electron in an orbit of large energy should, when it jumped to an adjacent orbit, radiate a photon whose frequency was equal to the frequency of rotation of the electron itself. He also insisted that any special properties that an electron might have 'inside' an atom must pass naturally to the classical properties when the electron is far from the centre of the atom.

To Bohr, the general method of solving a problem was clear. One had to calculate from an assumed classical model, and then adjust the necessary formulae such that the change was negligible for large quantum numbers, but was in good agreement with experiment for low quantum numbers. Classical electrodynamics provided a complete knowledge of the intensities and states of polarization of spectral lines, and in the manner just described Bohr was able to give a full description of the radiation emitted by the motion of electrons in atoms. This method of accounting for the actual situation by means of the corresponding classical situation was called the correspondence principle by Bohr. He realised that the classical theory of radiation was the limiting case of a more general theory, but this theory had then still to be discovered.

5) The Rise of Modern Quantum Theory

Although the Bohr-Sommerfeld theory gave an excellent account of atomic structure in the case of the hydrogen atom, it often failed in its application to the more complicated atoms and molecules. The theory did not for example predict the electronic energy levels of the H_2^+ molecule correctly. The Bohr-Sommerfeld quantum theory was essentially based on classical mechanics, and by the correspondence principle just discussed the description it provides when quantum numbers are high is perfectly adequate, however the theory has no real justification in the case of small quantum numbers. This was realised by many people at the time and indeed completely new theories were developed by Schrödinger and Heisenberg and the product of these theories is what we now call the theory of quantum mechanics.

Schrödinger's approach had its origins in the wave-particle properties of both radiation and matter. The famous Schrödinger wave equation for matter waves was the culmination of work done by Debye and de Broglie. Debye noted that whenever the refractive index of a medium changes slowly over distances comparable with the wavelength, then the scalar wave equation of optics reduces to the eikonal equation of geometrical optics (see for example Goldstein 1964, chap. 9, §8). De Broglie conjectured that since geometrical optics was the limiting case of wave optics then perhaps the Hamilton-Jacobi equation of classical mechanics was the limiting form of an equation representing matter waves, and he showed in 1924 that if one supposes waves to be associated with matter, then the wavelength λ of the matter waves is given by

$$\lambda = h/mv \qquad (1.6)$$

where v is the particle velocity. Schrödinger in 1926 obtained the equation of matter waves which gave the wavelength in accordance with de Broglie's result. Schrödinger pointed out that just as wave optics must be used whenever the refractive index changes considerably over a wavelength, then wave mechanics must be considered whenever the path of the system changes considerably over the dimensions of the associated de Broglie wavelength, as it does for the electron in an atom.

At the same time as these advances in wave mechanics were taking place, Heisenberg took a decisive step in the formulation of matrix mechanics. He rejected the idea of the path of an electron on the grounds that no one had actually observed it, and he developed a theory based on observed quantities such as frequencies and intensities. By using the correspondence principle once and for all he was able to guess the complete mathematical scheme of the quantum theory.

The main feature of this new theory was the fact that physical quantities such as position and momentum were represented by sets of time-dependent complex numbers - the sets being infinite-dimensional matrices. Further the theory predicted that a simultaneous knowledge of both the momentum and position coordinates of a system was impossible and the famous uncertainty relations have never been disproved. Heisenberg's theory of matrix mechanics was shown to be equivalent to the wave-mechanical approach by Schrödinger himself, and the two theories were later combined and put on a rigorous axiomatric basis by Dirac, Jordan and Hilbert,to name but a few.

6) The Correspondence Identities

When we consider the Bohr-Sommerfeld theory of atomic structure in the light of quantum mechanics, it is easy to understand its failures. The idea of electrons in atoms moving in well defined orbits, so essential in the Bohr-Sommerfeld theory, is in direct contradiction to Heisenberg's uncertainty principle and to the basic assumptions of wave mechanics. It is extremely difficult to account for the fact that in the case of the hydrogen atom the Bohr-Sommerfeld theory did prove to be successful and indeed gave results which were only to be confirmed by quantum mechanics. The theory was based on the nuclear model of the atom which as we have seen was strongly substantiated by the results of Rutherford's scattering experiments with α-particles. The success of both the Bohr-Sommerfeld theory of the hydrogen atom and Rutherford's work on the nuclear structure of the elements can be attributed to two correspondence identities:

(1) The Rutherford Scattering Identity. The quantum-mechanical and classical angular differential cross sections for the scattering of a charged particle by a fixed charge are the same.

(2) The Bohr-Sommerfeld Identity. The electronic energy levels of the hydrogen atom and the hydrogenic ions as predicted by the theories of Bohr and Sommerfeld are the same as those predicted by quantum mechanics.

In the case of α-particles scattered by nuclei, the action integrals associated with the interaction are large compared with Planck's constant and the approximation of classical mechanics is valid. The success of Rutherford's work can be accounted for in this manner. But this argument cannot be applied to the case of electrons or positrons being scattered by a central Coulomb potential, where the value of the angular differential cross section is still the same as that given by the Rutherford formula (see Mott and Massey 1965, p.53). The Rutherford scattering identity as it applies to the scattering of an electron by a fixed proton will be considered in this thesis and corresponds to the problem of the hydrogen atom for positive values of the total energy.

The Bohr-Sommerfeld identity concerns the bound-state problem of the hydrogen atom, and whenever the atom is in a highly excited level, the good agreement between the two theories can be understood by means of the correspondence principle. Why the identity holds for all quantum numbers, large and small, will be explained in this thesis. This correspondence identity obviously had a major effect on the development of the quantum theory. Transitions between low levels of the hydrogen atom could be studied, and the frequencies of the various spectral lines predicted accurately. Those lines predicted in the far ultraviolet were discovered in 1914 by Lyman, and the lines of ionized helium, corresponding to the Pickering series were found experimentally by Bohr and Evans. It was successes like these which suggested that the Bohr-Sommerfeld theory held all the answers to problems of atomic structure. Indeed, the success of the theory and Sommerfeld's account of the fine structure of hydrogen lines in terms of the relativistic change in mass of the electron were probably responsible for the delay in discovery of spin.

There is a third correspondence identity associated with the hydrogen atom which played no part in the early development of quantum mechanics. It was due to Fock in 1935 and is an identity between the classical- and quantum-mechanical bound-state momentum distributions of the electron in the hydrogen atom. Suppose that a statistical assembly of hydrogen atoms all have the same negative energy E_n. Then quantum-mechanically, neglecting spin, there are n^2 states belonging to this level. If we assume that each of these states is equally populated in this assembly, then we have a quantal microcanonical distribution. Fock (1935) showed that for such an assembly, the distribution in momentum $\rho_n(\underset{\sim}{p})$ is given by

$$\rho_n(\underset{\sim}{p}) = \frac{8\, p_n^5}{\pi^2 (p_n^2 + p^2)^4} \qquad (1.7)$$

and has the same form for all values of n. In this equation p_n^2 is the mean square momentum whose value is $-2\mu E_n$.

The corresponding momentum distribution obtained from the classical microcanonical distribution is

$$\rho_E(\underset{\sim}{p}) = \frac{8\, p_E^5}{\pi^2 (p_E^2 + p^2)^4} \qquad (1.8)$$

and is identical to the quantal momentum distribution for every value of the classical energy equal to the levels E_n. We shall refer to this correspondence identity as the Fock identity. It is interesting to note that no identity exists between distributions in position, since the classical orbits in position space for a given negative energy are bounded.

The Fock identity is of particular importance in the study of p-H and e-H collisions by means of classical mechanics (Abrines and Percival 1966a,b; Abrines, Percival and Valentine 1966). Here the target atoms are chosen from a microcanonical assembly of hydrogen atoms for which the distribution in momentum of the electron will be that of equation (1.8). In particular, when the assembly is chosen so that each atom has the ground state value of the energy, then the classical distribution in electronic momentum will be identical to the quantum-mechanical (1s) distribution. The p-H ionization and charge transfer cross sections obtained by Abrines and Percival when the atom is originally in its ground state agree with the experimentally obtained values to within the error bars. This good agreement has been attributed in part to the Rutherford scattering identity. However, to what extent the agreement is due also to the Fock identity has not been considered, and at this stage, it is still safest to regard the agreement as one more special feature of the Coulomb potential. The three correspondence identities to be considered in this thesis are special features of the Coulomb potential which must be understood before more complex problems can be considered!

CHAPTER 2

METHODS OF CLASSICAL MECHANICS

1) Introduction

The correspondence identities are relations between classical and quantum mechanics which hold for all quantum numbers and values of the classical action. One way of explaining the three correspondence identities mentioned in Chapter I is to obtain a complete correspondence identity whereby the full quantum dynamics of the hydrogen atom for both positive and negative energies is completely determined by the solution of the corresponding classical problem. Energy levels, state vectors and the evolution of the system with time must all be obtained from the classical solution and the other correspondence identities should then follow. In this chapter the necessary techniques of classical mechanics that are needed in the study of correspondence identities are explained, and for the purposes of reference a fairly detailed account will be given, however an excellent and full account can be found in either Corben and Stehle (1966), Goldstein (1950), or Landau and Lifshitz (1960).

Many problems arising in classical mechanics can be considered in the light of Lagrangian or Hamiltonian dynamics. Let us consider first of all the Lagrangian formulation of dynamics.

2) Lagrangian Dynamics

The instantaneous configuration of a system with n degrees of freedom can be described by the values of n generalised coordinates $q_1, q_2, .., q_i, .., q_n$. The relations between q_i, $\dot{q}_i$ and $\ddot{q}_i$ are the equations of motion which determine how the system point moves in configuration space as time elapses. The equations of motion can be obtained from Hamilton's principle: out of all possible paths by which the system point could travel from its position $q^{(1)}$ at time t_1 to its position $q^{(2)}$ at time t_2, it will travel along that path for which the integral

$$S = \int_{t_1}^{t_2} L(q_i, \dot{q}_i, t)\, dt \tag{2.1}$$

where $L(q_i, \dot{q}_i, t)$ is the classical Lagrangian of the system, is an extremum. This stationary value is known as Hamilton's principal function.

To derive the differential equations of motion we assume that $q_i = q_i(t)$ are the coordinates for which S

is stationary. We now vary $q_i(t)$ so that they become:

$$q_i(t) + \delta q_i(t) \; . \tag{2.2}$$

Since the coordinates of the system point at times t_1 and t_2 are $q^{(1)}$ and $q^{(2)}$, then it follows that:

$$\delta q_i(t_1) = \delta q_i(t_2) = 0 \quad ; \quad \text{all } i \; . \tag{2.3}$$

The principle may be written in the form

$$\delta S = \delta \int_{t_1}^{t_2} L(q_i, \dot{q}_i, t)\, dt = 0 \tag{2.4}$$

which, on carrying out the variation gives

$$\delta S = \sum_{i=1}^{n} \left[\frac{\partial L}{\partial \dot{q}_i} \delta q_i \right]_{t_1}^{t_2} + \int_{t_1}^{t_2} \sum_{i=1}^{n} \left(\frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} \right) \delta q_i \, dt$$

$$= 0 \; . \tag{2.5}$$

By virtue of the condition (2.3) the first term on the right-hand side of equation (2.5) is zero, and since this equation holds good for all arbitrary δq_i we must have

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i} \right) - \frac{\partial L}{\partial q_i} = 0 \quad ; \quad i = 1, 2, \ldots, n \; . \tag{2.6}$$

These are Lagrange's equations of motion and mathematically they constitute a set of n second order equations for n

unknown functions $q_i(t)$.

What is important about Lagrange's equations is that they remain valid, in the same form, in any coordinate system which can be related to the original coordinate system by a point transformation. Such a transformation can be regarded as a mapping of the n-dimensional configuration space onto itself such that the new (barred) coordinates may be expressed in terms of the original in the following way

$$\bar{q}_j = f_j(q_1, q_2, .., q_i, .., q_n) \; ; \; j = 1, 2, .., n. \qquad (2.7)$$

The functions $f_1, .., f_j, .., f_n$ must be single valued and differentiable so that to a definite point P in the original space there corresponds a definite point $\bar{P}$ in the new space. In this way we are at liberty to choose the most convenient coordinate system in which the equations of motion are easiest to integrate.

3) Hamiltonian Dynamics

An alternative formulation of classical mechanics, which has a much broader application, is due to Hamilton. In this formulation the independent variables are the n generalised coordinates q_i together with n generalised momenta p_i, defined by

$$p_i = \frac{\partial L}{\partial \dot{q}_i} \tag{2.8}$$

where L is the Lagrangian function. The aim is now to obtain both the coordinates and generalised momenta as explicit functions of time. The motion of the system is represented by a path in phase space of $2n$-dimensions. The motion may start from any point of phase space, but after specifying one point in this space, the motion is subsequently determined.

The equations of motion may be formulated in terms of the Hamiltonian function

$$H = H(q_i, p_i, t) \tag{2.9}$$

which is related to the Lagrangian L by a Legendre transformation (see, for example, Goldstein 1950):

$$H = \sum_{i=1}^{n} p_i \dot{q}_i - L \quad . \tag{2.10}$$

The equations of motion then arise from a modified Hamilton's principle:

$$\delta S = \delta \int_{t_1}^{t_2} \left\{ \sum_{i=1}^{n} p_i \dot{q}_i - H \right\} dt = 0 \quad . \tag{2.11}$$

The δ -variation here implies that the variations $\delta q_i(t)$ and $\delta p_i(t)$ are to be regarded as independent. The varied curve in phase space must be such that

$$\delta q_i(t_1) = \delta q_i(t_2) = 0 \quad . \tag{2.12}$$

Carrying out this type of variation we obtain:

$$\begin{aligned} \delta S &= \int_{t_1}^{t_2} \Big\{ \sum_{i=1}^{n} (\dot{q}_i \delta p_i + p_i \delta \dot{q}_i) - \sum_{i=1}^{n} \Big(\frac{\partial H}{\partial q_i} \delta q_i + \frac{\partial H}{\partial p_i} \delta p_i \Big) \Big\} dt \\ &= \int_{t_1}^{t_2} \Big\{ \sum_{i=1}^{n} (\dot{q}_i \delta p_i - \dot{p}_i \delta q_i) - \sum_{i=1}^{n} \Big(\frac{\partial H}{\partial q_i} \delta q_i + \frac{\partial H}{\partial p_i} \delta p_i \Big) \Big\} dt \\ &\qquad + \Big[\sum_{i=1}^{n} p_i \delta q_i \Big]_{t_1}^{t_2} \\ &= 0 \quad . \end{aligned} \tag{2.13}$$

Because of condition (2.12) the last term vanishes, and since the independent variations δp_i and δq_i are quite arbitrary, we must have:

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \quad ; \quad \dot{p}_i = -\frac{\partial H}{\partial q_i} \quad . \tag{2.14}$$

These are Hamilton's equations of motion and together comprise a set of $2n$ first-order differential equations for the coordinates and momenta. Neither the coordinates q_i nor the momenta p_i are to be considered as the more fundamental set of variables.

4) Principle of Least Action

The variational methods so far described are due to Hamilton. However, if we are dealing with a system in which the Hamiltonian is conserved, so that time is absent from H, then we can determine the path of the system, without any particular reference to time, by utilising the principle of least action due originally to Maupertius. This principle was correctly formulated by Euler and Lagrange, and we consider the variation of the function $\int \sum_i p_i dq_i$. In this type of variation we require that the variations of the end points are zero so that

$$\delta q^{(1)} = \delta q^{(2)} = 0 \qquad (2.15)$$

where (1) and (2) refer to initial and final values of the coordinates. The times of the end points are in fact allowed to vary. This is due to the fact that each of the varied paths must have the same value of the energy, and as a result the system point may have to speed up or slow down in order to keep the Hamiltonian constant. Provided the varied paths all have the same energy, then it can be shown (Goldstein 1950, p.228) that

$$\Delta \int_{q^{(1)}}^{q^{(2)}} \sum_i p_i \, dq_i = 0 \qquad (2.16)$$

where the Δ variation allows for variations in the time of the end points.

The condition of least action is in principle sufficient to obtain the actual path of the system. The value of $\int \sum_i p_i \, dq_i$, taken over the path of the system, is known as Hamilton's characteristic function and only yields a knowledge of the path when combined with the condition

$$H(p,q) = E = \text{constant} . \qquad (2.17)$$

The path is a curve on a $(2n-1)$-D energy surface in phase space, but can be treated as a curve in q-space, since the various p_i have to be known functions of the q_i before $\int \sum_i p_i \, dq_i$ may be evaluated. We shall also refer to this function as the energy-dependent action function. The same quantity is also referred to as the abbreviated action (Landau and Lifshitz 1960), or simply as the action function (Plumpton and Chirgwin 1966).

5) Canonical Transformations

The differential equations which arise out of the Hamiltonian formulation of mechanics are usually no easier to solve than those appearing in the Lagrangian formulation. In the first case we have $2n$ first-order equations to solve, and in the latter case n second-order equations. We have already seen how Lagrange's equations of motion can sometimes be made easier to solve by a change of variable brought about by a point transformation. In the Hamiltonian formulation, however, the generalised momenta as well as the coordinates are regarded as the variables and the concept of 'change of variable' is now the simultaneous transformation of both q_i and p_i to $\bar{q}_i$ and $\bar{p}_i$ say, where

$$\left.\begin{aligned} \bar{q}_i &= \bar{q}_i(p_j, q_j, t) \\ \bar{p}_i &= \bar{p}_i(p_j, q_j, t) . \end{aligned}\right\} \qquad (2.18)$$

Transformations of this type are less restrictive than point transformations and may be used to formulate classical mechanics in various representative spaces, for example momentum space, as well as making the solution of the equations of motion easier in certain cases.

In the new transformed space we naturally require $\bar{q}_i$ and $\bar{p}_i$ to be canonical variables. We thus need some new Hamiltonian function $\bar{H}(\bar{q}_i, \bar{p}_i, t)$ with the property:

$$\dot{\bar{q}}_i = \frac{\partial \bar{H}}{\partial \bar{p}_i} \quad ; \quad \dot{\bar{p}}_i = -\frac{\partial \bar{H}}{\partial \bar{q}_i} \quad . \qquad (2.19)$$

When equations (2.19) are valid, then transformations of the kind (2.18) are said to be canonical (or contact) transformations. If q_i , p_i and $\bar{q}_i , \bar{p}_i$ are related by a canonical transformation, then they each must satisfy:

$$\left.\begin{aligned} \delta\int_{t_1}^{t_2}\sum_i\left\{\bar{p}_i\dot{\bar{q}}_i - \bar{H}\right\}dt &= 0 \\ \delta\int_{t_1}^{t_2}\sum_i\left\{p_i\dot{q}_i - H\right\}dt &= 0 \,. \end{aligned}\right\} \qquad (2.20)$$

The two integrals therefore differ at most by a total time derivative of an arbitrary function ϕ , say, called the generating function of the transformation. When ϕ is given the transformation is completely specified.

ϕ is at first sight a function of $4n$ variables as well as time. However, by virtue of the transformation equations (2.18) only $2n$ of these are independent and the generating function may be a function of either :

$$(q,\bar{q},t)\ ,\ (q,\bar{p},t)\ ,\ (p,\bar{q},t)\ \text{or}\ (p,\bar{p},t)\,. \qquad (2.21)$$

The type of problem will usually indicate what the form of the generating function must be. The most important generating function, by analogy with unitary transformations in quantum mechanics, is the one where $q, \bar{q}$ are the independent variables. In this case

$$\phi = \phi(q,\bar{q},t)\,. \qquad (2.22)$$

Equation (2.20) then gives

$$\sum_i p_i\dot{q}_i - H = \sum_i \bar{p}_i\dot{\bar{q}}_i - \bar{H} + \frac{d}{dt}\phi(q_i,\bar{q}_i,t)\,. \qquad (2.23)$$

However :

$$\frac{d\phi}{dt} = \sum_i \frac{\partial\phi}{\partial q_i}\dot{q}_i + \sum_i \frac{\partial\phi}{\partial\bar{q}}\dot{\bar{q}}_i + \frac{\partial\phi}{\partial t} \qquad (2.24)$$

and when this relation is used in equation (2.23), together with the condition that q_i and $\bar{q}_i$ are independent variables, we obtain

$$\left.\begin{aligned} p_i &= \frac{\partial\phi}{\partial q_i} \\ \bar{p}_i &= -\frac{\partial\phi}{\partial\bar{q}_i} \\ \bar{H} &= H + \partial\phi/\partial t . \end{aligned}\right\} \qquad (2.25)$$

These equations together with (2.18) provide sufficient information to establish a Hamiltonian dynamics in the new space of variables.

In problems where the independent variables are to be q_i and $\bar{p}_i$, then the transition from $(q, \bar{q})$ to $(q, \bar{p})$ as independent variables may be carried out by a Legendre transformation and we obtain

$$\psi(q, \bar{p}, t) = \phi(q, \bar{q}, t) + \sum_i \bar{p}_i\bar{q}_i \quad , \qquad (2.26)$$

It is easily shown that ψ generates the transformation and we have now:

$$p_i = \frac{\partial\psi}{\partial q_i}$$

$$\left.\begin{aligned} \bar{q}_i &= \frac{\partial \Psi}{\partial \bar{p}_i} \\ \bar{H} &= H + \partial\Psi/\partial t. \end{aligned}\right\} \qquad (2.27)$$

A third type of generating function of the form $\Psi'(p, \bar{q}, t)$, where p and $\bar{q}$ are to be regarded as independent, may be constructed from ϕ as follows :

$$\phi(q,\bar{q},t) = \sum_i q_i p_i + \Psi'(\bar{q}, p, t) \qquad (2.28)$$

and this leads to

$$\left.\begin{aligned} q_i &= -\frac{\partial \Psi'}{\partial p_i} \\ \bar{p}_i &= -\frac{\partial \Psi'}{\partial \bar{q}_i} \\ \bar{H} &= H + \partial\Psi'/\partial t. \end{aligned}\right\} \qquad (2.29)$$

Finally, when p and $\bar{p}$ are to be taken as independent variables the corresponding generating function ϕ' is related to ϕ by a double Legendre transformation:

$$\phi'(p,\bar{p},t) = \phi(q,\bar{q},t) + \sum_i \bar{p}_i\bar{q}_i - \sum_i p_i q_i \quad . \tag{2.30}$$

The transformation equations are

$$\left.\begin{aligned} q_i &= -\frac{\partial\phi'}{\partial p_i} \\ \bar{q}_i &= \frac{\partial\phi'}{\partial \bar{p}_i} \\ \bar{H} &= H + \partial\phi'/\partial t \, . \end{aligned}\right\} \tag{2.31}$$

In considering these transformations we have assumed them to be dependent on time. However in cases of conservative systems, where time is of secondary importance, nothing is lost in considering time-independent transformations. In each case we see that the value of the new Hamiltonian remains the same. The value of the energy-dependent action is then related to its new value in terms of the change in ϕ . This follows from equation (2.23) and we have

$$\int_a^b \sum_i p_i dq_i = \int_a^b \sum_i \bar{p}_i d\bar{q}_i + \Big[\phi(q,\bar{q})\Big]_a^b \tag{2.32}$$

where a and b stand for initial and final values. It is shown by many authors that the generating functions of the type $\phi(q, \bar{q})$ form a group, and when $\phi = 0$ as in the case of a point or identity transformation, we see that the value of the energy-dependent action function remains unchanged. Their functional forms, however, are in general completely different.

In the light of contact transformations, we see that no representative space is necessarily more important for the formulation of Hamilton's equations of motion. The only criterion we use in choosing one particular representation as opposed to another is that we require the simplest possible solution to the problem.

6) The Hamilton-Jacobi Equation

One way of obtaining a solution to a problem is to seek a canonical transformation from the coordinates and momenta (q, p) at time t, to a new set of constant quantities which could be the $2n$ initial values (q_0, p_0) at time $t = 0$. The equations of the transformation are then the solution to the mechanical problem:

$$\left.\begin{aligned} q &= q(q_0, p_0, t) \\ p &= p(q_0, p_0, t)\,. \end{aligned}\right\} \qquad (2.33)$$

We have then the coordinates and momenta as functions of their original values and time.

To avoid confusion with what has been said in the previous section, we shall label this constant (new) set of initial values by $(\bar{q}, \bar{p})$. To ensure that these variables are constants, we require that the new Hamiltonian function is zero. Then we have:

$$\left.\begin{aligned} \frac{\partial \bar{H}}{\partial \bar{p}_i} &= \dot{\bar{q}}_i = 0 \\ -\frac{\partial \bar{H}}{\partial \bar{q}_i} &= \dot{\bar{p}}_i = 0\,. \end{aligned}\right\} \text{all } i. \qquad (2.34)$$

The new Hamiltonian is related to the old Hamiltonian by means of the generating function ϕ :

$$\bar{H} = H + \partial\phi/\partial t \qquad (2.35)$$

and equations (2.34) will be satisfied if

$$H(q,p,t) + \partial\phi/\partial t = 0 \quad . \tag{2.36}$$

If we use the generating function $\phi(q, \bar{q}, t)$, we see that equation (2.36) may be written by virtue of equation (2.25) in the form:

$$H\left(q_1, \ldots, q_n, \frac{\partial\phi}{\partial q_1}, \ldots, \frac{\partial\phi}{\partial q_n}, t\right) + \frac{\partial\phi}{\partial t} = 0 \, . \tag{2.37}$$

This is the well known Hamilton-Jacobi equation. It is a first-order partial differential equation and will depend on $n+1$ arbitrary constants. The solution, ϕ , is called Hamilton's principal function. It is not unique since we could equally well have obtained the same Hamilton-Jacobi equation by using the ψ type of generating function as described in the previous section. But in this case ψ differs only from ϕ by an additive constant $(\sum_i \bar{p}_i \bar{q}_i)$. Ignoring this, we may write ϕ as $\phi(q_1, q_2, \ldots, q_n, \alpha_1, \alpha_2, \ldots, \alpha_n, t)$. The α_i are the new constant variables $\bar{q}_i$. The equations

$$-\frac{\partial\phi}{\partial\alpha_i} = \bar{p}_i = \beta_i \tag{2.38}$$

then provide the solution of q_i in terms of α_i , β_i and t , and finally the equations

$$p_i = \frac{\partial\phi}{\partial q_i} \tag{2.39}$$

then give the momenta p_i as functions of q_i and α_i , and therefore as functions of t , α_i and β_i . We have thus obtained a solution to the problem in the form of equation (2.33). To show that ϕ is in fact Hamilton's principal function we note that

$$\frac{d\phi}{dt} = \sum_i \frac{\partial\phi}{\partial q_i}\dot{q}_i + \sum_i \frac{\partial\phi}{\partial\bar{q}_i}\dot{\bar{q}}_i + \frac{\partial\phi}{\partial t}$$

and as the $\bar{q}_i$ coordinates are constants in time then

$$\frac{d\phi}{dt} = \sum_i \frac{\partial\phi}{\partial q_i}\dot{q}_i + \frac{\partial\phi}{\partial t} = \sum_i p_i\dot{q}_i - H = L\,. \tag{2.40}$$

To within an additive constant, then:

$$\phi = \int L\,dt \quad . \tag{2.41}$$

In the case when the Hamiltonian is conserved, the time t is absent from the Hamiltonian and the Hamilton-Jacobi equation becomes:

$$\frac{\partial\phi}{\partial t} + H\left(q_i, \frac{\partial\phi}{\partial q_i}\right) = 0 \,. \tag{2.42}$$

ϕ depends on time only through $\partial\phi/\partial t$, and we separate out the time by writing

$$\phi(q_i, \alpha_i, t) = -Et + W(q_i, \alpha_i) \tag{2.43}$$

where E is the constant value of the conserved Hamiltonian. The Hamilton-Jacobi equation now reduces to

$$H\left(q_i, \frac{\partial W}{\partial q_i}\right) = E \tag{2.44}$$

and the function W generates a time-independent contact transformation: the momenta being given by $p_i = \dfrac{\partial W}{\partial q_i}$ from equations (2.43) and (2.39). In equation (2.43), the generating function ϕ is a function of the time, the n generalised coordinates q_i, and n constants α_i. The constant energy E cannot be then independent of the α_i. It is usual to make E one of the constants α_n, say. The remaining equations of the transformation give

$$\left.\begin{aligned} -\frac{\partial W}{\partial \alpha_i} &= \beta_i = \bar{P}_i \; ; \; i = 1, \ldots, n-1 \\ \text{and} \\ -\frac{\partial W}{\partial E} &= \beta_n - t = \bar{P}_n \;. \end{aligned}\right\} \tag{2.45}$$

The β_i are all constants. The first $n-1$ equations describe the path of the system and the final equation gives its time dependence. W is just the energy dependent action function or Hamilton's characteristic function. This is easily seen since:

$$\frac{dW}{dt} = \sum_i \frac{\partial W}{\partial q_i} \cdot \frac{dq_i}{dt} = \sum_i p_i \frac{dq_i}{dt} \tag{2.46}$$

and so, to within an additive constant

$$W = \int \sum_i p_i \, dq_i \;. \tag{2.47}$$

The important point to remember in solving the Hamilton-

Jacobi equation is that a knowledge of either ϕ or W is sufficient to provide a solution. Alternatively, once we have obtained the equivalent action functions we have in principle a solution to the problem.

7) Extended Phase Space

We have seen how time-dependent contact transformations usually lead to a new Hamiltonian whose value is different to that of the old one. It is not unreasonable on symmetrical grounds, to expect that when contact transformations depend on energy, the new value of the time will be changed. The usual concept of time as a parameter must now be altered and we have to regard time as one of the variables. t may be labelled as the $(n+1)$ th coordinate and accordingly we make $-H$ the corresponding conjugate momentum. Canonical transformations which are energy dependent have to be treated later on in this thesis and so it is worth while outlining the changes in outlook that occur in dealing with the $(2n+2)$- dimensional phase space, called extended phase space by Lanczos (1966).

In this space we take as variables $q_1, \dots, q_n, q_{n+1} = t$ and $p_1, p_2, \dots, p_n, p_{n+1} = -H$. For convenience we make the first $n+1$ variables the generalised coordinates, and the remainder are the generalised momenta. Instead of constructing a Hamiltonian function H, we now construct an energy equation

$$\Omega(p_i, q_i) = 0 . \tag{2.48}$$

The solution to the problem in this extended space is going to be one which involves expressing all the variables in terms of some parameter, s, say. The relevant equations of motion arise from a variational principle of the type

$$\delta \int_{s_1}^{s_2} \Big(\sum_{i=1}^{n+1} p_i \frac{dq_i}{ds} - \lambda(s)\Omega(p_i, q_i) \Big) ds = 0 \tag{2.49}$$

where the end values of q_i remain fixed and any variation is subject to condition (2.48). We obtain the following canonical equations of motion:

$$\left. \begin{aligned} \frac{dq_i}{ds} - \lambda(s)\frac{\partial\Omega}{\partial p_i} &= 0 \\ \frac{dp_i}{ds} + \lambda(s)\frac{\partial\Omega}{\partial q_i} &= 0 \end{aligned} \right\} i = 1, 2, \ldots, n+1 . \tag{2.50}$$

By proper choice of s we can make $\lambda = 1$, and s is then a special parameter (see Synge 1960). By making the time t , in general, one of the variables we may then say that the systems are always conservative in the sense that Ω is conserved and is zero.

When considering canonical transformations we have to treat the parameter s in the same light as we did t previously. That is, the role of s as a parameter holds in both the old and new representative spaces. The energy function Ω is also to be regarded as an invariant so that

$$\Omega(p,q) = \bar{\Omega}(\bar{p},\bar{q}) \quad . \qquad (2.51)$$

This does not mean, of course, that $H = \bar{H}$. The treatment of canonical transformations is exactly analogous to that already given, but now, of course, we have two more variables, the time and the energy.

CHAPTER 3

METHODS OF QUANTUM MECHANICS

This chapter is devoted to the methods of quantum mechanics that are necessary for the study of correspondence identities. As well as considering the quantum-mechanical evolution and Green operators, we also consider the generalised function operator $\delta(E-H)$ which is the spectral operator of a system whose Hamiltonian is H and whose total energy is E. Changes of representation by means of unitary operators are also discussed.

1) Description of a State in Quantum Mechanics

In classical mechanics we saw that it was necessary to know both the values of the coordinates and momenta for a complete description of the state of a system. In quantum mechanics Heisenberg's uncertainty principle indicates the impossibility of a simultaneous knowledge of both coordinates and momenta and in quantum mechanics the state of a system has to be described by fewer quantities. The maximum number of independent observable quantities whose values can all be measured simultaneously constitute what is known as a complete set of observable quantities and in quantum mechanics the state of a system is described most fully in terms of states which arise as a result of the simultaneous measurement of such a complete set. If all the possible states of a system corresponding to the simultaneous measurements of a complete set of observables are labelled ψ_i , then the most general state can be written as

$$\psi = \sum_n \alpha_n \psi_n \tag{3.1}$$

if $i = n$ is a discrete label, or, if $i = \eta$ is a continuous label, as

$$\psi = \int d\eta \, \alpha(\eta) \psi_\eta \quad . \tag{3.2}$$

2) Operators in Quantum Mechanics

Measuring processes in quantum mechanics are represented mathematically by Hermitian operators. For every observable quantity there is a Hermitian operator. The results of measurement are the eigenvalues of the operator, and the states which lead to these results are the eigenstates. If the operator is L, and the eigenvalues are λ, then

$$L\psi_n = \lambda_n \psi_n \, ; \quad n = 1, 2, \ldots \tag{3.3}$$

if the spectrum of L is discrete, or

$$L\psi_\lambda = \lambda \psi_\lambda \tag{3.4}$$

if the values of λ form a continuous set. If there is more than one eigenstate corresponding to a given eigenvalue, then the eigenvalue is degenerate. In this section we shall assume that eigenvalues are non-degenerate and only deal with degeneracy when it arises.

Expanding the wave function representing the state ψ in terms of the eigenfunctions of L we may write, assuming the spectrum to be discrete,

$$\psi(\underset{\sim}{q}) = \sum_n \alpha_n \psi_n(\underset{\sim}{q}) \, . \tag{3.5}$$

Assuming that the eigenfunctions $\psi_n(\underset{\sim}{q})$ are normalized, the expansion coefficients α_n can then be evaluated in the usual manner, so that equation (3.5) becomes:

$$\Psi(\underset{\sim}{q}) = \sum_n \int d\underset{\sim}{q}' \, \Psi_n(\underset{\sim}{q}) \Psi_n^*(\underset{\sim}{q}') \Psi(\underset{\sim}{q}') \tag{3.6}$$

which we may express as:

$$\Psi(\underset{\sim}{q}) = \sum_n \int d\underset{\sim}{q}' \, P_n(\underset{\sim}{q},\underset{\sim}{q}') \Psi(\underset{\sim}{q}') \; . \tag{3.7}$$

The function $P_n(\underset{\sim}{q}, \underset{\sim}{q}')$ is known as the kernel of the projection operator P_n . The completeness relation of the eigenfunctions can be expressed in the form

$$\sum_n P_n(\underset{\sim}{q},\underset{\sim}{q}') = \delta(\underset{\sim}{q}-\underset{\sim}{q}') \tag{3.8}$$

where the delta function is the usual Dirac delta function (see Dirac 1958, Lighthill 1960).

Operating on both sides of equation (3.6) with L we obtain:

$$\begin{aligned} L\Psi(\underset{\sim}{q}) &= \sum_n \int d\underset{\sim}{q}' \, L\Psi_n(\underset{\sim}{q}) \Psi_n^*(\underset{\sim}{q}') \Psi(\underset{\sim}{q}') \\ &= \sum_n \int d\underset{\sim}{q}' \, \lambda_n \Psi_n(\underset{\sim}{q}) \Psi_n^*(\underset{\sim}{q}') \Psi(\underset{\sim}{q}') \\ &= \sum_n \int d\underset{\sim}{q}' \, \lambda_n P_n(\underset{\sim}{q},\underset{\sim}{q}') \Psi(\underset{\sim}{q}') \end{aligned} \tag{3.9}$$

so that in the form of an operator equation

$$L = \sum_n \lambda_n P_n \, . \qquad (3.10)$$

This is the spectral resolution of the operator L and provides us with a knowledge of the eigenstates and eigenvalues of the operator. It can easily be shown that for functions of operators:

$$f(L) = \sum_n f(\lambda_n) P_n \qquad (3.11)$$

and we shall assume that this is true also for generalised functions of operators (Schönberg 1951).

In the case of L having a continuous spectrum, we assume that we can choose λ itself to label the states. The eigenfunctions $\psi_\lambda(\underset{\sim}{q})$ are then normalised as

$$\int d\underset{\sim}{q}\, \psi_\lambda(\underset{\sim}{q}) \psi^*_{\lambda'}(\underset{\sim}{q}) = \delta(\lambda - \lambda') \, . \qquad (3.12)$$

In terms of these eigenfunctions the wave functions of the system may be expressed

$$\psi(\underset{\sim}{q}) = \int d\lambda\, \alpha(\lambda) \psi_\lambda(\underset{\sim}{q}) \qquad (3.13)$$

where the expansion coefficients $\alpha(\lambda)$ are given by

$$\alpha(\lambda) = \int d\underset{\sim}{q}' \, \psi(\underset{\sim}{q}') \, \psi_\lambda^*(\underset{\sim}{q}') \, . \tag{3.14}$$

The wave function may now be written

$$\psi(\underset{\sim}{q}) = \int d\lambda \int d\underset{\sim}{q}' \, P_\lambda(\underset{\sim}{q}, \underset{\sim}{q}') \, \psi(\underset{\sim}{q}') \tag{3.15}$$

where $P_\lambda(\underset{\sim}{q}, \underset{\sim}{q}')$ is the corresponding projection operator kernel onto the states corresponding to λ . The completeness relation may be written

$$\int d\lambda \, P_\lambda(\underset{\sim}{q}, \underset{\sim}{q}') = \delta(\underset{\sim}{q} - \underset{\sim}{q}') \tag{3.16}$$

and the analogue of equation (3.11) is just

$$f(L) = \int d\lambda \, f(\lambda) \, P_\lambda \, . \tag{3.17}$$

The wave functions and operator kernels in both the discrete and continuous case are different in different representations; however operator equations hold independently of representation.

3) The Evolution Operator

In classical mechanics we can regard a problem as solved when the state at any given time t may be expressed in terms of the state at some given initial time t_0 say, as in equation (2.33). In quantum mechanics if we can express any state $\Psi(t)$ at time t in terms of the state $\Psi(t_0)$ at time t_0, then we also have, in effect, solved the problem.

If the system is not subjected to any measuring process, then it will evolve in an exactly predictable manner. We assume that the evolution of the state of the system can be represented by a linear operator $U(t, t_0)$ called the evolution operator, so that

$$\Psi(t) = U(t,t_0)\Psi(t_0) \quad ; \quad \text{all } t, t_0 \ . \qquad (3.18)$$

We shall also assume, without proof, that the state $\Psi(t)$ at any instant t satisfies the Schrödinger equation:

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi \qquad (3.19)$$

where H is the Hamiltonian operator and $\hbar$ is Planck's constant divided by 2π. And so:

$$i\hbar \frac{\partial}{\partial t} U(t,t_0) = H\, U(t,t_0) \ . \tag{3.20}$$

If we restrict our discussion to systems where the Hamiltonian is conserved, we can solve this last equation together with the condition

$$U(t_0\, , t_0) = I \tag{3.21}$$

and obtain:

$$U(t\, , t_0) = \exp\left\{-\frac{i}{\hbar} H(t-t_0)\right\} \ . \tag{3.22}$$

Since the Hamiltonian operator is Hermitian, then the evolution operator is unitary.

Using the relation (3.11) or (3.17) we see that the evolution operator may be expressed in the form

$$U(t,t_0) = \sum_n P_n \exp\left\{-\frac{i}{\hbar} E_n(t-t_0)\right\} \tag{3.23}$$

if the energy spectrum is discrete, or in the form

$$U(t,t_0) = \int dE \exp\left\{-\frac{i}{\hbar} E(t-t_0)\right\} P_E \tag{3.24}$$

if it is continuous. If the spectrum is mixed, then the evolution operator is given as a sum over the discrete spectrum together with an integral over the continuous spectrum. Should the energy levels be degenerate, then the different states belonging to the particular level, have to be distinguished with further labels (continuous or discrete) k , l , m , . . . , and the projection operator P_n is then given by

$$P_n = \sum_{k,l,m,\ldots} P_{n,k,l,m,\ldots} \quad . \tag{3.25}$$

where '$\sum$' here, means sum over the discrete labels together with integration over the continuous ones (over the appropriate ranges of each). The same applies for P_E . The normalization of the states has also to be adjusted accordingly and equation (3.12) would read, in the case of λ being the energy:

$$\int d\underset{\sim}{q}\, \Psi_{E,k,l,m,\ldots}(\underset{\sim}{q})\, \Psi^{*}_{E',k',l',m',\ldots}(\underset{\sim}{q}) = \delta(E-E')\,\delta(k,k')\ldots \tag{3.26}$$

where the delta functions are either Kronecker or Dirac delta functions.

Thus the kernel of the evolution operator may be evaluated either by using the fact that it is a solution of Schrödinger's equation with boundary condition (3.21), or by means of the expansions (3.23) and (3.24).

In general the evolution operator $U(t, t_0)$ is defined for all times t, t_0. We may define the forward evolution operator, $U^+(t, t_0)$ by:

$$U^+(t,t_0) = \left\{ \begin{array}{cc} U(t,t_0) & ; t \geqslant t_0 \\ 0 & ; t < t_0 \end{array} \right\} \qquad (3.27)$$

and similarly the backward evolution operator $U^-(t,t_0)$ by:

$$U^-(t,t_0) = \left\{ \begin{array}{cc} U(t,t_0) & ; t \leqslant t_0 \\ 0 & ; t > t_0 \end{array} \right\} \qquad (3.28)$$

so that:

$$U(t,t_0) = \left\{ \begin{array}{cc} U^+(t,t_0) + U^-(t,t_0) & ; t \neq t_0 \\ I & ; t = t_0 . \end{array} \right\} \qquad (3.29)$$

The backward and forward evolution operators are related by:

$$U^-(t,t_0) = \left[U^+(t_0,t)\right]^* \qquad (3.30)$$

and we shall refer to the kernel of $U^+(t,t_0)$ as the propagator.

4) Green Operators and Spectral Operator

If we take the Fourier transformation of the forward evolution operator with factors of the type $(2\pi\hbar)^{-\frac{1}{2}}\exp\frac{i}{\hbar}Et$, then we can define an operator denoted by $U^{+}(E,E_0)$ as follows:

$$U^{+}(E,E_0)=\frac{1}{(2\pi\hbar)}\int_{-\infty}^{\infty}dt\int_{-\infty}^{\infty}dt_0\exp\frac{iEt}{\hbar}U^{+}(t,t_0)\exp-\frac{iE_0t_0}{\hbar}\,. \quad (3.31)$$

Using equation (3.27) together with equation (3.22), we can write $U^{+}(E,E_0)$ as

$$U^{+}(E,E_0)=\frac{1}{(2\pi\hbar)}\int_{t_0}^{\infty}dt\int_{-\infty}^{\infty}dt_0\exp\frac{iEt}{\hbar}\exp-\frac{iH}{\hbar}(t-t_0)\exp-\frac{iE_0t_0}{\hbar}\,. \quad (3.32)$$

Putting $t-t_0=\tau$, this reduces to

$$U^{+}(E,E_0)=\frac{1}{(2\pi\hbar)}\int_{0}^{\infty}d\tau\int_{-\infty}^{\infty}dt_0\exp\frac{i}{\hbar}(E-E_0)t_0\exp\frac{i}{\hbar}(E-H)\tau\,. \quad (3.33)$$

Carrying out the integration over t_0, the right-hand side of equation (3.33) becomes

$$\delta(E-E_0)\int_0^\infty d\tau \exp \frac{i}{\hbar}(E-H)\tau \quad . \qquad (3.34)$$

To evaluate this latter integral we have to assume that the parameter E is complex with a positive imaginary part (Feynman and Hibbs 1965, p. 103) so that

$$E = E + i\varepsilon \quad ; \quad \varepsilon > 0 \quad . \qquad (3.35)$$

The value of the integral then exists and we have

$$U^+(E,E_0) = \lim_{\varepsilon \to 0} \frac{\delta(E-E_0)\, i\hbar}{(E - H + i\varepsilon)} \quad . \qquad (3.36)$$

If the parameter E is chosen to be the energy of the system whose Hamiltonian is H , then the operator $(E - H + i\varepsilon)^{-1}$ is just the Green operator G_E^+ which in the case of potential scattering corresponds to the Green operator for outgoing waves (Roman 1965, chap. 3; Newton 1966, chap. 7). G_E^+ is thus related to $U^+(E, E_0)$ by

$$U^+(E, E_0) = i\hbar\, G_E^+\, \delta(E - E_0) \quad . \qquad (3.37)$$

We can similarly take the Fourier transform of the backward evolution operator $U^{-}(t,t_0)$ and obtain an operator $U^{-}(E,E_0)$ which is related to the Green operator G_E^{-} (the Green operator for incoming waves) and we have :

$$U^{-}(E,E_0) = -i\hbar\, G_E^{-}\, \delta(E-E_0) \tag{3.38}$$

where now

$$G_E^{-} = \lim_{\varepsilon\to 0} (E-H-i\varepsilon)^{-1} \; ; \; \varepsilon > 0 . \tag{3.39}$$

The Green operators may be expressed in terms of the projection operators in the usual way. If the spectrum is discrete and the energy levels non-degenerate we may write

$$G_E^{\pm} = \sum_n \frac{P_n}{(E-E_n \pm i\varepsilon)} . \tag{3.40}$$

If the spectrum is continuous, then we have

$$G_E^{\pm} = \int \frac{dE'\, P_{E'}}{(E-E' \pm i\varepsilon)} . \tag{3.41}$$

The integrands of equation (3.41) have poles at $E' = E \pm i\varepsilon$ respectively. If we regard the energy E' as a complex variable, the integral over the continuous spectrum can be evaluated without too much difficulty (see, for example, appendix A). If the spectrum is mixed, the Green operators are then expressed as a sum over the discrete spectrum together with an integral over the continuous spectrum as before. We require, by the definition of the projection operators that in this case (and for the evolution operator):

$$\sum_n P_n + \int P_{E'}\, dE' = I \ . \qquad (3.42)$$

Degeneracy is to be treated in exactly the same way as for the evolution operator.

As functions of complex E, the Green operators have poles at the bound state energy levels E_n, and cuts along the real axis corresponding to the continuous spectrum. The operators $G_E^{\pm}$ are defined only in the upper and lower half-planes respectively. In the case of the discrete spectrum $G_E^{\pm}$ as $\varepsilon \rightarrow 0$ are equal except near the bound state energy levels, and in the case of the continuous spectrum the Green operators are discontinuous across the cut in the complex E-plane.

We can define an operator $U(E, E_0)$ for real values of the energy E by taking the Fourier transform of the full evolution operator $U(t,t_0)$:

$$U(E,E_0) = \frac{1}{(2\pi\hbar)}\int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt_0 \exp\frac{iEt}{\hbar}\, U(t,t_0) \exp -\frac{iE_0 t_0}{\hbar}$$

$$= \frac{1}{(2\pi\hbar)}\int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt_0 \exp\frac{iEt}{\hbar} \exp -\frac{iH}{\hbar}(t-t_0) \exp -\frac{iE_0 t_0}{\hbar} \; . \quad (3.43)$$

To evaluate the transform we again use the substitution $\tau = t - t_0$ and obtain

$$U(E,E_0) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dt_0 \int_{-\infty}^{\infty} d\tau \exp\frac{i}{\hbar}(E-E_0)t_0 \exp\frac{i}{\hbar}(E-H)\tau$$

$$= 2\pi\hbar\, \delta(E-E_0)\, \delta(E-H)$$

$$= 2\pi\hbar\, \delta(E-E_0)\, I_E \quad (3.44)$$

where the generalised function operator I_E is called the spectral operator. It follows from the Fourier transform of equation (3.29) that

$$I_E = \lim_{\varepsilon\to 0} \frac{1}{2\pi i}\left(G_E^- - G_E^+ \right) . \quad (3.45)$$

In future we shall omit the limiting process $\varepsilon \to 0$ when it is obvious that it applies.

Expressed in terms of the projection operators the spectral operator may be written, in the general case of a mixed spectrum, as

$$I_E = \sum_n P_n \delta(E-E_n) + \underbrace{\int dE' P_{E'} \delta(E-E')}_{\text{continuous spectrum}}$$

$$= \sum_n P_n \delta(E-E_n) + \mathcal{E}(E) P_E \qquad (3.46)$$

where $\mathcal{E}(E) = 1$ if E is in the continuous spectrum and zero otherwise. The completeness relation of the states may be expressed by

$$\int \delta(E-H)\, dE = I \quad . \qquad (3.47)$$

Again, the problem of degeneracy is taken care of in the manner previously described. A knowledge of the spectral operator or the Green operators of a system is sufficient to determine the energy spectrum of the system and the projection operators onto the states corresponding to the various values of the energy. The evolution of the state of the system with time can be obtained by evaluating the inverse Fourier transforms of these operators which then give the corresponding evolution operators.

From equation (3.45) we see that the spectral operator at the n th energy level E_n of the discrete spectrum is determined by the residue of $(E - H)^{-1}$ and in the continuous spectrum it is just given by the discontinuity of $(E - H)^{-1}$ across the cut divided by $2\pi i$. Finally it should be pointed out that the operator $\delta(E-H)$ is not to be confused with the operator

$$G_E = \frac{1}{2}(G_E^+ + G_E^-) \qquad (3.48)$$

which is known as the standing wave Green operator. It is in fact the principal value of $(E - H)^{-1}$ and provides a definition of the spectral operator in terms of either $G_E^\pm$ in the following ways:

$$\left.\begin{aligned} G_E^+ &= \text{p.v.}\,(E-H)^{-1} - \pi i\,\delta(E-H) \\ G_E^- &= \text{p.v.}\,(E-H)^{-1} + \pi i\,\delta(E-H). \end{aligned}\right\} \qquad (3.49)$$

5) Change of Representation

In classical mechanics we saw that no particular representative space had any real advantage over another for the formulation of the subject. The same is true in quantum mechanics. The theory may be formulated in any representation, and usually the representation which is chosen is the one best suited to the problem. In quantum mechanics the transformations which play the part of canonical transformations are unitary transformations.

In classical mechanics we required Hamilton's equations of motion to hold in the new representation. In quantum mechanics we require the results of measurement to be the same in all representations. That is to say, we require the eigenvalues of operators representing physical quantities to be the same. Also we require the expectation values of the operators to remain unchanged, and in particular we require the normalization of wave functions to be unaltered in different representations. Whenever the transformation from one representation to another is brought about by a unitary operator, the above conditions will be automatically satisfied. If X is the unitary operator specifying the transformation then operators and states transform as follows:

$$\left.\begin{aligned} L \rightarrow L' &\equiv X L X^{\dagger} \\ \Upsilon \rightarrow \Upsilon' &\equiv X \Upsilon . \end{aligned}\right\} \qquad (3.50)$$

In actually changing from one representation to another the operator X can be obtained by knowing how the states of some physical quantity transform, for by linearity we then know how any arbitrary state transforms, and the transformation is specified. Transformations that are not unitary do arise in quantum mechanics and we shall have to consider such transformation in this thesis. However, since no hard and fast rules apply to non-unitary transformations we shall not discuss them here, and we shall deal with the difficulties that arise as we meet them.

It is quite customary to speak of different representations in quantum mechanics, whilst the term 'representation' in classical mechanics is not widely used, although it was mentioned in Chapter 2. In quantum mechanics, for example, it is well known what is meant by momentum representation: all operator kernels and wave functions are expressed as functions of the (momentum) variable $\underset{\sim}{p}$. In this thesis we shall use freely the term 'representation' in classical mechanics, meaning, in the case of momentum representation,the classical phase space (P, Q) whose coordinates Q_i are the generalized momenta p_i of usual phase space (p, q). The name of the representation will usually refer to the variables that play the role of the coordinates in the representative space.

CHAPTER 4

RELATING THE TWO THEORIES

It is clear from the previous two chapters that the methods of classical and quantum mechanics have very little in common, and at first sight the only link between the two theories is through the correspondence principle. Whenever quantum numbers are small we know that the classical equations of motion can no longer be used to describe the system adequately and we have to resort to quantum mechanics. However, the results of classical mechanics in such a situation need not be discarded since it is possible to obtain a quantum-mechanical solution to a problem by calculating from an assumed classical model. Several ways of doing this are described in this chapter. Some of the resulting solutions are only approximations which depend for validity on conditions concerning the associated de Broglie wavelength, whilst others are exact solutions. The correspondence identities for the hydrogen atom are explained by the fact that the quantum-mechanical solution can be expressed exactly in terms of the classical solution.

1) The W.K.B. Method

When Schrödinger (1928) applied his wave-mechanical approach to the hydrogen atom he obtained the same atomic energy levels as did Bohr and Sommerfeld previously. His method however indicated the serious inadequacies of using classical mechanics for such a problem and the question arose as to why the Bohr-Sommerfeld theory had been so successful in this case. Interested in seeing to what extent the quantum-mechanical solution could be obtained from the classical solution to the problem, Wentzel, Brillouin and Kramers introduced a new wave-mechanical approximation method: the W.K.B. method.

The W.K.B. method is easiest to consider mathematically in one dimension. We can write the time-independent Schrödinger equation in the usual notation as

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\psi = 0 \qquad (4.1)$$

and the wave function $\psi(x)$ in the form

$$\psi(x) = e^{i/\hbar\, \sigma(x)} . \qquad (4.2)$$

$\sigma(x)$ then satisfies the equation

$$\left(\frac{d\sigma}{dx}\right)^2 - i\hbar\left(\frac{d^2\sigma}{dx^2}\right) = 2m(E - V(x)) . \qquad (4.3)$$

If we neglect the term in $\hbar$, then this equation is just the time-independent, one-dimensional, Hamilton-Jacobi equation of classical mechanics. The value of σ then corresponds to Hamilton's characteristic function discussed in Chapter 2. To solve equation (4.3) as it stands we expand $\sigma(x)$ as a power series in $(\hbar/i)$:

$$\sigma = \sigma_0 + \frac{\hbar}{i}\sigma_1 + \left(\frac{\hbar}{i}\right)^2\sigma_2 + \cdots + \left(\frac{\hbar}{i}\right)^n\sigma_n + \cdots \qquad (4.4)$$

and substitute back into equation (4.3). Equating powers of $\hbar$ we obtain for the first two terms:

$$\left.\begin{aligned} \sigma_0 &= \pm\int_{x_0}^{x}\left\{2m(E-V(x'))\right\}^{1/2}dx' \\ \sigma_1 &= -\frac{1}{2}\log\left\{2m(E-V(x))\right\}^{1/2} . \end{aligned}\right\} \qquad (4.5)$$

The term σ_0 is the classical action function and the wave function corresponding to the first two terms in (4.4) is given by

$$\Psi(x) = c_1 p^{-1/2}\exp\frac{i}{\hbar}\int_{x_0}^{x}p\,dx' + c_2 p^{-1/2}\exp-\frac{i}{\hbar}\int_{x_0}^{x}p\,dx' \qquad (4.6)$$

where

$$p = \left\{2m(E-V(x))\right\}^{1/2} \qquad (4.7)$$

and C_1 and C_2 are arbitrary constants.

The wave function $\psi(x)$ in (4.6) is an approximation to the full solution of equation (4.1). Nevertheless it has been shown that provided

$$\left| \frac{d}{dx}\left(\frac{\hbar}{p}\right) \right| \ll 1 \qquad (4.8)$$

then the approximation involving only σ_0 and σ_1 is valid. This is the same as insisting that the de Broglie wavelength vary only slightly over distances of the order of itself. (A more rigorous treatment on the validity of the W.K.B. approximation is given in Fröman and Fröman 1965).

What is important about the W.K.B. method is the fact that one can obtain an approximate quantum-mechanical wave function in terms of the classical action and momentum, that will provide a truer description of the state of the system than that given by the equations of classical mechanics. For example interference phenomena can be accounted for within the framework of the W.K.B. approximation (just as interference in optics can be described by means of geometrical optics, which also is a ray theory). The Sommerfeld quantization conditions may be interpreted as interference effects, and Wentzel showed that the condition

$$\oint p\,dq = nh \qquad (4.9)$$

arises naturally in the W.K.B. approximation (see, for example, Jammer 1966). A more detailed investigation leads to the condition

$$\oint p\,dq = \left(n + \tfrac{1}{2}\right)h \qquad (4.10)$$

and this is shown in many books on quantum mechanics, for example Landau and Lifshitz (1965). However, why the quantization conditions (4.9) and (4.10) happen to give the exact energy levels for the hydrogen atom and harmonic oscillator has always been considered more of a coincidence than of a more general relation between the classical and quantal solutions for each of these systems.

2) The Feynman Approach to Quantum Mechanics: Path Integrals

The W.K.B. method relates quantum-mechanical wave functions to classical action functions. An alternative way of relating the two theories is through quantum-mechanical operator kernels as opposed to the wave functions. Feynman (1948) first of all showed how the quantum-mechanical evolution operator kernel could be related to the time-dependent action function. His approach is related to the Lagrangian formulation of classical mechanics and is directed at expressing the propagator of equation (3.18) and (3.27) in terms of an integral over all possible paths from a given point to another of terms involving the action for that path. The method is discussed fully in Feynman and Hibbs (1965) and can be described here without any loss of generality in the case of a particle moving in one dimension.

The propagator $U(x,t\,;x_0,t_0)$ is such that

$$\Psi(x,t) = \int_{x_0} U(x,t\,;x_0,t_0)\Psi(x_0,t_0)\,dx_0,\; t>t_0 \quad (4.11)$$

and Feynman's recipe for evaluating the propagator is as follows:

We denote by Ω the set of all continuous, piecewise differentiable functions $x(t')$, which satisfy the conditions $x(t_0) = x_0$, $x(t) = x$. For each function of the set Ω we evaluate the action integral:

$$S[x(t')] = \int_{t_0}^{t} L\,dt' = \int_{t_0}^{t} \left\{ \tfrac{1}{2} m\dot{x}(t')^2 - V(x(t')) \right\} dt'. \quad (4.12)$$

The action function $S[x(t')]$ is a function of the particular path $x(t')$ and will only be equal to Hamilton's principal function along the classical paths in Ω. The propagator can then be written in a shorthand version as

$$U(x,t\,;x_0,t_0) = \int_{\Omega} \exp\left\{ i/\hbar\, S[x(t')] \right\} d[x(t')]. \quad (4.13)$$

To evaluate this integral we partition the time interval $(t - t_0)$ so that the N th partition corresponds to:

$$t_0 = t_0 < t_1 < t_2 \ldots \qquad < t_{N-1} < t_N = t \ . \quad (4.14)$$

We can assume for convenience that each time interval $t_{j+1} - t_j$ is equal, and has the value ε. For this partition, a typical path in Ω will be as shown in Figure 4.1.

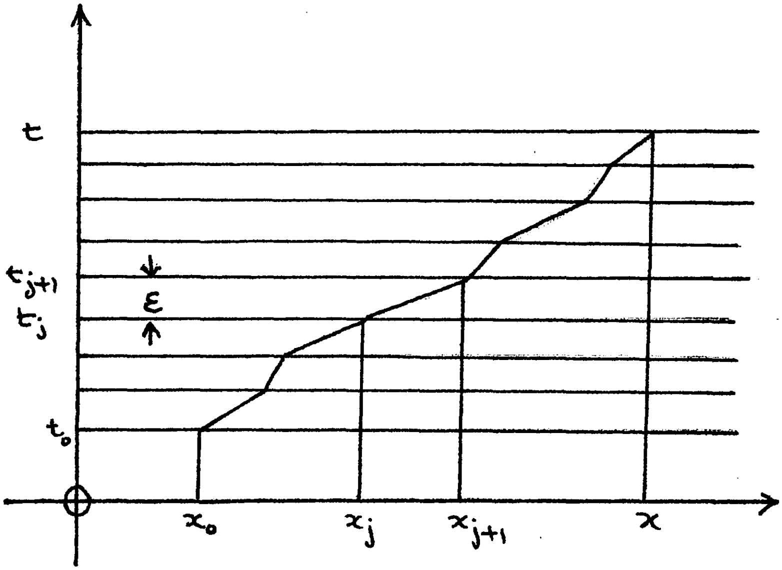

Figure 4.1. Typical path in Ω.

The paths from $x_j(t_j)$ to $x_{j+1}(t_{j+1})$ can be taken as straight lines and the action along these paths correct to the first order in ε is

$$\frac{1}{2} m \varepsilon \left(\frac{x_{j+1} - x_j}{\varepsilon} \right)^2 - \varepsilon V\left(\frac{x_{j+1} + x_j}{2} \right) . \qquad (4.15)$$

The action along the path in Figure 4.1 is thus

$$\sum_{j=0}^{N-1} \left\{ \frac{1}{2} m \varepsilon \left(\frac{x_{j+1} - x_j}{\varepsilon} \right)^2 - \varepsilon V\left(\frac{x_j + x_{j+1}}{2} \right) \right\} = S_N[x(t')] . \qquad (4.16)$$

The N th. approximation to the propagator is defined to be:

$$\frac{1}{A} \iint \cdots \int \frac{dx_1}{A} \frac{dx_2}{A} \cdots \frac{dx_{N-1}}{A} \exp \frac{i}{\hbar} S_N[x(t')] \qquad (4.17)$$

where A is a normalization factor which ensures that $U(x,t\,;\,x_0,t_0)$ is unitary. Its value in this case is $\{2\pi i \hbar \varepsilon / m\}^{1/2}$. The exact value of the propagator is then given by the limit of the expression (4.17) as $N \rightarrow \infty$ (or $\varepsilon \rightarrow 0$), such that $N\varepsilon = t - t_0$, and can be shown to satisfy Schrödinger's equation (3.20) for times $t > t_0$.

Feynman has considered the classical limit of the propagator as given by equation (4.13). As the action functions $S[x(t')]$ become large in comparison with $\hbar$, then both the real and imaginary parts of $\exp i/\hbar\, S[x(t')]$ are rapidly oscillating functions with respect to changes in $x(t')$. The only contributions to the propagator arise from the paths $x(t')$ for which $S[x(t')]$ is stationary, and these are the classical paths. In the classical limit, then, the propagator can be expressed as a sum over only the classical paths (which we can label by c):

$$U(x,t\,;\,x_0,t_0) = \sum_c f_c(x,t\,;\,x_0,t_0)\exp \frac{i}{\hbar} S_c(x,t\,;\,x_0,t_0) \quad (4.18)$$

where f_c are smoothly varying amplitude factors. Whenever the action functions are comparable with $\hbar$, then contributions from all paths arise and no one particular path can be singled out as being more important than the next.

Feynman's approach to quantum mechanics is different to both Schrödinger's and Heisenberg's and again it illustrates the inadequacies of classical mechanics whenever values of action functions are small. Paths are, however, an important feature in this approach, and it is easier to follow through the transition from quantum to classical mechanics since the notion of a path is perhaps easier to conceive of than that of a wave function.

3) Hamiltonian Path-Integral Method

The Feynman formulation of quantum mechanics is related to Lagrangian rather than Hamiltonian dynamics. Garrod (1966) has shown how the Feynman approach can be generalised to include path integrals over phase-space trajectories and his method is briefly as follows:

We consider this time the set Ω' of all phase-space trajectories which satisfy the condition $x(t_0) = x_0$, $x(t) = x$, with no condition on the energy or initial and final values of the momentum. The action function now considered is

$$S\left[x(t'),p(t')\right] = \int_{t_0}^{t} \left\{ p\dot{x} - H(x(t'),p(t')) \right\} dt' \qquad (4.19)$$

and the propagator is written:

$$U(x,t\,;x_0,t_0) = \int_{\Omega'} \exp \frac{i}{\hbar} S\left[x(t'),p(t')\right] d\left[x(t')\right] d\left[p(t')\right] . \qquad (4.20)$$

A typical phase-space trajectory corresponding to the N th. partition of the time interval is shown in Figure 4.2.

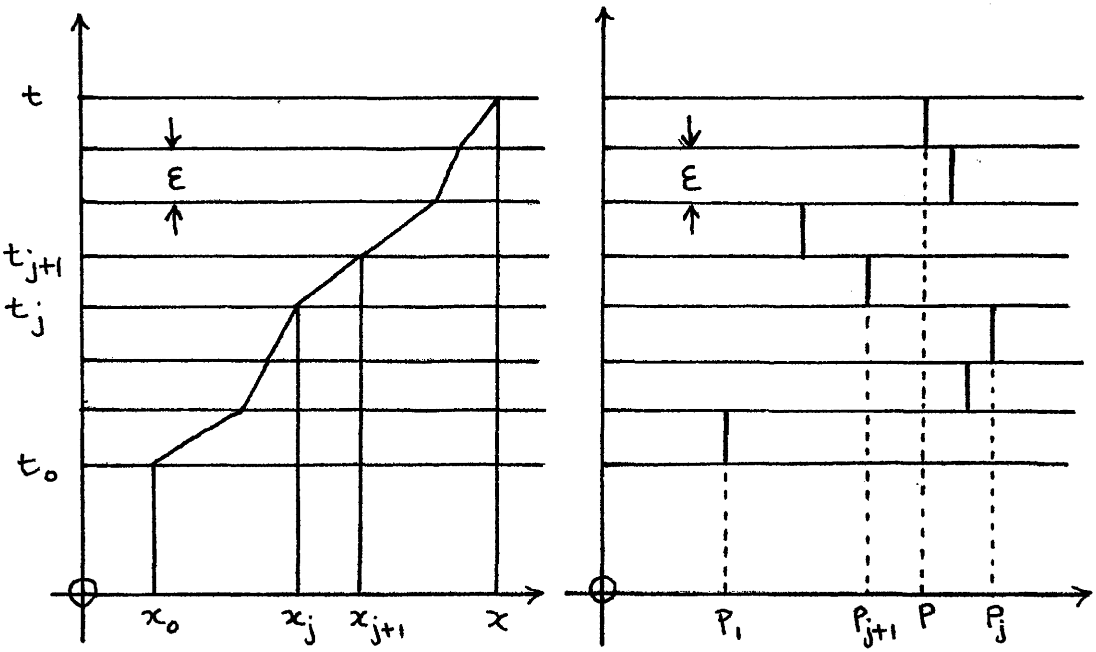

Figure 4.2. The Nth approximation to the phase-space path.

The values of the momenta are now no longer required to be continuous. The N th. approximation to the action is

$$S_N[p(t'),x(t')] = \sum_{j=0}^{N-1} \left\{ p_{j+1}(x_{j+1}-x_j) - \frac{p_{j+1}^2 \varepsilon}{2m} - \int_{t_j}^{t_{j+1}} V dt' \right\} \qquad (4.21)$$

and the propagator is given by the limit $N \to \infty$ of the expression:

$$\iint\ldots\int dp_1 dp_2 \ldots dp_N \iint\ldots\int dx_1 dx_2 \ldots dx_{N-1} \exp\frac{i}{\hbar}\left\{ S[x(t'),p(t')]\right\} . \quad (4.22)$$

There is no need to introduce any normalization constant A as in equation (4.17), and Garrod rightly points out that the constant A arises from the integration over momentum. The propagator obtained in this manner is automatically unitary.

Garrod also considers the spectral operator kernel in the light of phase-space trajectories. He takes the Fourier transform (to energy representation) of the full evolution operator kernel of equation (3.29) and shows that the resulting kernel is given by:

$$I_E(x,x_0) = \lim_{N\to\infty} \iint..dp_1 dp_2..dp_N \iint..dx_1..dx_{N-1}\,\delta(E-\tilde{H})\exp\frac{i}{\hbar}\left[\int_{x_0}^{x} p\,dx'\right] . \quad (4.23)$$

Now, only those trajectories for which the average value, $\hat{H}$, of the Hamiltonian is equal to the energy of the system contribute to the spectral operator kernel, and the action function in the exponential is that corresponding to the energy-dependent action of equation (2.16). The condition that the average value of H be equal to E is the energy analogue of the condition that all trajectories in the time-dependent representation have the same time interval $t - t_0$.

Garrod has not been the only person to consider path integrals in phase space and some interesting work has been done by Davies (1963). His approach is much more restrictive than Garrod's and he assumes from the start that the system under consideration may be described by coordinates in such a way that the Hamiltonian is identically zero. In this representation he obtains the result that the propagator may be expressed exactly in terms of the classical path. This is important because it shows that there are instances, other than the classical limit, when only the classical paths contribute to the propagator.

4) <u>The Phase-Integral Approximation</u>

Although the propagator can sometimes be expressed in terms of the classical paths in certain representations, it has in general to be expressed as a sum over all paths between the two given points. However, the approximation of summing over only the classical paths has been considered and is often used to obtain approximate values of operator kernels. This approach, which is closely related to the W.K.B. method, is known as the phase-integral approximation and we shall discuss it here as it applies to general motion in three dimensions. In this approximation the propagator is expressed in the form of equation (4.18) and the problem is then that of obtaining the amplitude factors corresponding to the functions f_c .

The phase-integral approximation is reviewed by Gutzwiller (1967), who uses as a starting point Pauli's result that the propagator of a particle moving in a potential which has no singularities may be written for small time intervals $t - t_0$ as:

$$U(q,t;q_0,t_0) = (2\pi i\hbar)^{-\frac{3}{2}}(D_s)^{\frac{1}{2}} \exp\frac{i}{\hbar}S(q,t;q_0,t_0) \qquad (4.24)$$

where $S(q,t;q_0,t_0)$ is the action evaluated along the classical trajectory from q_0 to q , and D_s is the determinant of mixed derivatives:

$$D_s = (-1)^3 \det|\partial^2 S/\partial q\partial q_0| \; . \qquad (4.25)$$

The propagator as given in equation (4.24) satisfies Schrödinger's equation up to a remainder of the order of $\hbar^2$, and it is assumed in the phase-integral approximation that this is also going to be the form of the propagator in the classical limit. However, we saw (equation 4.18) that in the classical limit, the propagator is given as a sum over all classical paths leading from q_0 to q, and so whenever there is more than one classical path joining q_0 to q, we take as the phase-integral approximation to the propagator a sum of terms, each one having the same form as that given in equation (4.24), and each one evaluated along one of the classical trajectories. Gutzwiller gives as the phase-integral approximation to the propagator an expression involving terms similar to those in equation (4.24):

$$U(q,t;q_0,t_0) = (2\pi i\hbar)^{-\frac{3}{2}} \sum_{\text{classical paths}} (D_s)^{\frac{1}{2}} \exp \frac{i}{\hbar}\left[S_c(q,t;q_0,t_0) + \text{Phases}\right] . \quad (4.26)$$

The only difference is the presence of the phases in the exponential term. These phases are usually multiples of $\hbar\pi/2$ and are inserted to provide a convenient way of absorbing the different weighting factors, multiples of i, associated with each term in equation (4.26). These weighting factors apparently arise naturally from the limiting process $\hbar \to 0$ of the Feynman expression for the propagator. Gutzwiller investigates the singularities of the determinant D_s and relates the phases to the points along the classical trajectories which produce these singularities. These singular points are the focal points.

The phase-integral method can be employed to obtain approximate Green functions, and this too has been considered by Gutzwiller. The approximate Green function is now a sum over classical paths of terms involving the energy-dependent action together with an amplitude factor involving another determinant of mixed derivatives. In the phase-integral approximation the operator kernel is always related to the classical action function appropriate to the particular representation. This is shown by Gutzwiller who evaluates the Green function in momentum representation and shows it to be expressible in terms of the energy-dependent action function of momentum space.

It is interesting to note that the phase-integral approximation sometimes leads to results that are correct. Gutzwiller's aim of developing the phase-integral approximation was to obtain approximate analytic wave functions for electrons in atoms and simple molecules. His application of the method to the bound state problem of the hydrogen atom in momentum space actually gives the correct bound state energy levels and associated projection operator kernels. However, although the poles and residues of his approximate Green function happen to coincide with those of the actual Green function, it does not follow that the approximate Green function is in fact identical to the actual one. Nevertheless, Gutzwiller's result suggests that there is a possibility of expressing the kernel of a quantum-mechanical operator exactly in terms of classical path sums if the operator is zero everywhere except at the poles of the Green function. Such an operator is the spectral operator $\delta(E-H)$ and, as we shall show, we do obtain a complete correspondence identity between this operator kernel and the classical solution in momentum representation for the hydrogen atom.

5) Providing a Complete Correspondence Identity

In the introduction to Chapter 2 we considered how the correspondence identities for the hydrogen atom were going to be explained, and the method put forward was to obtain a complete correspondence identity. One method of obtaining a complete correspondence identity is to express either the propagator, Green functions or spectral operator kernel exactly and precisely in terms of sums over classical paths of terms involving the classical action. For the purposes of this thesis the fact that we can express the spectral operator kernel in this way is sufficient to explain the three correspondence identities. Why we can only obtain a complete correspondence identity for this operator and not the others, and why we can only do this in momentum representation are difficult questions to answer. However, we are guided by the Fock identity in choosing to work in momentum representation, and by Gutzwiller's work in choosing the spectral operator.

The problem of finding out when an operator kernel is expressible exactly in terms of the classical paths has been considered by others, but only as far as we are aware for the propagator. Feynman and Hibbs (1965) have shown (see appendix B) that if the classical Lagrangian is a quadratic function of position and velocities, then the propagator is given exactly in terms of the classical paths. The propagator of the free particle and the harmonic oscillator can thus be obtained explicitly in terms of the classical paths in configuration space and we shall do this for the free particle in Chapter 5. Also, to provide a simple introduction to the mathematics needed later in dealing with the Coulomb potential, we shall obtain the free-particle Green functions and spectral operator kernel explicitly as sums over classical paths.

Clutton-Brock (1964) has also considered the problem of expressing the propagator exactly in terms of classical paths and shows that even in the general case the propagator can be determined exactly by the classical paths. His method is to assume that the kernel is first of all obtained in the representation for which the Hamiltonian is identically zero (so that it is determined by the classical paths as mentioned previously). The action in this representation is (to use Clutton-Brock's notation)

$$\int_{t_0}^{t} P\dot{Q}\,dt' \tag{4.27}$$

and the action in any other representation is related to this by the generating function of the transformation, so that (see equation (2.23) and (2.26))

$$\int_{t_0}^{t} \left(p\dot{q} - H(p,q,t')\right)dt' = \int_{t_0}^{t} P\dot{Q}\,dt' + \Big[\Psi(q,P,t')\Big]_{t_0}^{t} . \tag{4.28}$$

Clutton-Brock then considers Feynman path integration in phase space of terms of the form

$$\exp\left[\frac{i}{\hbar}\int_{t_0}^{t} P\dot{Q}\,dt'\right] \exp\left[\frac{i}{\hbar}\Psi(q,P,t\,;q_0,P_0,t_0)\right] \tag{4.29}$$

and shows that only the classical paths contribute to the propagator. However, his result is incorrect, since equation (4.28) only holds for the classical paths and not the generalised paths in phase space as shown in Figure 4.2, over which the terms given in (4.29) have to be summed.

It is unfortunate that Clutton-Brock's result is invalid, as problems in classical mechanics are often easier to solve than in quantum mechanics. We have to be content with the fact that operator kernels can only sometimes be expressed in terms of sums over classical paths. When this turns out to be the case, and we do have a complete correspondence identity, we find that there are usually other correspondence identities associated with the system which are consequences of this complete correspondence identity. However we do not know if the reverse is necessarily true, namely, when a system possesses correspondence identities does it follow that we can obtain a complete correspondence identity? For the hydrogen atom we have been able to do this, but the existence of such an identity does depend crucially on the particular choice of operator and also on the choice of representation.

CHAPTER 5

OBTAINING A COMPLETE CORRESPONDENCE IDENTITY FOR THE FREE PARTICLE, AS A SIMPLE EXAMPLE

1) Introduction

In appendix B it is shown that if the classical Lagrangian of a system is a quadratic function of the co-ordinates and velocities, then the quantum-mechanical propagator can be expressed precisely in terms of the classical action function. The classical Lagrangian of a free particle moving in one dimension along the x-axis is

$$L = \frac{1}{2} m \dot{x}^2 \qquad (5.1)$$

and the quantum-mechanical propagator can thus be expressed in this manner. This result is in keeping with the fact that a theory based on classical paths (or rays) is entirely adequate for the treatment of free particles in quantum mechanics provided that a phase is associated with each path between two points in space-time. The analogy in geometrical optics is of light waves passing through a homogeneous medium where it is well known that the eikonal approximation is sufficient to furnish the exact plane-wave solution of the scalar wave equation.

In this chapter we shall provide a complete correspondence identity through each of the kernels of the evolution operator, the Green operators and the spectral operator. In each case we shall express the kernel as a sum over classical paths of terms involving the appropriate action for the path. The original de Broglie relations between momentum and wavelength, and between frequency and energy are correspondence identities which follow from either of the complete correspondence identities.

2) The Concept of a Particle on a Ring

The system of electron and proton to be discussed in the following chapters possesses both a continuous and a discrete energy spectrum according to whether the total energy of the system is positive or negative. A free particle can also exist in states for which the energy spectrum is either continuous or discrete, depending on the boundary conditions. To provide a simple introduction to the more difficult theory of the Coulomb potential we shall consider the free particle with both types of energy spectrum.

The simplest example of a continuous spectrum is that of a free particle moving in one dimension, and we take the motion to be along the x-axis. If we insist that the motion be periodic in x, with period $x = 2\pi a$ say, then the spectrum of the free particle will be discrete (see for example Merzbacher 1961, p. 85). The periodic motion is then equivalent to that of a free particle moving on a ring of radius a, as in Figure 5.1.

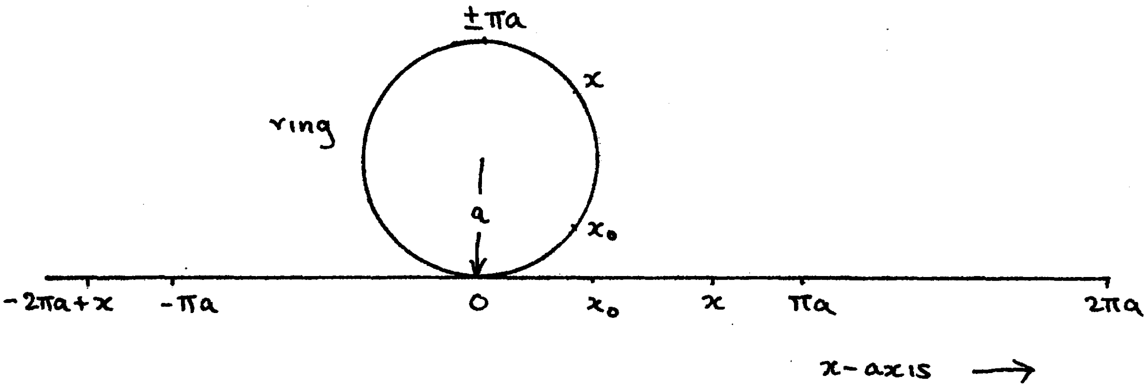

Figure 5.1. The point x on the ring is identified with the points $2\pi ca + x$ on the x-axis.

The distance around the ring is denoted by x, where $|x| \leqslant \pi a$, and quantum-mechanically the motion can be described by free-particle wave functions which satisfy the periodic boundary conditions:

$$\left.\begin{aligned}\psi(x)(\text{at } x = \pi a) &= \psi(x)(\text{at } x = -\pi a)\\ \psi'(x)(\text{at } x = \pi a) &= \psi'(x)(\text{at } x = -\pi a)\,.\end{aligned}\right\} \qquad (5.2)$$

For any time interval $\tau \neq 0$, the particle may move classically along an infinite number of paths between two points x_0 and x on the ring. In the figure, the direct path from x_0 to x corresponds to the path from x_0 to x on the x-axis. The path from x_0, through πa, past the origin c times then to x, corresponds to the path from x_0 to $2\pi ca + x$ on the x-axis. Alternatively the path from x_0, past the origin c times and then to x, corresponds to the path on the x-axis from x_0 to $-2\pi ca + x$. In this way we can relate each path on the ring to a path between the points x_0 and $2\pi ca + x$ on the x-axis, where c is a positive or negative integer. We shall label each classical path on the ring by c so that the magnitude and sign of the integer c defines the number of times that the particle passes around the ring in a clockwise or anti-clockwise sense. Each one of the points $x + 2\pi ca$, on the x-axis is identified with the point x on the ring, so that the ring can be regarded as the x-axis coiled up onto itself. This device is useful, as we shall see, in expressing the quantum-mechanical propagator of a particle on the ring in terms of sums over classical paths. In the time-dependent treatment of the problem the energy is different for each path: the energy being large for large values of $|c|$. In the time-independent treatment the energy for each path is the same, but the times are now different.

3) Evaluating the Classical Action Functions

The time-dependent Hamilton-Jacobi equation for the free particle may be written:

$$\frac{1}{2m}\left(\frac{\partial\phi}{\partial x}\right)^2 + \frac{\partial\phi}{\partial t} = 0 \quad . \qquad (5.3)$$

Assuming a separable solution for ϕ we obtain

$$\phi = \frac{m}{2}\frac{(x-A)^2}{(t-B)} \qquad (5.4)$$

where A and B are constants to be determined. By requiring that the initial values of x and t be x_0 and t_0 we obtain as Hamilton's principal function the following expression for ϕ :

$$\phi(x,t\,;x_o,t_o) = \frac{m}{2}\frac{(x-x_o)^2}{(t-t_o)} \quad . \tag{5.5}$$

This is the value of the classical action function $S(x,t\,;x_o,t_o)$ of a free particle travelling from x_o at time t_o , to x at time t . The value of Hamilton's principal function for a particle travelling along the x-axis from x_o to $2\pi ca + x$ in the same time is thus going to be

$$\phi(x+2\pi ca,t\,;x_o,t_o) = \frac{m}{2}\frac{(x-x_o+2\pi ca)^2}{(t-t_o)} \quad . \tag{5.6}$$

Since all points $x + 2\pi ca$ are identified with the point x on the ring, then the value of the classical action S_c for the path c from x_o to x in the time $t - t_o$ is going to be

$$S_c(x,t\,;x_o,t_o) = \frac{m}{2}\frac{(x-x_o+2\pi ca)^2}{(t-t_o)}; \; c=0,\pm 1,\pm 2,\ldots \tag{5.7}$$

where $|x|, |x_o| \leqslant \pi a$.

The value of the time-independent action for the motion between x_0 and x can be obtained by considering the time-independent Hamilton-Jacobi equation. The H-J equation for the characteristic function W now reads:

$$\frac{1}{2m}\left(\frac{\partial W}{\partial x}\right)^2 = E \tag{5.8}$$

so that

$$W = \pm\sqrt{2mE}\,x + C \tag{5.9}$$

where C is a constant to be determined. We have two solutions depending on the sign of the square root:

$$\left.\begin{aligned} W^+ &= \sqrt{2mE}\,x + C^+ \\ W^- &= -\sqrt{2mE}\,x + C^- . \end{aligned}\right\} \tag{5.10}$$

The constants $C^\pm$ can be obtained by again assuming that the initial value of x is x_0. Since $W^\pm = 0$ when $x = x_0$ we have

$$\left.\begin{aligned} W^+ &= \sqrt{2mE}\,(x - x_0) \\ W^- &= \sqrt{2mE}\,(x_0 - x) . \end{aligned}\right\} \tag{5.11}$$

We note that the value of the momentum at x is given by $\partial W^{\pm}/\partial x$, and is positive for motion in the positive x direction. Thus we conclude that W^{+} and W^{-}, as given by equation (5.11), are respectively the characteristic functions for $x > x_0$ and $x < x_0$. We may therefore write for the characteristic function the expression

$$W(x,x_0) = \sqrt{2mE}\,|x - x_0| \,. \tag{5.12}$$

This is the value of the energy-dependent action function $S_E(x,x_0)$ of a free particle moving along the x-axis from x_0 to x with energy E. The corresponding value of the action along the path c on the ring for values of $|x|, |x_0| \leq \pi a$ is then

$$S_{cE}(x,x_0) = \sqrt{2mE}\,|x - x_0 + 2\pi c a| \,;\; c = 0, \pm 1, \pm 2, \ldots \tag{5.13}$$

4) The Kernels of the Quantum-Mechanical Evolution Operator, Green Operators and Spectral Operator

The solutions of the free-particle time-independent Schrödinger equation for a given value of the energy E, may be written as

$$\left.\begin{aligned} \psi_E^{+}(x) &= A^{+} \exp i/_\hbar (2mE)^{1/2} x \\ \psi_E^{-}(x) &= A^{-} \exp - i/_\hbar (2mE)^{1/2} x \end{aligned}\right\} \tag{5.14}$$

where $A^{\pm}$ are arbitrary constants involving the energy E. If we choose to normalise $\psi_E^{\pm}(x)$ according to equation (3.12), so that

$$\int dx\, A^{+}(E)\left[A^{+}(E')\right]^{*} \psi_E^{+}(x)\left[\psi_{E'}^{+}(x)\right]^{*} = \delta(E-E') \tag{5.15}$$

and

$$\int dx\, A^{-}(E)\left[A^{-}(E')\right]^{*} \psi_E^{+}(x)\left[\psi_{E'}^{+}(x)\right]^{*} = \delta(E-E') \tag{5.16}$$

we obtain for the normalised solutions $\psi_E^{\pm}(x)$ the following (Merzbacher 1961, chap. 6):

$$\psi_E^{\pm}(x) = \left(\frac{1}{2\pi\hbar}\sqrt{\frac{m}{2E}}\right)^{1/2} \exp \pm i/_\hbar (2mE)^{1/2} x \,. \tag{5.17}$$

The kernel of the evolution operator, given by equation

(3.24) for the free particle will now be

$$U(x,t\,;x_0,t_0) = \int_0^\infty \frac{dE}{2\pi\hbar}\left(\frac{m}{2E}\right)^{1/2} \exp -\frac{i}{\hbar}E(t-t_0)\, \exp\frac{i}{\hbar}(2mE)^{1/2}(x-x_0)$$

$$+\int_0^\infty \frac{dE}{2\pi\hbar}\left(\frac{m}{2E}\right)^{1/2} \exp -\frac{i}{\hbar}E(t-t_0)\, \exp -\frac{i}{\hbar}(2mE)^{1/2}(x-x_0)\,. \qquad (5.18)$$

With the substitution $2mE = p_0^2$, equation (5.18) becomes:

$$U(x,t\,;x_0,t_0) = \int_{-\infty}^{\infty} \frac{dp_0}{2\pi\hbar} \exp -\frac{ip_0^2}{2m\hbar}(t-t_0)\, \exp\frac{i}{\hbar}p_0(x-x_0)$$

$$= \left(\frac{m}{2\pi i\hbar(t-t_0)}\right)^{1/2} \exp\frac{i}{\hbar}\cdot\frac{m}{2}\cdot\frac{(x-x_0)^2}{(t-t_0)} \qquad (5.19)$$

which is the well known expression for the free-particle evolution operator kernel (see, for example, Feynman and Hibbs 1965, Kurşunoğlu 1962).

The evolution operator kernel for the particle on a ring may be obtained in two quite distinct ways. The more conventional approach is to solve the time-independent Schrödinger equation with periodic boundary conditions.

The normalised solutions in the interval $-\pi a \lesssim x \lesssim \pi a$ are then:

$$\psi_\nu(x) = \frac{1}{(2\pi a)^{1/2}} \exp \frac{i\nu x}{a} \quad ; \quad \nu = 0, \pm 1, \ldots \qquad (5.20)$$

where the discrete energy spectrum is given by

$$E_\nu = \frac{\nu^2 \hbar^2}{2a^2 m} \quad . \qquad (5.21)$$

The evolution operator for a discrete spectrum is given by equation (3.23) and in this case the kernel is:

$$U(x,t;x_0,t_0) = \sum_{\nu=-\infty}^{\infty} (2\pi a)^{-1} \exp \frac{i\nu(x-x_0)}{a} \exp -\frac{i\nu^2\hbar^2}{\hbar 2a^2 m}(t-t_0) \, . \qquad (5.22)$$

The other, more convenient approach, is to use the device of coiling the x-axis upon itself as mentioned before. We consider a wave packet $\psi(x_0, t_0)$ on the ring at time t_0 , whose value and whose derivative at $x_0 = \pm a\pi$ is zero. We can consider also the same wave packet on the x-axis itself. For times $t > t_0$ this wave packet will move into regions where $|x| > \pi a$

and the motion will be determined by the evolution operator kernel of (5.19). If we distinguish wave functions and kernels on the x-axis by the superscript SL (straight line) we have:

$$\psi^{SL}(x,t) = \int dx_0 U^{SL}(x,t\,;x_0,t_0)\psi^{SL}(x_0,t_0),\ t>t_0$$

$$= \int dx_0 U^{SL+}(x,t\,;x_0,t_0)\psi(x_0,t_0)\,. \qquad (5.23)$$

The value of the amplitude on the ring is obtained by the interference (constructive and destructive) of each of the segments of the wave packet between $(2c-1)\pi a$ and $(2c+1)\pi a$ on the x-axis for every value of the integer c :

$$\left.\begin{aligned}\psi(x,t) &= \sum_c \psi^{SL}(x+2\pi ca,t)\\ &= \sum_c \int dx_0 U^{SL+}(x+2\pi ca,t\,;x_0,t_0)\psi(x_0,t_0)\end{aligned}\right\}|x|,|x_0|\leqslant\pi a \qquad (5.24)$$

Therefore, the propagator for the particle on the ring is given by

$$U^{+}(x,t;x_0,t_0) = \sum_c U^{SL+}(x+2\pi ca,t;x_0,t_0)$$

$$= \varepsilon(t-t_0)\sum_c \left\{\frac{m}{2\pi i\hbar(t-t_0)}\right\}^{1/2} \exp \frac{im}{\hbar 2}\frac{(x-x_0+2\pi ca)^2}{(t-t_0)} \; . \quad (5.25)$$

The ε function is present in equation (5.25) since this expression only holds for $t > t_0$. However the backward evolution operator kernel can be obtained from this equation by the relation (3.30) and the full evolution operator kernel is

$$U(x,t;x_0,t_0) = \sum_c \left\{\frac{m}{2\pi i\hbar(t-t_0)}\right\}^{1/2} \exp \frac{im}{\hbar 2}\frac{(x-x_0+2\pi ca)^2}{(t-t_0)} \; . \quad (5.26)$$

The two expressions (5.26) and (5.22) are different expansions of the same operator kernel, and their effect on an arbitrary wave function is the same. There is, however, no direct connection between the summation indices ν and c as we shall see.

The Green functions can be evaluated directly by summing (or integrating) over the energy states as given by equations (3.40) and (3.41). This is done in appendix A for the free particle moving along the x-axis. However, we can make use of the relations (3.37) and (3.38), and obtain the Green functions $G_E^{\pm}(x, x_0)$ by taking the respective Fourier transforms of equations (5.19) and (5.26). Noting that $G_E^{\pm}(x, x_0)$ come from $U^{\pm}(x,t\ ; x_0, t_0)$ respectively, we obtain for the free particle moving along the x-axis:

$$\left.\begin{aligned} G_E^{+}(x,x_0) &= \frac{1}{i\hbar}\left(\frac{m}{2E}\right)^{\frac{1}{2}} \exp \frac{i}{\hbar}|x-x_0|(2mE)^{\frac{1}{2}} \\ \text{and:} & \\ G_E^{-}(x,x_0) &= \frac{-1}{i\hbar}\left(\frac{m}{2E}\right)^{\frac{1}{2}} \exp -\frac{i}{\hbar}|x-x_0|(2mE)^{\frac{1}{2}}. \end{aligned}\right\} \quad (5.27)$$

For the particle on the ring the Green functions are:

$$\left.\begin{aligned} G_E^{+}(x,x_0) &= \sum_c \frac{1}{i\hbar}\left(\frac{m}{2E}\right)^{\frac{1}{2}} \exp \frac{i}{\hbar}|x-x_0+2\pi ca|(2mE)^{\frac{1}{2}} \\ \text{and:} & \\ G_E^{-}(x,x_0) &= \sum_c -\frac{1}{i\hbar}\left(\frac{m}{2E}\right)^{\frac{1}{2}} \exp -\frac{i}{\hbar}|x-x_0+2\pi ca|(2mE)^{\frac{1}{2}}. \end{aligned}\right\} \quad (5.28)$$

The spectral operator kernel $I_E(x, x_0)$ is now given by the result (3.45), so that for the free particle:

$$I_E(x,x_0) = \varepsilon(E)\frac{1}{\pi\hbar}\left(\frac{m}{2E}\right)^{1/2}\cos\frac{(x-x_0)(2mE)^{1/2}}{\hbar} \qquad (5.29)$$

and for the free particle on the ring:

$$I_E(x,x_0) = \varepsilon(E)\frac{1}{\pi\hbar}\left(\frac{m}{2E}\right)^{1/2}\sum_c \cos\frac{(x-x_0+2\pi ca)(2mE)^{1/2}}{\hbar}. \qquad (5.30)$$

5) A Complete Correspondence Identity

We can provide a complete correspondence identity through the kernels of either the evolution operator, the Green operators or the spectral operator. In the case of the evolution operator, the quantum-mechanical kernel is related to the solutions of the classical time-dependent Hamilton-Jacobi equation. In this way the operator kernel is related directly to the classical time-dependent action functions $S(x, t; x_0, t_0)$ and $S_c(x, t; x_0, t_0)$ given in the two cases by equations (5.5) and (5.7). The kernels of the Green operators and spectral operator are related to the solutions of the time-independent Hamilton-Jacobi equation which are the time-independent action functions $S_E(x,x_0)$, $S_{cE}(x,x_0)$ of equations (5.12) and (5.13).

For the free particle moving along the x-axis a complete correspondence identity is obtained for each of the operators as follows:

For the propagator:

$$U^+(x,t;x_0,t_0) = \varepsilon(t-t_0)\left\{\frac{m}{2\pi i\hbar(t-t_0)}\right\}^{1/2}\exp\frac{i}{\hbar}S(x,t;x_0,t_0). \qquad (5.31)$$

For the Green functions and spectral operator kernel:

$$G_E^{\pm}(x,x_0) = \pm\frac{1}{i\hbar}\left(\frac{m}{2E}\right)^{1/2}\exp\pm\frac{i}{\hbar}S_E(x,x_0) \qquad (5.32)$$

and

$$I_E(x,x_0) = \varepsilon(E)\frac{1}{\pi\hbar}\left(\frac{m}{2E}\right)^{1/2}\cos\left\{S_E\frac{(x,x_0)}{\hbar}\right\}. \qquad (5.33)$$

For the free particle on the ring the respective complete correspondence identities are very similar but involve sums over all classical paths c from x_0 to x :

$$U^+(x,t;x_0,t_0) = \varepsilon(t-t_0)\left\{\frac{m}{2\pi i\hbar(t-t_0)}\right\}^{1/2}\sum_c \exp\frac{i}{\hbar}S_c(x,t;x_0,t_0). \quad (5.34)$$

$$G_E^{\pm}(x,x_0) = \pm\frac{1}{i\hbar}\left(\frac{m}{2E}\right)^{1/2}\sum_c \exp\pm\frac{i}{\hbar}S_{cE}(x,x_0) . \qquad (5.35)$$

$$I_E(x,x_0) = \varepsilon(E)\frac{1}{\pi\hbar}\left(\frac{m}{2E}\right)^{1/2}\sum_c \cos\frac{S_{cE}(x,x_0)}{\hbar}. \qquad (5.36)$$

For completeness, we can also express the external factors $\left\{\frac{m}{2\pi i\hbar(t-t_0)}\right\}^{1/2}$ and $\frac{1}{i\hbar}\left(\frac{m}{2E}\right)^{1/2}$ of equations (5.31), (5.34) and (5.32), (5.35) in terms of the classical action functions. For the free particle on the x-axis the two factors are given by

$$\left\{\frac{m}{2\pi i\hbar(t-t_0)}\right\}^{1/2} = (2\pi i\hbar)^{-\frac{1}{2}}\left|(-1)\frac{\partial^2 S(x,t;x_0,t_0)}{\partial x\,\partial x_0}\right|^{1/2} \qquad (5.37)$$

and

$$\frac{1}{i\hbar}\left(\frac{m}{2E}\right)^{1/2} = \frac{1}{i\hbar}\left|\frac{\partial^2 S_E(x,x_0)}{\partial E\,\partial x}\cdot\frac{\partial^2 S_E(x,x_0)}{\partial x_0\,\partial E}\right| . \qquad (5.38)$$

The same applies for the particle on a ring, but $S(x,t\,;x_0,t_0)$ and $S_E(x,x_0)$ are replaced by $S_c(x,t\,;x_0,t_0)$ and $S_{cE}(x,x_0)$. These results are just those given by the phase-integral approximation, which also leads to the same results for the kernels of the evolution and Green operators.

6) Discussion of the Results

The free particle and particle on a ring have been considered by Norcliffe and Percival (1968, to be referred to as I). Most of the results are well known and have been obtained by others. Feynman and Hibbs (1965) evaluate the propagator for a free particle in one dimension and relate the kernel to the classical action function. They also consider the propagator for a free particle with periodic boundary conditions. However they express the propagator as a sum over quantum states as in equation (5.22), which cannot easily be expressed as a sum over classical paths as compared with the expression (5.26).

Green functions as sums over classical paths are considered by Gutzwiller (1967) and as we have stated the phase-integral approximation leads to the correct Green functions for the free particle. Gutzwiller does not evaluate the free particle Green functions in his review paper and is concerned solely with the Coulomb potential. However his general formula for the Green functions does lead to the expressions (5.32) and (5.35).

Garrod (1966) using Feynman path summation in phase space evaluates the spectral operator kernel for the free particle and his result is the same as that given by equation (5.29). Bezák (1968) evaluates the kernel of the spectral operator (his 'energy-level density function') for a free particle moving in a one-dimensional square well potential with perfectly reflecting walls. He expresses the result in terms of sums over classical paths and shows (see also I) that there is no simple connection between sums over classical paths and sums over quantum states.

The relation between sums over classical paths and sums over quantum states is worth considering here and the expansion in terms of quantum states can be obtained from the expansion in terms of classical paths. If we consider the spectral operator kernel for a particle on a ring (equation (5.36)) we can expand the cosine term and obtain:

$$I_E(x,x_0) = \frac{\mathcal{E}(E)}{\pi\hbar}\left(\frac{m}{2E}\right)^{1/2}\cos\left\{\frac{(2mE)^{\frac{1}{2}}(x-x_0)}{\hbar}\right\}\left\{1+\sum_{c=1}^{\infty}2\cos(\frac{(2mE)^{\frac{1}{2}}2\pi ac}{\hbar}\right\}. \quad (5.39)$$

Now, in terms of Dirac δ -functions (Lighthill 1960, p. 68)

$$1 + 2\sum_{c=1}^{\infty}\cos\frac{(2mE)^{\frac{1}{2}}2\pi ac}{\hbar} = \sum_{\ell=-\infty}^{\infty}\delta\left\{\frac{(2mE)^{\frac{1}{2}}a}{\hbar} - \ell\right\} \qquad (5.40)$$

where ℓ is an integer. From the properties of the δ - function we obtain

$$I_E(x,x_0) = \sum_{\ell=-\infty}^{\infty}\frac{1}{2\pi a}\exp\frac{i\ell}{a}(x-x_0)\,\delta(E-\frac{\ell^2\hbar^2}{2a^2m}) \quad . \qquad (5.41)$$

The integer ℓ is just the quantum-mechanical label ν and so

$$I_E(x,x_0) = \sum_{\nu=-\infty}^{\infty}\frac{1}{2\pi a}\exp\frac{i\nu}{a}(x-x_0)\,\delta(E-E_\nu) \qquad (5.42)$$

which is the kernel equation analogous to equation (3.46). The only connection between ν and c is therefore through equation (5.40) with $\nu = \ell$.

The expansion in terms of classical paths can often be more useful than summing over quantum states. The Green functions, for example, for the particle moving on a ring may be obtained in closed form. The sums over classical paths in equation (5.35) is a geometric series whose sum can be evaluated and the Green functions may be written (see for example I):

$$\left.\begin{aligned} G_E^{+}(x,x_0) &= \lim_{\varepsilon\to 0}\frac{1}{\hbar}\left(\frac{m}{2E}\right)^{1/2}\frac{\cos\{(\pi a-|x-x_0|)(2mE)^{1/2}/\hbar\}}{\sin\{\pi a(2mE)^{1/2}/\hbar\}}\,;\, E=E+i\varepsilon \\[2em] G_E^{-}(x,x_0) &= \lim_{\varepsilon\to 0}\frac{1}{\hbar}\left(\frac{m}{2E}\right)^{1/2}\frac{\cos\{(\pi a-|x-x_0|)(2mE)^{1/2}/\hbar\}}{\sin\{\pi a(2mE)^{1/2}/\hbar\}}\,;\, E=E-i\varepsilon. \end{aligned}\right\} \quad (5.43)$$

Although the Green functions $G_E^{\pm}(x,x_0)$ are apparently equal they are defined only in the upper and lower halves of the complex E plane. Along the real axis as $\varepsilon \to 0$ they are equal everywhere except at the poles

$E_\nu = \nu^2\hbar^2(2a^2m)^{-1}$, where ν is an integer. At the poles, themselves, the Green functions are related directly to the spectral operator kernel, as given by equation (3.49).

Finally, for the particle on a ring, the expansion in terms of classical paths of the spectral operator kernel shows how the spectrum is formed from the amplitudes of the classical paths by constructive interference at the energy levels E_ν and by destructive interference elsewhere. The onset of such interference is shown by the partial summation of equation (5.36) for $I_E(x,x)$ in Figure 5.2.

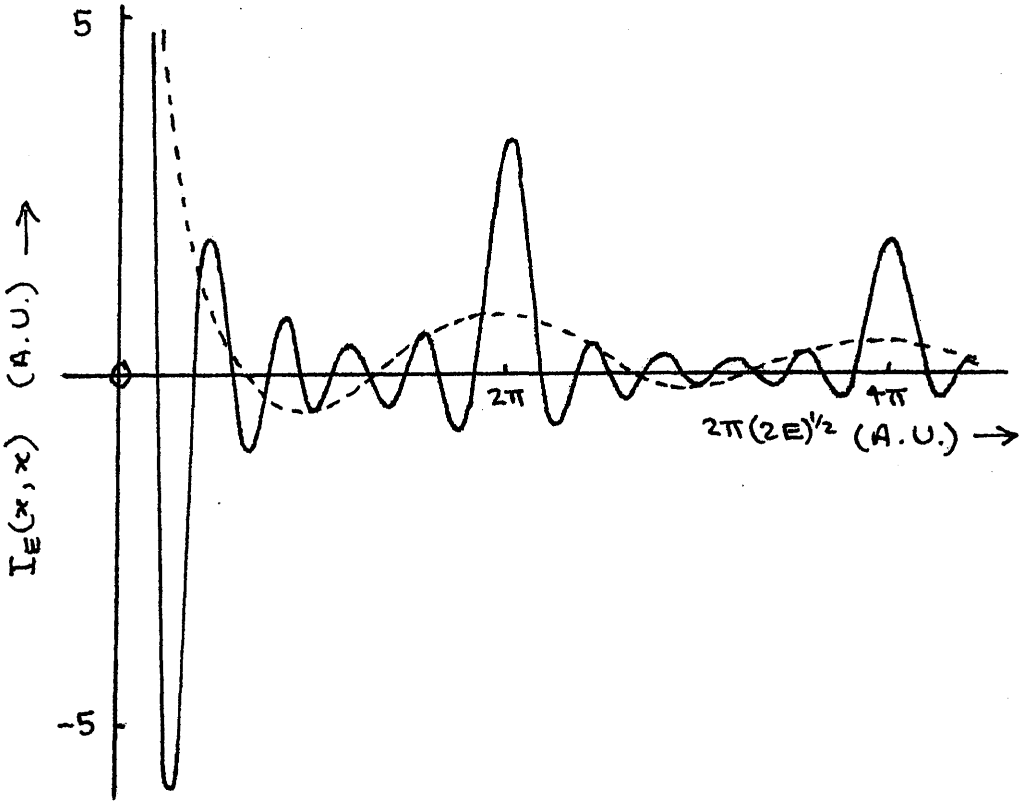

Figure 5.2. Partial summation of equation (5.36) for $I_E(x,x)$ (atomic units) against $2\pi(2E)^{1/2}$ (atomic units), a = 1. The curve ---- is the partial summation for 3 paths, and the curve —— for eleven paths.

Bezák (1968) also considers the partial summation of the spectral operator kernel and comments on the utilization of such an approximation for the estimation of energy levels. He claims that the peaks give approximate values of the energy which are lower than the actual values E_ν, in contrast to the variational methods, which provide energies greater than the actual values.

CHAPTER 6

THE BOHR-SOMMERFELD AND FOCK IDENTITIES

1) Introduction

In chapter 1 we discussed the three correspondence identities associated with the hydrogen atom and considered their role in the development of quantum mechanics and in present-day atomic physics. The two identities which concern the bound states of the hydrogen atom are the Bohr-Sommerfeld identity and the Fock identity, and in this chapter we shall explain how both these identities arise. They follow from a complete correspondence identity between the kernel of the quantum-mechanical spectral operator and the solution of the classical problem. As described in chapter 5 we shall express the kernel of this operator explicitly as a sum over classical paths of terms involving the classical action function for the path, and thus show that for the hydrogen atom a theory based on rays is sufficient to describe the behaviour of matter waves.

We shall represent the hydrogen atom by an electron moving in the field of a central potential due to the nucleus, which we shall take as having infinite mass in comparison with the electron, and we shall neglect all relativistic effects.

2) Choosing The Representation and The Operator for A Complete Correspondence Identity

An electron of mass μ moving in the field of a central potential

$$V(\underset{\sim}{r}) = -k/r = -Ze^2/r \qquad (6.1)$$

is described by a time-independent Hamiltonian. Classically the motion can be determined by solving the time-independent Hamilton-Jacobi equation. Amongst other things we find that the motion in position space is bounded: the energy equation may be written as

$$\begin{aligned} E &= T + V \\ &= \frac{p^2}{2\mu} - \frac{k}{r} \qquad (6.2) \end{aligned}$$

and since T must always be a positive quantity we see that r can only vary from 0 to r_{max}. as illustrated in Figure 6.1.

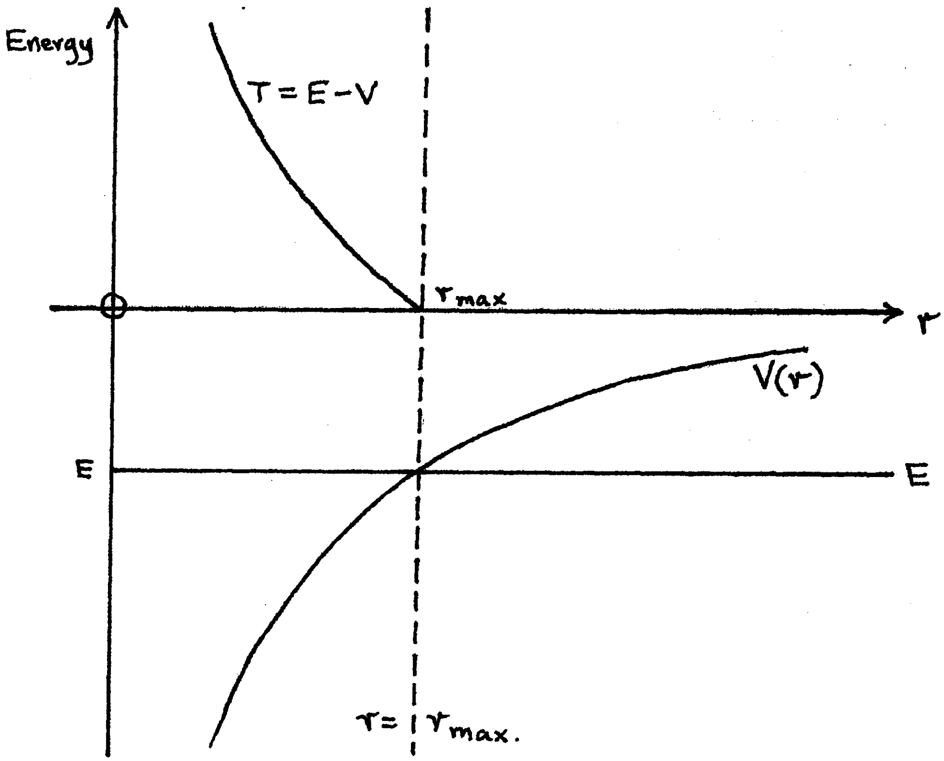

Figure 6.1. Graph showing values of the potential energy V and kinetic energy T as functions of r for a given negative value of the total energy E .

Quantum-mechanically, wave functions and operator kernels have non-zero values for $r > r_{max.}$ and consequently to express an operator kernel in terms of classical paths is not possible in position representation since between two points $\underset{\sim}{r_0}$ and $\underset{\sim}{r}$ which lie outside the sphere $|\underset{\sim}{r}| = r_{max.}$ there is no classical path.

In momentum representation we do not run into this difficulty since for a given value of the energy there is always a classical trajectory between any two points in momentum space. We shall therefore choose this representation in which to obtain a complete correspondence identity. Gutzwiller (1967), using the phase-integral method to obtain approximate Coulomb Green functions also chose to work in momentum representation because of the difficulty encountered in position space.

When the research on the hydrogen atom was initiated it was decided to try and express the Green functions as sums over classical paths. Following a method similar to that of Schwinger (1964) to obtain the Coulomb Green functions in momentum representation, we found that only part of the Green functions could be expressed in this way. We have already seen (equation 3.49) that the Green operators may be expressed in the form

$$G_E^{\pm} = \mathrm{p.v.}(E-H)^{-1} \mp \pi i\,\delta(E-H)$$

and it was concluded that the part not expressible in terms of the classical path sums arose from the principal value of the Green operator $\mathrm{p.v.}\,(E-H)^{-1}$ and not from the spectral operator $\delta(E-H)$. We thus turned our attention to the possibility of obtaining a complete correspondence identity for the spectral operator kernel instead of the Green functions.

As we have already mentioned in chapter 4 Gutzwiller's work also lends support to the possibility of expressing the kernel of $\delta(E-H)$ exactly in terms of classical path sums, since the spectral operator is non zero only for those values of the energy for which the phase-integral approximation is exact, namely at the bound-state energy levels.

3) The Symmetric Representation

When we come to evaluate the quantum-mechanical spectral operator kernel and the classical action functions of momentum space we shall find it easier to consider the Coulomb problem in a new representation, the symmetric representation. This representation is due to Fock (1935) who used it to show that the accidental degeneracy with respect to l of the energy levels of the hydrogen atom is connected with the four-dimensional rotation group $O(4)$. The symmetric representation is considered in the literature by Schwinger (1964), Bander and Itzykson (1966a), Kurşunoğlu (1962) and others. The treatment of this representation by each of these authors varies and the symmetric representation used here will be as follows:

Any point in momentum space is represented by a momentum vector $\underset{\sim}{p}$. This vector is then scaled by some parameter p_E so that $\underset{\sim}{p}$ now becomes the vector $\underset{\sim}{p}/p_E$. The scaled vector is now represented by a unit 4-vector $\underset{\sim}{u}$ obtained by the stereographic projection of $\underset{\sim}{p}/p_E$ onto the surface of a four-dimensional unit hypersphere (centred at the origin) from the north pole given by $\underset{\sim}{n} = (0, 0, 0, 1)$. Two examples of the projection are shown in Figure 6.2 restricted to three dimensions for simplicity. Using four-dimensional

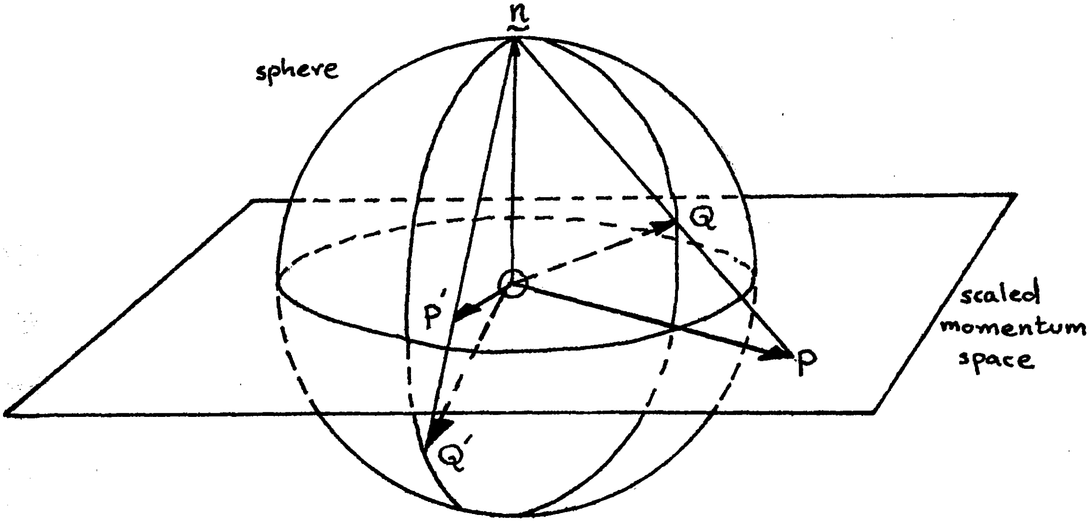

Figure 6.2. Two examples of the stereographic projection. The points P, P' in the scaled momentum space become the points Q, Q' on the sphere.

coordinate geometry we obtain the coordinates u_1, u_2, u_3, u_4 of the unit vector $\underset{\sim}{u}$ in terms of the parameter p_E and the coordinates p_x, p_y, p_z of $\underset{\sim}{p}$:

$$\left.\begin{aligned} u_1 &= \frac{2p_E p_x}{p_E^2 + p^2} \\ u_2 &= \frac{2p_E p_y}{p_E^2 + p^2} \\ u_3 &= \frac{2p_E p_z}{p_E^2 + p^2} \\ u_4 &= \frac{p^2 - p_E^2}{p_E^2 + p^2} . \end{aligned}\right\} \qquad (6.3)$$

Any point on the three-dimensional surface is most conveniently represented by the angles α, θ, ϕ where θ and ϕ are the usual spherical coordinates in momentum space, and we have

$$\left.\begin{aligned} u_1 &= \sin\alpha \sin\theta \cos\phi \\ u_2 &= \sin\alpha \sin\theta \sin\phi \\ u_3 &= \sin\alpha \cos\theta \\ u_4 &= \cos\alpha \end{aligned}\right\} 0 \leqslant \alpha \leqslant \pi . \qquad (6.4)$$

In terms of these spherical polar coordinates the line element $\underset{\sim}{ds}$ on the sphere is given by

$$\underset{\sim}{ds} = d\alpha\,\underset{\sim}{\hat{\alpha}} + \sin\alpha\, d\theta\,\underset{\sim}{\hat{\theta}} + \sin\alpha\sin\theta\, d\phi\,\underset{\sim}{\hat{\phi}} . \qquad (6.5)$$

The surface element is thus

$$d\Omega = \sin^2\alpha\, \sin\theta\, d\alpha\, d\theta\, d\phi \qquad (6.6)$$

and is related to the volume element in momentum space by the relation

$$d^3p = p^2 dp \sin\theta\, d\theta\, d\phi = \frac{(p_E^2 + p^2)^3}{8p_E^3}\, d\Omega . \qquad (6.7)$$

Finally, if we define a new variable ω by

$$\cos\omega = \underset{\sim}{u}\cdot\underset{\sim}{u}_0 \qquad (6.8)$$

then for values $0 \leq \omega \leq \pi$, it represents the shortest arc length along the surface of the sphere from $\underset{\sim}{u}_0$ to $\underset{\sim}{u}$. The actual distance between $\underset{\sim}{u}_0$ and $\underset{\sim}{u}$ is given by

$$|\underset{\sim}{u} - \underset{\sim}{u}_0|^2 = 4\sin^2\frac{\omega}{2} = \frac{4p_E^2\,|\underset{\sim}{p} - \underset{\sim}{p}_0|^2}{(p^2+p_E^2)(p_0^2+p_E^2)} . \qquad (6.9)$$

4) The Classical Theory of the Hydrogen Atom

The Hamiltonian describing the classical motion of the electron in the hydrogen atom is

$$H(\underset{\sim}{p},\underset{\sim}{r}) = \frac{p^2}{2\mu} - \frac{k}{r} = E . \tag{6.10}$$

For bound motion, when the value of E is negative, the electron moves around the nucleus in an elliptic orbit. The Kepler problem for elliptic orbits in position representation is considered in almost every book on classical mechanics and will not be considered here in any more detail.

In momentum representation the Kepler problem is simpler. From the virial theorem of both classical and quantum mechanics it follows that $p_E^2 = -2\mu E$ is the mean square momentum of the electron in a bound state of energy E, and it can be shown (Sommerfeld 1952) that the momentum vector $\underset{\sim}{p}$ traces out a circle whose radius is $p_E(1 - \varepsilon^2)^{-1/2}$ and whose centre is at a distance $p_E\,\varepsilon\,(1 - \varepsilon^2)^{-1/2}$ from the origin which is enclosed by the circle (see Figure 6.3). ε is the eccentricity of the elliptic orbit in position space.

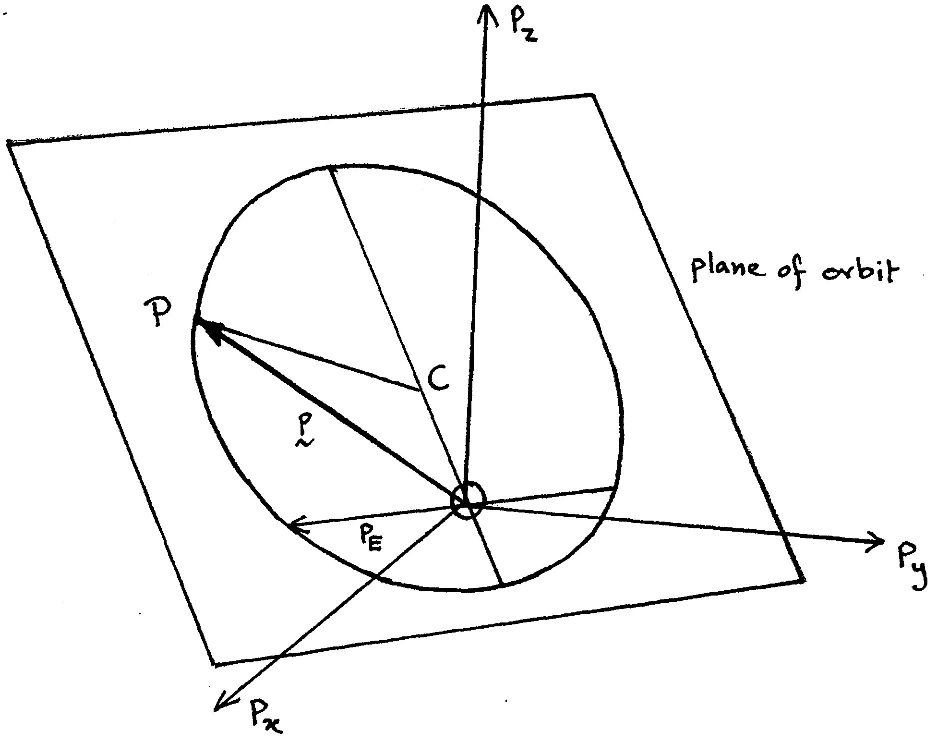

Figure 6.3. The circular orbit in momentum space. The centre C is at a distance $p_E\,\varepsilon(1-\varepsilon^2)^{-1/2}$ from the origin and the radius CP is $p_E(1-\varepsilon^2)^{-1/2}$.

The properties of this motion may be obtained by formulating and solving the H-J equation in momentum representation. The value of the characteristic function is the same as the time-independent action function $S_E(\underset{\sim}{p}, \underset{\sim}{p}_0)$ given by

$$S_E(\underset{\sim}{p},\underset{\sim}{p}_0) = \int_{\underset{\sim}{p}_0}^{\underset{\sim}{p}} -\underset{\sim}{r}\cdot d\underset{\sim}{p}' \quad . \qquad (6.11)$$

Gutzwiller (1967) has evaluated this integral directly, but we shall obtain it by now considering the problem in symmetric representation.

We obtain the motion in symmetric representation by scaling all coordinates in momentum space by the quantity p_E which is now the square root of the mean square momentum $p_E^2 = -2\mu E$. The transformation relating momentum and symmetric space is now energy dependent since the equations (6.3) contain the energy E explicitly. We shall thus consider the Coulomb problem in its greatest generality in extended phase space.

The generalised coordinates of the extended momentum space are now p_x, p_y, p_z and $-E$, and we can take α, θ, ϕ and E as the coordinates of the extended symmetric space. A simple geometric picture of the extended symmetric space is that of a cylinder whose cross section is the unit hypersphere, and whose axis is taken as the E -axis. The connection between the two spaces is shown in Figure 6.4. As the momentum-energy vector moves in momentum-energy space, the vector $(\underset{\sim}{u}, E)$ will trace out some curve on the surface of the cylinder; for a particular fixed value of the energy E , the motion will be restricted to lie on the unit hypersphere.

The two extended spaces can be related by means of

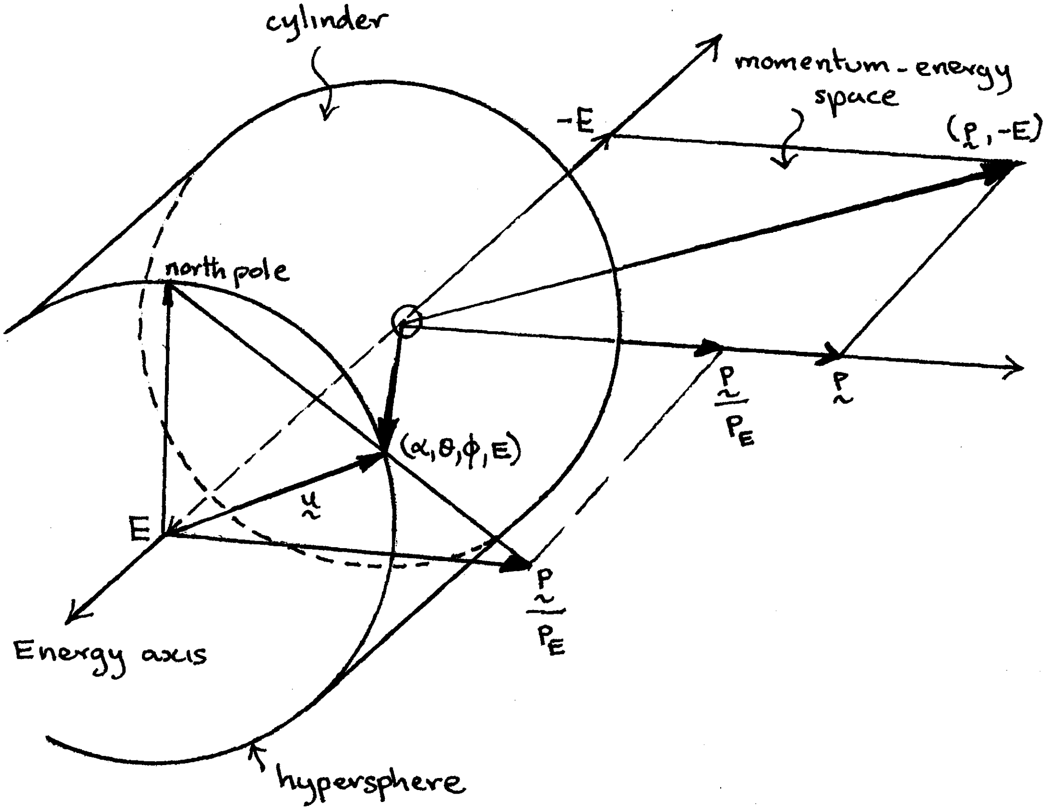

Figure 6.4. Diagram showing how the point $(\underset{\sim}{p}, -E)$ becomes the point $(\alpha, \theta, \phi, E)$.

a canonical transformation. The transformation is given by equations (6.3) and (6.4) or more explicitly by:

$$\left.\begin{aligned}
p_x &= (-2\mu E)^{1/2}\,\frac{\sin\alpha\sin\theta\cos\phi}{1-\cos\alpha}\\
p_y &= (-2\mu E)^{1/2}\,\frac{\sin\alpha\sin\theta\sin\phi}{1-\cos\alpha}\\
p_z &= (-2\mu E)^{1/2}\,\frac{\sin\alpha\cos\theta}{1-\cos\alpha}\\
-E &= -(E)\,.
\end{aligned}\right\} \qquad (6.12)$$

We shall generate the transformation by means of a function ψ' of the type given by equation (2.28), that is ψ' is a function of the (new) hyperspherical-energy coordinates and the (old) conjugate momenta of momentum-energy representation, which in this case are $-x, -y, -z, -t$. We choose ψ' to have the form:

$$\psi' = f_1(\alpha,\theta,\phi,E)x + f_2(\alpha,\theta,\phi,E)y + f_3(\alpha,\theta,\phi,E)z + f_4(\alpha,\theta,\phi,E)t \qquad (6.13)$$

where the functions f_1, f_2, f_3, f_4 can be obtained by the transformation equations. Using equations (2.29) we have

$$p_x = \partial\psi'/\partial x \text{ etc.}; \quad -E = \partial\psi'/\partial t \qquad (6.14)$$

so that:

$$\Psi' = \frac{(-2\mu E)^{1/2}}{(1-\cos\alpha)}\{x\sin\alpha\sin\theta\cos\phi + y\sin\alpha\sin\theta\sin\phi + z\sin\alpha\cos\theta\} - Et. \quad (6.15)$$

Corresponding to the generalised coordinates α, θ, ϕ we can define the conjugate momenta $P_\alpha, P_\theta, P_\phi$ and conjugate to E a fourth canonical momentum τ. For convenience we shall regard $P_\alpha, P_\theta, P_\phi$ as being the coordinates of a hyperspherical momentum vector given by:

$$\underset{\sim}{P_u} = P_\alpha \underset{\sim}{\hat{\alpha}} + \frac{P_\theta \underset{\sim}{\hat{\theta}}}{\sin\alpha} + \frac{P_\phi \underset{\sim}{\hat{\phi}}}{\sin\alpha\sin\theta} \quad (6.16)$$

and τ as being the new 'time' variable. These canonical momenta are given in terms of the independent variables of the transformation by means of the other transformation equations:

$$P_\alpha = -\frac{\partial\Psi'}{\partial\alpha} \text{ etc. }; \quad \tau = -\frac{\partial\Psi'}{\partial E} \quad . \quad (6.17)$$

In particular, the new time variable is given by:

$$\tau = t - \frac{\underset{\sim}{p}\cdot\underset{\sim}{r}}{2E} = t - \frac{P_\alpha \sin\alpha}{2E} \, . \tag{6.18}$$

The values of P_α , P_θ and P_ϕ may be expressed in a similar fashion and it can be shown (Norcliffe and Percival 1968, to be referred to as II) that

$$P_u = \frac{+(-2\mu E)^{1/2}}{(1 - \cos\alpha)} \tag{6.19}$$

so that the value of the Hamiltonian is now going to be

$$H = -E\left(\frac{1 + \cos\alpha}{1 - \cos\alpha}\right) - \frac{k(-2\mu E)^{1/2}}{(1 - \cos\alpha)P_u} \, . \tag{6.20}$$

We are now equipped to set up a Hamiltonian dynamics in the extended symmetric space. We shall take as our energy equation corresponding to Ω of equation (2.48) the expression $H - E$, so that

$$\begin{aligned} \Omega &= -E\left(\frac{1 + \cos\alpha}{1 - \cos\alpha}\right) - \frac{k(-2\mu E)^{1/2}}{(1 - \cos\alpha)\,P_u} - E \\ &= \frac{-2E}{(1 - \cos\alpha)} - \frac{k(-2\mu E)^{1/2}}{(1 - \cos\alpha)\,P_u} \, . \end{aligned} \tag{6.21}$$

To parameterize the variables we shall choose the time t. We are quite at liberty to do this providing it is understood that in terms of the parameter t the variable t is given by:

$$t(\text{variable}) = f(t(\text{parameter})) = t. \tag{6.22}$$

Hamilton's equations of motion in terms of a Lagrange multiplier $\lambda(t)$ are thus

$$\left.\begin{aligned} \frac{d\alpha}{dt} &= \lambda(t)\,\frac{\partial\Omega}{\partial p_\alpha}\,, \text{ etc.} \\ \frac{dp_\alpha}{dt} &= -\lambda(t)\,\frac{\partial\Omega}{\partial\alpha}\,, \text{ etc.}\,. \end{aligned}\right\} \tag{6.23}$$

These equations will determine the properties of the classical trajectory on the surface of the cylinder. However if we now consider the value of the energy E to be fixed so that the motion is restricted to the unit hypersphere, we can obtain the path of motion on the hypersphere by means of the principle of least action. To evaluate the classical action we need to obtain the direction of the line element $d\underset{\sim}{s}$ on the hypersphere. We note that

$$\frac{d\underset{\sim}{s}}{dt} = \frac{d\alpha}{dt}\,\underset{\sim}{\hat{\alpha}} + \sin\alpha\frac{d\theta}{dt}\,\underset{\sim}{\hat{\theta}} + \sin\alpha\sin\theta\frac{d\phi}{dt}\,\underset{\sim}{\hat{\phi}} \qquad (6.24)$$

and using the first set of Hamilton's equations together with the identity:

$$P_u = \left(P_\alpha^2 + \frac{P_\theta^2}{\sin^2\alpha} + \frac{P_\phi^2}{\sin^2\alpha\sin^2\theta}\right)^{1/2} \qquad (6.25)$$

we have:

$$d\underset{\sim}{s} = \frac{\lambda(t)\,k P_E\,dt\,\underset{\sim}{P_u}}{P_u^3(1-\cos\alpha)} \quad . \qquad (6.26)$$

The line element $d\underset{\sim}{s}$ is thus in the same direction as the hyperspherical momentum vector $\underset{\sim}{P_u}$. The path on the hypersphere will be determined by the least action principle:

$$\Delta\int(P_\alpha d\alpha + P_\theta d\theta + P_\phi d\phi) = 0$$

that is:

$$\Delta\int \underset{\sim}{P_u}\cdot d\underset{\sim}{s} = 0 \quad . \qquad (6.27)$$

Since both $\underset{\sim}{ds}$ and $\underset{\sim}{p_u}$ have the same direction we consider

$$\Delta \int p_u ds = 0 . \tag{6.28}$$

Since, however, $\Omega = 0$, the magnitude of the hyperspherical momentum vector is

$$p_u = \frac{\mu k}{p_E} \tag{6.29}$$

which, for a given value of E , is constant. The least action principle thus reduces to

$$p_u \Delta \int ds = 0 \tag{6.30}$$

and the path on the hypersphere is therefore a geodesic, that is, a great circle, and the action is just the product of p_u and the path length s .

We saw by considering the motion in extended symmetric space that the new time variable was $\tau = t - p_\alpha \sin\alpha / 2E$, and we shall treat this for fixed E as the new time variable associated with the motion on the hypersphere. The second of Hamilton's equations tells us that

$$\frac{d\tau}{dt} = -\lambda(t)\frac{\partial\Omega}{\partial E} .$$

The value of $d\tau/dt$ for fixed E is then

$$\frac{d\tau}{dt} = \frac{\lambda(t)}{(1-\cos\alpha)} \tag{6.31}$$

so that the rate at which $\underset{\sim}{u}$ traces out the great circle is given by

$$\left|\frac{d\underset{\sim}{s}}{d\tau}\right| = \left|\frac{d\underset{\sim}{s}}{dt}\cdot\frac{dt}{d\tau}\right| = \left|\frac{k\rho_E\lambda(t)(1-\cos\alpha)\underset{\sim}{\rho_u}}{\rho_u^3(1-\cos\alpha)\lambda(t)}\right| \tag{6.32}$$

which is constant. This uniform motion on the hypersphere has been obtained by Györgyi (1968). The situation is very similar to that of the free particle moving on a ring, but now the path is traced out uniformly with respect to τ and not t .

Just as there was an infinite number of paths joining two points on the ring, there is also an infinite number joining two points on the hypersphere. The geodesic between two points $\underset{\sim}{u}_0$ and $\underset{\sim}{u}$ is of length ω , so the lengths $s_c(\underset{\sim}{u}, \underset{\sim}{u}_0)$ of the possible paths c between these two points are given by

$$s_c(\underset{\sim}{u}, \underset{\sim}{u}_0) = |\omega + 2\pi c| \quad c = 0, \pm 1, \pm 2, \ldots \qquad (6.33)$$

and the corresponding action functions are just

$$S_{cE}(\underset{\sim}{u}, \underset{\sim}{u}_0) = \frac{\mu k}{p_E}|\omega + 2\pi c| \quad . \qquad (6.34)$$

Since we need the value of the action function in momentum representation it should be noted that the contact transformation relating momentum and symmetric representation is a coordinate transformation: the coordinates of momentum and symmetric representation are related by equations which do not involve the conjugate momenta (see equation (6.12) for constant energy E). The value of the classical action is consequently the same in either representation as was mentioned in chapter 2. Thus if $\underset{\sim}{u}_0$ and $\underset{\sim}{u}$ in symmetric representation correspond to $\underset{\sim}{p}_0$ and $\underset{\sim}{p}$ in momentum representation, then

$$\begin{aligned} S_{cE}(\underset{\sim}{u}, \underset{\sim}{u}_0) &= S_{cE}(\underset{\sim}{p}, \underset{\sim}{p}_0) \\ &= \frac{\mu k|\omega + 2\pi c|}{p_E} \qquad (6.35) \end{aligned}$$

where now, in terms of momenta

$$\omega = \cos^{-1}\left\{\frac{4p_E^2\, \underset{\sim}{p}\cdot\underset{\sim}{p}_0 + (p^2-p_E^2)(p_0^2-p_E^2)}{(p^2+p_E^2)(p_0^2+p_E^2)}\right\} . \qquad (6.36)$$

5) The Quantum-Mechanical Theory

To evaluate the spectral operator kernel in momentum representation we shall again consider the problem first of all in the symmetric representation. The quantum-mechanical Coulomb problem has been considered in this representation by Schwinger (1964), Bander and Itzykson (1966a), Fock (1935) and Kurşunoğlu (1962). Schwinger makes use of this representation to obtain the Coulomb Green functions in momentum representation. The other authors are concerned mainly with the group theoretical aspects of the Coulomb problem and show that the Schrödinger equation in symmetric representation is none other than the integral equation for the spherical harmonics of four-dimensional potential theory. We shall use the symmetric representation to provide an expression for the kernel of the spectral operator which is expressible directly in terms of classical path sums.

In chapter 3 we saw that different representative spaces in quantum mechanics were in general related by unitary transformations. This is true of position and momentum representations, but unfortunately momentum and symmetric representations cannot be related by a unitary transformation. This does not mean that we cannot formulate the problem in symmetric representation, it just means that properties of operators and kernels which hold in one space need not necessarily hold in the other.

We shall label wave functions by the energy E which has a negative value, but which need not be an energy level of the hydrogen atom, and we shall represent the transformation from momentum to symmetric representation by $\mathcal{S}$. Any momentum wave function $\psi(\underset{\sim}{p},E)$ will be related to the wave function $\psi_s(\underset{\sim}{u},E)$ of symmetric representation by

$$\psi_s(\underset{\sim}{u},E) = \mathcal{S}\,\psi(\underset{\sim}{p},E)$$

$$= \frac{\pi}{\sqrt{8}}\, p_E^{-\frac{5}{2}} \left(p_E^2 + p^2\right)^2 \psi(\underset{\sim}{p},E) \,. \qquad (6.37)$$

The factor in equation (6.37) is chosen so that if $\psi(\underset{\sim}{p},E)$ is a normalised solution of the Coulomb

Schrödinger equation in momentum space belonging to the energy E, then $\psi_s(\underset{\sim}{u}, E)$ will also be normalised:

$$\begin{aligned}\int \frac{d\Omega}{2\pi^2} |\psi_s(\underset{\sim}{u}, E)|^2 &= \int d^3p \, \frac{p_E^2 + p^2}{2p_E^2} |\psi(\underset{\sim}{p}, E)|^2 \\ &= \int d^3p \, |\psi(\underset{\sim}{p}, E)|^2 \\ &= 1 \quad . \end{aligned} \tag{6.38}$$

This result depends on the fact that the mean value of the quantity p^2 is p_E^2.

Now that we know how the wave functions are related, we can obtain the relation between operator kernels in the two representations. If $L(\underset{\sim}{p}, \underset{\sim}{p}_0)$ is the kernel of an integral operator L in momentum representation, and $L(\underset{\sim}{u}, \underset{\sim}{u}_0)$ is the kernel in symmetric representation, we have

$$\int \frac{d\Omega_0}{2\pi^2} L(\underset{\sim}{u}, \underset{\sim}{u}_0) \psi_s(\underset{\sim}{u}_0, E) = \mathcal{S} \int d^3p_0 \, L(\underset{\sim}{p}, \underset{\sim}{p}_0) \psi(\underset{\sim}{p}_0, E)$$

$$= \int \frac{d\Omega_0}{2\pi^2} \frac{(p_E^2 + p^2)^2 (p_E^2 + p_0^2) \, 2\pi^2}{8 p_E^3} L(\underset{\sim}{p}, \underset{\sim}{p}_0) \psi_s(\underset{\sim}{u}_0, E) \tag{6.39}$$

so that the two kernels are related by:

$$L(\underset{\sim}{u},\underset{\sim}{u}_0) = 2\pi^2\frac{(p_E^2+p^2)^2(p_E^2+p_0^2)}{8p_E^3}L(\underset{\sim}{p},\underset{\sim}{p}_0) \quad . \qquad (6.40)$$

The kernel of the spectral operator can now be obtained by deriving Schrödinger's equation in symmetric representation. In momentum space Schrödinger's equation has the form of the integral equation (Kurşunoğlu, 1962, p. 364):

$$\frac{p^2}{2\mu}\psi(\underset{\sim}{p},E) - \frac{k}{2\pi^2\hbar}\int\frac{d^3p_0\,\psi(\underset{\sim}{p}_0,E)}{|\underset{\sim}{p}-\underset{\sim}{p}_0|^2} = E\psi(\underset{\sim}{p},E) \quad . \qquad (6.41)$$

Thus, if H is the Hamiltonian of the hydrogen atom then

$$(E-H)\psi(\underset{\sim}{p},E) = \left(E-\frac{p^2}{2\mu}\right)\psi(\underset{\sim}{p},E) + \frac{k}{2\pi^2\hbar}\int\frac{d^3p_0\,\psi(\underset{\sim}{p}_0,E)}{|\underset{\sim}{p}-\underset{\sim}{p}_0|^2} \quad . \qquad (6.42)$$

The form of this equation in symmetric representation can be obtained via equations (6.3), (6.7) and (6.9) and is:

$$(E-H)\psi_s(\underset{\sim}{u},E) = \left(E-\frac{p^2}{2\mu}\right)(I-\nu Q)\psi_s(\underset{\sim}{u},E) \qquad (6.43)$$

where:

$$\nu = \frac{k\mu}{p_E \hbar} \quad ; \quad Q\psi_s(\underset{\sim}{u},E) = \int \frac{d\Omega_0}{2\pi^2} \frac{\psi_s(\underset{\sim}{u}_0, E)}{|\underset{\sim}{u} - \underset{\sim}{u}_0|^2} . \qquad (6.44)$$

The equation

$$(I - \nu Q)\psi_s(\underset{\sim}{u},E) = 0 \qquad (6.45)$$

is what is referred to by Fock and Kurşunoğlu as Schrödinger's equation in symmetric representation, and for positive integer values $\nu = n$ it is satisfied by the hyperspherical harmonics of order n, so that

$$Q\psi_{nlm}(\underset{\sim}{u}) = n^{-1}\psi_{nlm}(\underset{\sim}{u}) . \qquad (6.46)$$

These functions form a complete and orthonormal set on the sphere. The functions in momentum space corresponding to these harmonics also form a complete set, but are no longer orthogonal.

The operator equation corresponding to equation (6.43) is

$$(E - H) = \left(E - \frac{p^2}{2\mu}\right)(I - \nu Q) . \qquad (6.47)$$

and assuming we can construct generalised functions of both sides of this equation, we have in particular

$$\delta(E-H) = \delta\left(\left(E-\frac{p^2}{2\mu}\right)(I-\nu Q)\right). \qquad (6.48)$$

Since $\left(E-\frac{p^2}{2\mu}\right)$ is never zero for $E<0$, it can be shown (appendix C) that

$$\delta(E-H) = -\delta(I-\nu Q)\left(E-\frac{p^2}{2\mu}\right)^{-1}. \qquad (6.49)$$

The spectral operator is thus given by

$$I_E = J_\nu\left(E-\frac{p^2}{2\mu}\right)^{-1} \qquad (6.50)$$

where:

$$J_\nu = -\delta(I-\nu Q). \qquad (6.51)$$

J_ν plays the analogous role in symmetric representation as does the spectral operator I_E in momentum representation. It should be noted that although the operator

I_E has a symmetric kernel in momentum representation, it is J_ν and not I_E which has a symmetric kernel in symmetric space. Again this is due to the fact that the two representations are connected by a transformation which is not unitary.

In terms of the projection operators onto the levels $\nu = n$ in symmetric space we can express the operator J_ν as (see equation (3.11):

$$J_\nu = -\sum_{n=1}^{\infty} P_n \delta(I - \nu/n)$$

$$= -\sum_{n=1}^{\infty} n P_n \delta(n-\nu) . \qquad (6.52)$$

The kernel of the projection operator P_n can be obtained directly from the spherical harmonic addition theorem (Fock 1935):

$$P_n(\underset{\sim}{u}, \underset{\sim}{u_0}) = \sum_{l=0}^{n-1} \sum_{m=-l}^{l} \psi_{nlm}(\underset{\sim}{u}) \psi_{nlm}^*(\underset{\sim}{u_0})$$

$$= \frac{n \sin n\omega}{\sin \omega} \qquad (6.53)$$

where ω is the hyperspherical variable discussed previously, and the kernel of J_ν is thus

$$J_\nu(\underset{\sim}{u}, \underset{\sim}{u}_0) = -\sum_{n=1}^{\infty} n^2 \frac{\sin n\omega}{\sin\omega}\,\delta(n-\nu)$$

$$= -\sum_{n=-\infty}^{\infty} \varepsilon(\nu)\,\nu^2 \frac{\sin \nu\omega}{\sin\omega}\,\delta(\nu-n). \qquad (6.54)$$

This expression involves directly a sum over quantum states and as we have seen in chapter 5 for the particle on a ring the expansion in terms of quantum states bears little resemblance to the same expression involving sums over classical paths. An alternative expansion of equation (6.54) can be obtained by expressing the infinite sum of delta functions in terms of trigonometric functions as given in Lighthill (1960), p. 68. The kernel of J_ν can now be written as

$$J_\nu(\underset{\sim}{u}, \underset{\sim}{u}_0) = \frac{\varepsilon(\nu)\,\nu^2}{\sin\omega} \sum_{c=-\infty}^{\infty} \sin\{\nu(2\pi c-\omega)\} \qquad (6.55)$$

and as we shall see it is this expansion which is readily expressible in terms of sums over classical paths. The corresponding spectral operator kernel in momentum representation can now be obtained from this equation together with equation (6.50) and (6.40), and we have

$$I_E(\underset{\sim}{p}, \underset{\sim}{p}_0) = \frac{-8\mu^3 p_E k^2}{\pi^2 \hbar^2 (p^2+p_E^2)^2 (p_0^2+p_E^2)^2} \sum_{c=-\infty}^{\infty} \frac{\sin\{\nu(2\pi c-\omega)\}}{\sin\omega} \qquad (6.56)$$

where ω is given in terms of the momenta by equation (6.36).

6) A Compete Correspondence Identity

To provide a complete correspondence identity we shall now relate the kernel of J_ν as given by equation (6.55) to the classical action functions $S_{cE}(\underset{\sim}{u}, \underset{\sim}{u}_0)$ and the classical path lengths $s_c(\underset{\sim}{u}, \underset{\sim}{u}_0)$ of symmetric representation. We have explicitly:

$$J_\nu(\underset{\sim}{u}, \underset{\sim}{u}_0) = -\varepsilon(\nu)\nu^2 \sum_{c=-\infty}^{\infty} \frac{\sin\{S_{cE}(\underset{\sim}{u}, \underset{\sim}{u}_0)/\hbar\}}{\sin\{s_c(\underset{\sim}{u}, \underset{\sim}{u}_0)\}} \; . \qquad (6.57)$$

This expansion in terms of classical paths is an alternative expression for the kernel of J_ν as given in equation (6.54) which involves explicitly sums over quantum states.

As in the phase-integral approximation (see Gutzwiller 1967), the singularities of the expression $\sin\{s_c(\underset{\sim}{u}, \underset{\sim}{u}_0)\}$ give the focal points along the classical trajectory on the hypersphere. The zeros of $\sin\{s_c(\underset{\sim}{u}, \underset{\sim}{u}_0)\}$ occur when

$$s_c(\underset{\sim}{u}, \underset{\sim}{u}_0) = 0, \pi, 2\pi, \ldots \text{ etc.} \qquad (6.58)$$

That is when ω is 0 or π. The focal points thus occur at $\underset{\sim}{u}_0$, or its antipodal point. This is not surprising, since all paths leaving $\underset{\sim}{u}_0$ pass through the antipodal point and return to $\underset{\sim}{u}_0$.

Corresponding to the complete correspondence identity in symmetric representation, we also have a complete correspondence identity for the kernel of the spectral operator I_E in momentum representation. Since the values of the classical action in both momentum and symmetric representation are the same, then the spectral operator kernel of equation (6.56) may be expressed in terms of classical path sums as follows:

$$I_E(\underset{\sim}{p}, \underset{\sim}{p}_0) = \frac{8\mu^3 p_E k^2}{\pi^2 \hbar^2 (p^2+p_E^2)^2 (p_0^2+p_E^2)^2} \sum_{c=-\infty}^{\infty} \frac{\sin\{S_{cE}(\underset{\sim}{p}, \underset{\sim}{p}_0)/\hbar\}}{\sin|\omega + 2\pi c|} \, . \qquad (6.59)$$

Now, the term $\sin|\omega + 2\pi c|$ has no direct interpretation in momentum space. However if we expand $\sin\omega$ in terms of momenta $\underset{\sim}{p}, \underset{\sim}{p_0}$ and energy E, we may write equation (6.59) in the form:

$$I_E(\underset{\sim}{p},\underset{\sim}{p_0}) = \sum_{c=-\infty}^{\infty} \rho_{cE}(\underset{\sim}{p},\underset{\sim}{p_0})^{1/2} \frac{\sin\{S_{cE}(\underset{\sim}{p},\underset{\sim}{p_0})/\hbar\}}{\hbar^2} \qquad (6.60)$$

where

$$\rho_{cE}(\underset{\sim}{p},\underset{\sim}{p_0}) = \frac{16\mu^6 k^4}{\pi^4(p^2-2\mu E)^2(p_0^2-2\mu E)^2|\underset{\sim}{p}-\underset{\sim}{p_0}|^2(4\mu^2E^2+p^2p_0^2-4\mu E\,\underset{\sim}{p}\cdot\underset{\sim}{p_0})} \cdot \qquad (6.61)$$

In this form we can relate the density factor $\rho_{cE}(\underset{\sim}{p},\underset{\sim}{p_0})$ to the equivalent term obtained in the phase-integral approximation. It is in fact identical to the result obtained by Gutzwiller apart from a mass factor in the numerator of (6.61), which must be an error on Gutzwiller's part since the spectral operator kernel (6.60) has the correct dimensions of (energy)$^{-1}$ (momentum)$^{-3}$. The density becomes infinite now if $\underset{\sim}{p} = \underset{\sim}{p_0}$ (corresponding to $\underset{\sim}{u} = \underset{\sim}{u_0}$) or if $pp_0 = p_E^2$; $\hat{\underset{\sim}{p}}\cdot\hat{\underset{\sim}{p_0}} = -1$ (corresponding to the antipodal point of $\underset{\sim}{u_0}$). The sign of the square root of

$\rho_{cE}(\underset{\sim}{p}, \underset{\sim}{p}_0)$, which is given naturally by the sign of the expression $\sin|\omega + 2\pi c|$, can be determined by the focal points. If the path C from $\underset{\sim}{p}_0$ to $\underset{\sim}{p}$, passes the focal points in total an even number of times, then the sign associated with $\rho_{cE}(\underset{\sim}{p}, \underset{\sim}{p}_0)^{1/2}$ is positive. If the total number of times is odd, then the corresponding sign is negative.

The complete correspondence identity that we have obtained in momentum representation together with Gutzwiller's result for the density function $\rho_{cE}(\underset{\sim}{p}, \underset{\sim}{p}_0)$ suggests that the phase-integral method formulated in momentum representation for the spectral operator, and not the Green operators, will lead to a result which will be correct.

7) The Bohr-Sommerfeld Identity

Having obtained a complete correspondence identity in both symmetric and momentum representation for the kernels of J_ν and I_E respectively we are now able to explain the two correspondence identities associated with the bound states of the hydrogen atom. The Bohr-Sommerfeld identity follows at once:

From equation (6.54) we see that contributions to the kernel of J_ν only arise from positive integer values of ν . These correspond to the bound states and ν is the principal quantum number n . Since the kernel of J_ν in equation (6.57) is expressible exactly in terms of the classical action functions it follows by comparison with equation (6.54) that contributions only arise from those classical paths for which the energy is a bound state energy level. The value of the action for one complete orbit in these cases is going to be $2\pi n\hbar$. This value is independent of the representation and the value of the action for one orbit in position space is also $2\pi n\hbar$. This is how the Bohr-Sommerfeld identity arises, and indeed those orbits for which the total action is $2\pi n\hbar$ do have energy E_n given by

$$E_n = -\frac{k^2\mu}{2n^2\hbar^2} \qquad (6.62)$$

8) The Fock Identity

The Fock identity follows from dynamical symmetry. The kernel of J_ν in symmetric representation as given by equation (6.54) is invariant with respect to rotations on the hypersphere, and so is the kernel of the projection operator $\mathcal{P}_n$ of equation (6.53). It follows that the value of $\mathcal{P}_n(\underset{\sim}{u},\underset{\sim}{u})$ is thus constant over the hypersphere so that:

$$\sum_{l=0}^{n-1}\sum_{m=-l}^{l}\psi_{nlm}(\underset{\sim}{u})\,\psi^{*}_{nlm}(\underset{\sim}{u}) = \text{constant}\,. \tag{6.63}$$

In this sum each of the n^2 states corresponding to the different l and m occur with the same weighting or probability and the distribution in $\underset{\sim}{u}$ over the hypersphere is the quantal microcanonical distribution for the level $\nu = n$ (see Landau and Lifshitz 1958).

Because the kernel $J_\nu(\underset{\sim}{u},\underset{\sim}{u}_0)$ is expressible in terms of the classical action functions as given in equation (6.57), the classical action functions are thus also invariant with respect to rotations on the hypersphere. They are solutions of the Hamilton-Jacobi equation:

$$p_u = \left\{\left(\frac{\partial S}{\partial \alpha}\right)^2 + \left(\frac{\partial S}{\partial \theta}\right)^2\frac{1}{\sin^2\alpha} + \left(\frac{\partial S}{\partial \phi}\right)^2\frac{1}{\sin^2\alpha\,\sin^2\theta}\right\}^{1/2} = \frac{k\mu}{p_E} \tag{6.64}$$

which is also invariant with respect to rotations. The classical microcanonical distribution function corresponding to the quantum-mechanical operator $\mathcal{J}_y$, namely $\delta\left(\frac{k\mu}{p_E p_u} - 1\right)$ is consequently independent of $\underset{\sim}{u}$ and the distribution in $\underset{\sim}{u}$ for all negative values of the energy E is uniform.

Thus, for all values of E equal to E_n, the classical and quantal microcanonical distributions in $\underset{\sim}{u}$ (suitably normalised) will be equal. This is the origin of the Fock identity: from the properties of the transformation relating momentum and symmetric spaces, it then follows that the classical and quantal microcanonical distributions in $\underset{\sim}{p}$ are also equal. Now, of course, the distributions are no longer uniform but are given by

$$\rho(\underset{\sim}{p}) = \frac{8 p_E^5}{\pi^2 (p^2 + p_E^2)^4}, \quad E = E_n . \tag{6.65}$$

We have thus explained the two correspondence identities associated with the bound states of the hydrogen atom. The third identity, the Rutherford scattering identity, will be considered in the following chapters.

CHAPTER 7

THE CLASSICAL THEORY OF THE H-ATOM FOR POSITIVE ENERGIES AND RUTHERFORD SCATTERING

1) Introduction

The scattering of an electron by a fixed proton corresponds to the positive energy states of the hydrogen atom. The angular differential cross sections for this type of scattering as predicted by the theories of classical and quantum mechanics are identical, and this is the well known Rutherford scattering identity. The success of certain classical theories of scattering, where the collision of two particles is the dominating process, has been attributed to this identity (see, for example, Burgess and Percival, 1968). The Rutherford scattering identity is the third and final correspondence identity to be considered in this thesis and we shall show that it follows from a complete correspondence identity, whereby the non-relativistic quantum dynamics of the system is obtained from the solution of the corresponding classical problem.

In constrast to the bound states, we find that the classical theory is complicated by the need to consider not only classical trajectories, but also generalised classical trajectories. These generalised classical trajectories are the analytic continuation in energy of the classical paths of the bound state problem and are needed for the derivation of the complete correspondence identity. As we shall see, they are built up out of the paths which occur in the Rutherford scattering of both electrons and positrons by a fixed proton.

Since the complete correspondence identity involves these generalised classical paths (Norcliffe, Percival and Roberts 1969, to be referred to as III and IV), and since the quantal theory is also more complicated than for the bound states, the derivation of the complete correspondence identity, and the explanation of the Rutherford scattering identity has been left until the next chapter. In this chapter we will be concerned solely with the relevant classical theory.

2) Choice of Representation

We shall again obtain a complete correspondence identity through the kernel of the quantum-mechanical spectral operator. For the bound states one reason for choosing to work in momentum representation was the fact that a large region of position space was classically inaccessible to a particle of given negative energy E . For the positive energy states the reverse is true and a part of momentum space is now classically inaccessible as described in section 4. At first sight position representation would seem the obvious choice in which to obtain a complete correspondence identity. Nevertheless we still find that momentum representation as opposed to position representation is more convenient for this purpose.

Once again there is a symmetric representation for which the classical- and quantum-mechanical equations of motion remain invariant with respect to rotations in four dimensions. The symmetry group to which these rotations belong is now no longer the group $O(4)$ but the group of rotations $O(1,3)$. The treatment of both the classical- and quantum-mechanical problem in momentum representation is made easier by considering the problem in this symmetric representation and the classical theory will be given in section 4.

3) Classical and Generalised Classical Trajectories

Consider a particle of mass μ and positive energy $E = p_E^2/2\mu$ moving in an attractive Coulomb potential

$$V(\underset{\sim}{r}) = -k/r = -Ze^2/r \quad ; \quad k > 0 . \qquad (7.1)$$

The trajectory in position space is well known and is one branch of a hyperbola which has one focus at the origin. The momentum-space trajectory, or hodograph, is an arc of a circle whose radius is $p_E(\varepsilon^2-1)^{-1/2} = k\mu/bp_E$, and whose centre is at a distance $\varepsilon p_E(\varepsilon^2-1)^{-1/2}$ from the origin. The eccentricity of the orbit is ε and b is the impact parameter. The tangents to the circular hodograph at the extremities of the arc intersect at the origin at an angle Θ which is the scattering angle, as shown in Figure 7.1. The remaining arc of the circle is the hodograph of a particle having the same energy moving under the influence of a repulsive Coulomb potential $V(\underset{\sim}{r}) = k/r$. In position space this corresponds to a trajectory which is just the other branch of the same hyperbola, and would be the trajectory of a positron scattered by a fixed proton when the potential is e^2/r.

For attractive Coulomb scattering, as we have mentioned, the whole of position space is accessible to a particle of positive energy E, since between any two points there is always a classical trajectory. For

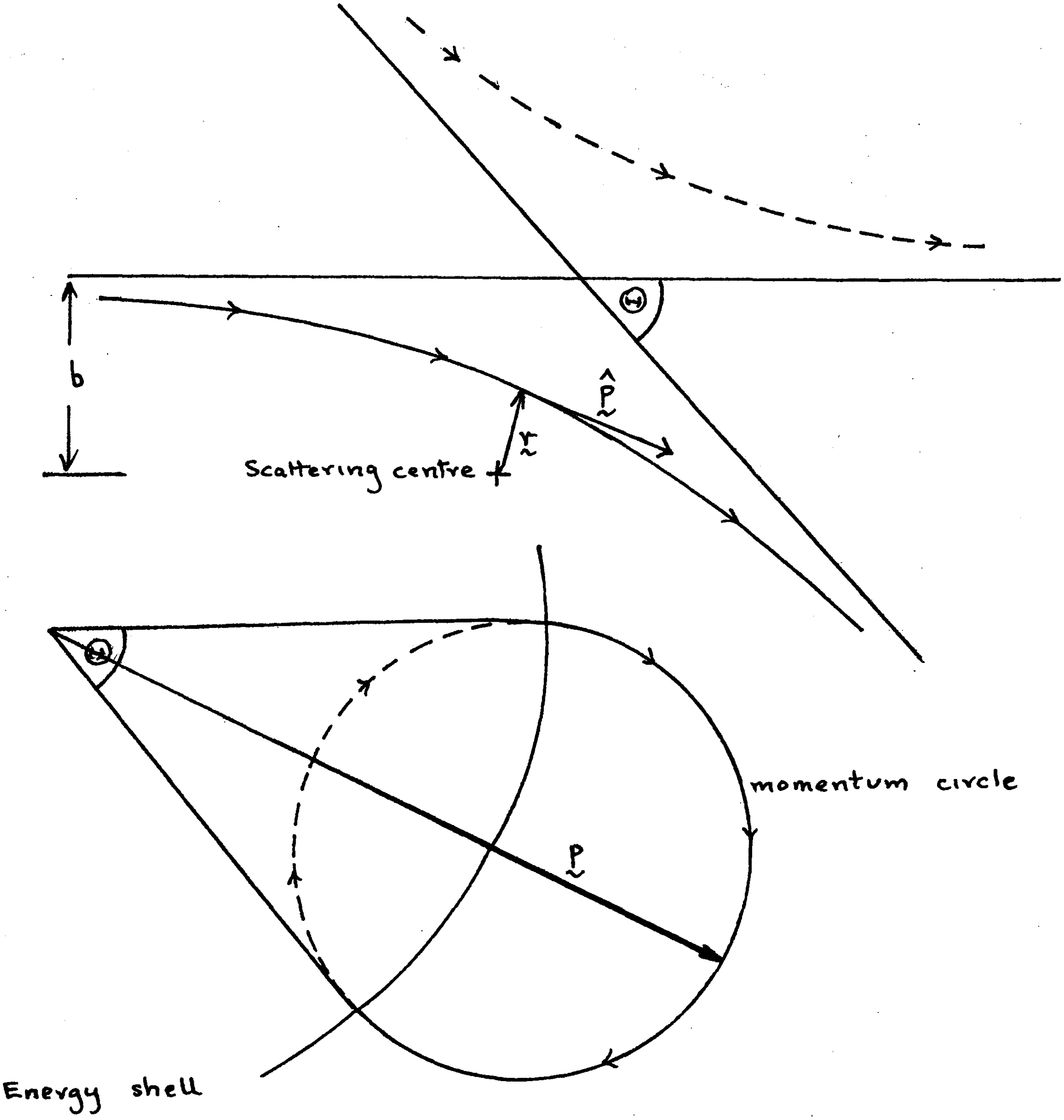

Figure 7.1. The hyperbolic trajectory in position space and the circular hodograph. The continuous curves are the trajectories for the attractive Coulomb potential and the dotted for the repulsive.

repulsive scattering this is not the case and a small part of position space is classically inaccessible to a particle having the same positive energy E. However in momentum space large regions are classically inaccessible in both types of scattering. As can be seen in Figure 7.1 the two regions $|\underset{\sim}{p}| \geqslant p_E$ and $|\underset{\sim}{p}| \leqslant p_E$ are inaccessible to a particle moving in a repulsive and an attractive Coulomb potential respectively. Consequently there is no classical trajectory in the normal sense joining two momenta $\underset{\sim}{p}_0$, $\underset{\sim}{p}$ when, for example, $|\underset{\sim}{p}| < p_E$ and $|\underset{\sim}{p}_0| > p_E$.

The two momenta, nevertheless, are joined by the arc of the complete momentum circle (see Figure 7.2) and we can regard this arc as a generalised classical trajectory leading from $\underset{\sim}{p}_0$ to $\underset{\sim}{p}$. The generalised classical path PFQ of Figure 7.2 is only one of an infinite number of generalised classical paths all leading from P to Q . For example any path from P through F or E to Q , having passed around the complete momentum circle c times, is also another such path.

It is through these generalised classical paths and the properties of the action functions evaluated along them that we are able to obtain a complete

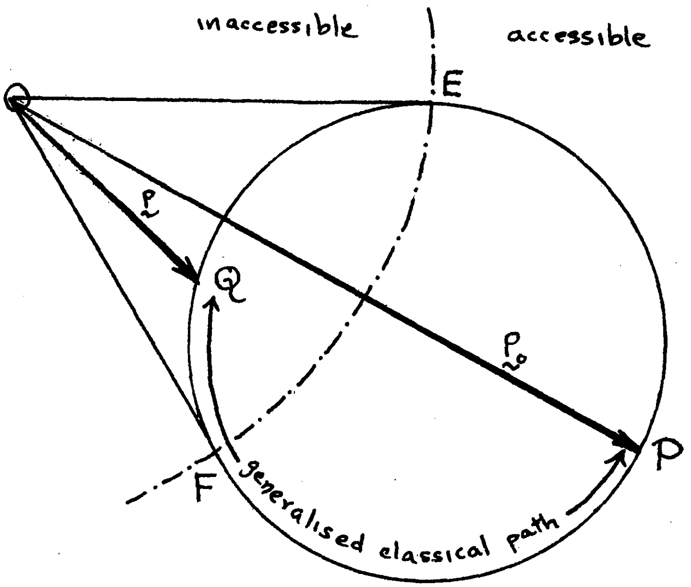

Figure 7.2. The arc PFQ joining $\underset{\sim}{p}_0$ and $\underset{\sim}{p}$ can be regarded as a generalised classical path leading from P to Q for attractive Coulomb scattering.

correspondence identity. The spectral operator kernel for the bound states is expressed as a sum over all paths in momentum representation which run between $\underset{\sim}{p}_0$ and $\underset{\sim}{p}$ (see equation 6.59) and it is obvious that the generalised classical paths are just the analogue of these paths. One would thus expect the spectral operator kernel for positive energies to include a sum over all the generalised classical paths; but this is not the case, and it turns out that we only take a subset of these paths. The number of paths in this subset is still infinite, however, but the reason for the particular choice of paths is a subtle one which depends on the relative positions of $\underset{\sim}{p}$ and $\underset{\sim}{p}_0$ and will be discussed in the next chapter.

Before the value of the action function along a generalised classical path is obtained, we shall evaluate the action between two points in the accessible region. The action along a generalised classical path is then obtained by analytic continuation. From canonical transformation theory the energy-dependent action function of momentum space is given by

$$S_E(\underset{\sim}{p}, \underset{\sim}{p}_0) = -\int_{\underset{\sim}{p}_0}^{\underset{\sim}{p}} \underset{\sim}{r} \cdot d\underset{\sim}{p}' \tag{7.2}$$

and this can be evaluated directly by using the parameterization by means of the eccentric anomaly as given in Landau and Lifshitz (1960). We shall obtain the value of the action by considering the classical theory of attractive Coulomb scattering in the symmetric representation.

4) The Symmetric Representation

The symmetric representation appropriate to the electron-proton system for positive energies has been discussed in the literature by Bander and Itzykson (1966b) and others (see for example III). Let u_λ $(\lambda = 0, 1, 2, 3)$ denote a position vector in the four-dimensional Minkowski space with a metric whose signature is $(1, -1, -1, -1)$. The surface $\mathcal{S}$ of a unit sphere in this space has the equation

$$u_\lambda u^\lambda = u_0^2 - u_1^2 - u_2^2 - u_3^2 = 1 \qquad (7.3)$$

and consists of two sheets $\mathcal{S}^+$ and $\mathcal{S}^-$ **defined** by $u_0 \geqslant 1$ and $u_0 \leqslant -1$ respectively. In four-dimensional Euclidean space $\mathcal{S}$ is just the surface of a rectangular hyperboloid. A point u_λ on $\mathcal{S}$ is associated with a point $\underset{\sim}{p}$ in momentum space by projecting the scaled momentum 4-vector $(0, \underset{\sim}{p}/p_E)$ from the the point $(-1, 0, 0, 0)$ on $\mathcal{S}^-$ onto the surface $\mathcal{S}$. For the time being we shall regard p_E **as a fixed parameter so that** the transformation between momentum and symmetric spaces is not explicitly energy dependent. Two examples of the projection are shown in Figure 7.3 in 3 dimensions for simplicity. Explicitly

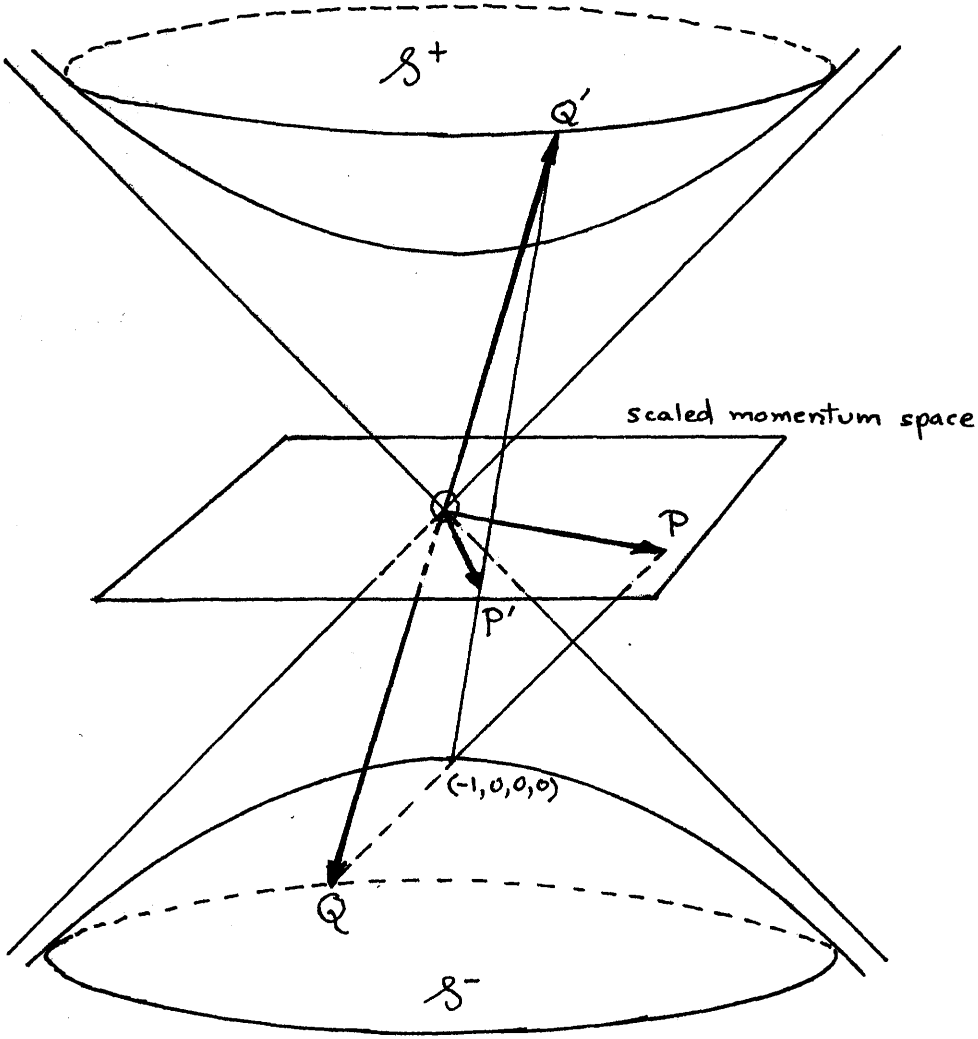

Figure 7.3. The stereographic projection. The points P and P′ in the scaled momentum space project onto the points Q and Q′ on the surface of the hyperboloid.

we have:

$$
\begin{aligned}
u_\lambda &= \left(\cosh\alpha,\ \sinh\alpha\cdot\hat{\underset{\sim}{p}}\right), \text{ where } \tanh\tfrac{1}{2}\alpha = p/p_E \\
&\qquad |\underset{\sim}{p}| \leqslant p_E \\
u_\lambda &= -\left(\cosh\alpha,\ \sinh\alpha\cdot\hat{\underset{\sim}{p}}\right), \text{ where } \tanh\tfrac{1}{2}\alpha = p_E/p \\
&\qquad |\underset{\sim}{p}| \geqslant p_E\,.
\end{aligned}
\tag{7.4}
$$

All points in the region of momentum space for which $|\underset{\sim}{p}| \geqslant p_E$ are projected on $\mathcal{S}^-$ and all those in the region $|\underset{\sim}{p}| \leqslant p_E$ onto $\mathcal{S}^+$. When we come to consider the Coulomb problem for positive values of the energy E, the transformation between the two spaces becomes energy dependent since p_E is now related to the energy by $p_E^2 = 2\mu E$. $\mathcal{S}^-$ and $\mathcal{S}^+$ are then respectively the classically accessible regions of the attractive and repulsive Coulomb potentials in the symmetric representation.

Considering, then, a particle moving in the influence of an attractive Coulomb potential we see that the motion is confined to $\mathcal{S}^-$. Since the transformation **is** energy dependent the full properties of the motion can only be obtained by considering the energy E and time t as further variables. So, as for the bound states, we shall regard $-E$ as the new coordinate in momentum space and $-t$ as its new conjugate momentum. In symmetric space the energy E is taken as the new coordinate. Motion in the four-dimensional momentum-energy space will correspond to motion on the surface of a cylinder whose cross section is the surface $\mathcal{S}^-$ of the Minkowski space (see for comparison Figure 6.3).

The two spaces can be related by means of a contact transformation generated by the function

$$\psi'(\alpha,\theta,\phi,E,x,y,z,t) = p_E \coth{}^1\!/\!_2\alpha\,(x\sin\theta\cos\phi + y\sin\theta\sin\phi + z\cos\theta) - Et. \quad (7.5)$$

We can define the generalised momenta of the extended symmetric space by the usual transformation equations:

$$\left.\begin{aligned} P_\alpha &= -\partial\psi'/\partial\alpha\text{, etc. for } P_\theta, P_\phi \\ \tau &= -\partial\psi'/\partial E\,. \end{aligned}\right\} \quad (7.6)$$

In particular τ, which may be thought of as the new time variable, is given by

$$\tau = t - \underset{\sim}{r}\cdot\underset{\sim}{p}/2E \quad (7.7)$$

and P_α, P_θ, P_ϕ satisfy the relation

$$r = 2\sinh^2 \tfrac{1}{2}\alpha . \Pi / P_E \qquad (7.8)$$

where:

$$\Pi = \left(P_\alpha^2 + P_\theta^2/\sinh^2\alpha + P_\phi^2/\sinh^2\alpha \sin^2\theta\right)^{1/2}. \qquad (7.9)$$

The value of the classical Hamiltonian is now given by

$$H = \frac{p^2}{2\mu} - \frac{k}{r} = \frac{P_E^2 \coth^2 \frac{1}{2}\alpha}{2\mu} - \frac{k P_E \operatorname{cosech}^2 \frac{1}{2}\alpha}{2\Pi} \qquad (7.10)$$

and to formulate a Hamiltonian dynamics in the extended symmetric space we construct the following energy equation:

$$\Omega = H - E$$

$$= \frac{P_E^2 \operatorname{cosech}^2 \frac{1}{2}\alpha}{2\mu} - \frac{k P_E \operatorname{cosech}^2 \frac{1}{2}\alpha}{2\Pi} . \qquad (7.11)$$

As for the bound states we parameterize the variables by the time t and obtain Hamilton's equations of motion in terms of a Lagrange multiplier:

$$\left.\begin{aligned} \frac{d\alpha}{dt} &= \lambda(t)\,\frac{\partial\Omega}{\partial p_\alpha}\,,\ \text{etc.}, \\ \frac{dp_\alpha}{dt} &= -\lambda(t)\,\frac{\partial\Omega}{\partial\alpha}\,,\ \text{etc.} \end{aligned}\right\} \qquad (7.12)$$

These equations will determine the properties of the classical trajectory on the surface of the cylinder. However for a fixed value of the energy, when the motion is restricted to $\mathcal{S}^-$ we can obtain the trajectory by means of the principle of least action. The element of distance along a path in $\mathcal{S}^-$ is given by

$$du_\lambda = d\alpha\,\hat{\alpha}_\lambda + \sinh\alpha\, d\theta\,\hat{\theta}_\lambda + \sinh\alpha \sin\theta\, d\phi\,\hat{\phi}_\lambda \qquad (7.13)$$

where $\hat{\alpha}_\lambda$, $\hat{\theta}_\lambda$, $\hat{\phi}_\lambda$ are mutually orthonormal vectors in the Minkowski space. By means of Hamilton's equations (7.12) the invariant distance s along the path is given by

$$\frac{ds}{dt} = \left(-\frac{du_\lambda}{dt}\frac{du^\lambda}{dt}\right)^{1/2} = \frac{\lambda(t)\, k\, p_E \operatorname{cosech}^2 \frac{1}{2}\alpha}{2\pi}\,. \qquad (7.14)$$

For fixed values of the energy, the condition $\Omega = 0$ implies that

$$\Pi = \text{constant} = k\mu / p_E \tag{7.15}$$

and a four-vector Π_λ can be defined by

$$\Pi_\lambda = \Pi \frac{du_\lambda}{ds} = P_\alpha \hat{\alpha}_\lambda + \frac{P_\theta \hat{\theta}_\lambda}{\sinh\alpha} + \frac{P_\phi \hat{\phi}_\lambda}{\sinh\alpha \sin\theta} \,. \tag{7.16}$$

This is consistent with the definition of Π, since

$$\Pi^2 = -\Pi_\lambda \Pi^\lambda \,. \tag{7.17}$$

The value of the classical energy-dependent action evaluated between two points $u_\lambda^{(0)}$, u_λ is given by

$$S_E(u_\lambda, u_\lambda^{(0)}) = \int_{\alpha_0,\theta_0,\phi_0}^{\alpha,\theta,\phi} P_{\alpha'} d\alpha' + P_{\theta'} d\theta' + P_{\phi'} d\phi' \tag{7.18}$$

$$= \int_{s_0}^{s} -\Pi^\lambda \frac{du_\lambda}{ds'} ds'$$

$$= \Pi \int_{s_0}^{s} ds' \,. \tag{7.19}$$

The principle of stationary action

$$\Pi \Delta \int_{s_0}^{s} ds' = 0 \tag{7.20}$$

implies that the trajectories on $\mathcal{S}^-$ are thus geodesics and in this case they are the curves in which planes through the origin intersect $\mathcal{S}^-$. In a Euclidean sense they are rectangular hyperbolae, and are analogous to the great circles on the unit hypersphere in the case of the bound states. If β is the Minkowski distance along a geodesic between $u^{(0)}_{\lambda}$ and u_{λ} on $\mathcal{S}^-$ then

$$\cosh\beta = u^{(0)}_{\lambda} u^{\lambda} = 1 + \frac{E|\underset{\sim}{p} - \underset{\sim}{p}_0|^2}{\mu(T_0 - E)(T - E)} \tag{7.21}$$

where the kinetic energies T and T_0 are

$$T = p^2/2\mu \ , \quad T_0 = p_0^2/2\mu \ . \tag{7.22}$$

β is thus the hyperbolic angle between the two points on $\mathcal{S}^-$ and is given by the analytic continuation, as we shall see in the next section, of the angle ω of equation (6.33). The value of the classical action is thus

$$S_E(u_\lambda, u_\lambda^{(0)}) = \pi\beta \qquad (7.23)$$

and once more, since the coordinates of both momentum and symmetric space may be expressed in terms of one another without involving the conjugate momenta (see equation (7.4)) the transformation relating the two spaces leaves the value of the classical action unaltered. Thus

$$S_E(u_\lambda, u_\lambda^{(0)}) = \pi\beta = S_E(\underset{\sim}{\rho}, \underset{\sim}{\rho_0});\ |\underset{\sim}{\rho}|, |\underset{\sim}{\rho_0}| \geqslant \rho_E \qquad (7.24)$$

where $\underset{\sim}{\rho}$ corresponds to u_λ and $\underset{\sim}{\rho_0}$ to $u_\lambda^{(0)}$.

5) The Analytic Continuation

In the case of the discrete spectrum where $E < 0$ the kernel $I_E(\underset{\sim}{\rho}, \underset{\sim}{\rho_0})$ of the spectral operator can be expressed as a sum over classical paths between $\underset{\sim}{\rho_0}$ and $\underset{\sim}{\rho}$, each path being characterised by the number c of times that the particle passes around the circular momentum orbit. The contribution from each classical path depends on the corresponding action $S_{cE}(\underset{\sim}{\rho}, \underset{\sim}{\rho_0})$ For the continuous spectrum we have seen that there is no classical path joining the points $\underset{\sim}{\rho}_0$ and $\underset{\sim}{\rho}$ if one of them or both lie in the inaccessible region of momentum space. We have to consider the generalised classical paths which pass through the inaccessible region and around the complete momentum circle any number of times. We shall again characterize each of these generalised classical paths by the integer c, and the corresponding classical actions $S_{cE}(\underset{\sim}{\rho}, \underset{\sim}{\rho}_0)$ for $E > 0$ must be obtained for all values of $\underset{\sim}{\rho}$ and $\underset{\sim}{\rho}_0$. The classical action functions $S_{cE}(\underset{\sim}{\rho}, \underset{\sim}{\rho}_0)$ for $E < 0$ are defined for all $\underset{\sim}{\rho}$ and $\underset{\sim}{\rho}_0$ and we shall obtain the result for $E > 0$ by analytic continuation.

The action $S_{cE}(\underset{\sim}{\rho}, \underset{\sim}{\rho}_0)$ treated as a function of complex energy is discontinuous across the positive energy axis, and this is because the action is given in terms of the square root of the energy. The value of ω, and hence of $S_{cE}(\underset{\sim}{\rho}, \underset{\sim}{\rho}_0)$ depends on whether we analytically continue above or below the cut along the positive energy axis and the two actions

$$S^{\pm}_{cE}(\underset{\sim}{\rho}, \underset{\sim}{\rho}_0) = \lim_{\varepsilon \to 0} S_{cE \pm i\varepsilon}(\underset{\sim}{\rho}, \underset{\sim}{\rho}_0) \; ; \quad E, \varepsilon > 0 \qquad (7.25)$$

are different.

From equation (6.35) we know that for the attractive Coulomb potential the value of the action along the shortest path joining the two momenta $\underset{\sim}{p}_0$ and $\underset{\sim}{p}$ for a negative energy E is given by

$$S_{0E}(\underset{\sim}{p},\underset{\sim}{p}_0) = \frac{\mu k \omega}{(-2\mu E)^{1/2}} \tag{7.26}$$

where

$$\cos\omega = 1 + \frac{E|\underset{\sim}{p}-\underset{\sim}{p}_0|^2}{\mu(E-T)(E-T_0)} . \tag{7.27}$$

If we look at the function $Z(\mathcal{E})$ of the complex energy variable $\mathcal{E}$ given by

$$Z(\mathcal{E}) = 1 + \frac{\mathcal{E}|\underset{\sim}{p}-\underset{\sim}{p}_0|^2}{\mu(\mathcal{E}-T)(\mathcal{E}-T_0)} = \cos\omega \tag{7.28}$$

we see that when $\mathcal{E}$ is real and negative, ω is real and lies between 0 and π as it should for the bound states. We require the value of ω for real positive values of $\mathcal{E}$ and what we shall now obtain is

$$\omega^+(\mathcal{E}) = \lim_{\varepsilon\to 0} \omega(E+i\varepsilon) \quad , (E,\varepsilon) > 0 \tag{7.29}$$

for $\underset{\sim}{p}_0$ fixed in the accessible region and $\underset{\sim}{p}$ on different parts of the momentum circle as shown in Figure 7.4.

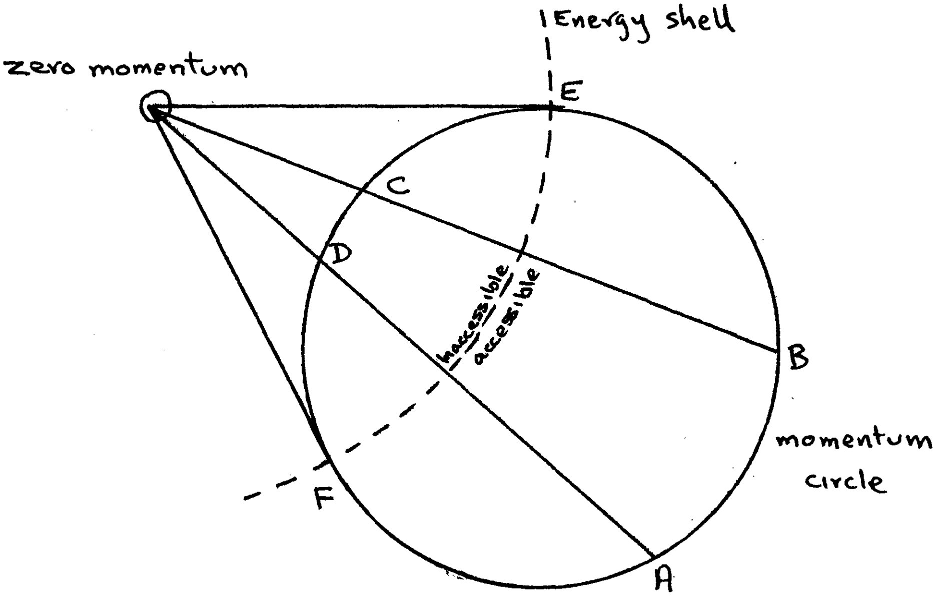

Figure 7.4. The different types of paths in momentum space. Between A and B we have the path in the accessible region and also AFDCEB which passes through the inaccessible region.

Inverting the relation (7.28) we obtain

$$\omega = \pm i \log\{Z + (Z^2-1)^{1/2}\} \tag{7.30}$$

which is a many-valued function of Z. The function $Z + (Z^2 - 1)^{1/2}$ is itself a double-valued function of Z and all its values are given on the Riemann surface consisting of two sheets R_1, R_2 joined by cuts from $-\infty$ to -1 and from 1 to ∞. On R_1 we define $\operatorname{Im}(Z^2 - 1)^{1/2} \geqslant 0$, then $(Z^2-1)^{1/2}$ is uniquely defined on the Riemann surface. On R_2, $(Z^2-1)^{1/2}$ takes on values of opposite sign to those at the corresponding points on R_1. The argument of $Z + (Z^2-1)^{1/2}$ then varies continuously from 0 to 2π as Z passes around the branch points ± 1 on the two sheets. If we now take an infinite set of such pairs of sheets joined in the same way along the cuts, then $\arg(Z + (Z^2-1)^{1/2})$ takes on all real values on the Riemann surface thus obtained, and ω is a single-valued function of Z on this surface given by

$$\omega = \arg\{Z + (Z^2-1)^{1/2}\} - i \log|Z + (Z^2-1)^{1/2}| . \qquad (7.31)$$

We now consider Z as a function of $E + i\varepsilon$, where $E > 0$, with $\underset{\sim}{\rho}_0$ fixed at $A(\underset{\sim}{\rho}_0)$ say, and $\underset{\sim}{\rho}$ varying around the momentum circle from A through E and F and back to A in Figure 7.4. By examining the real and imaginary parts of Z we find that Z describes the contour shown in Figure 7.5.

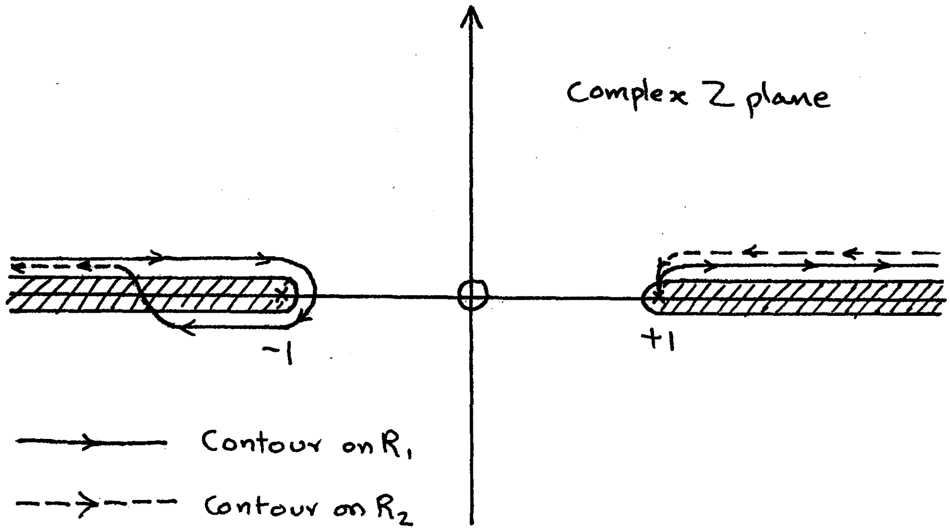

Figure 7.5. The path on the Riemann sheets R_1 and R_2 defined in equation (7.28) for $\mathcal{E} = E + i\varepsilon (E, \varepsilon > 0)$ and $\underset{\sim}{\rho}_0$ fixed in the accessible region, with $\underset{\sim}{\rho}$ varying round the hodograph.

The analytic continuation of ω for $\underset{\sim}{\rho}_0$ at A as $\underset{\sim}{\rho}$ lies on the different parts of the momentum circle is thus as follows:

$$\omega^+ = \begin{cases} i\beta\text{, for } \underset{\sim}{p} \text{ at } B\text{, where } B \text{ varies from } A(\beta=0) \text{ to } E\ (\beta=\infty)\text{, on path } ABE & \text{(a)} \\ \pi - i\beta\text{, for } \underset{\sim}{p} \text{ at } C\text{, where } C \text{ varies from } E(\beta=\infty) \text{ to } D\ (\beta=0)\text{, on path } ABED & \text{(b)} \\ \pi + i\beta \text{ for } \underset{\sim}{p} \text{ at } C\text{, where } C \text{ varies from } D(\beta=0) \text{ to } E(\beta=\infty)\text{, on path } AFDE & \text{(c)} \\ 2\pi + i\beta \text{ for } \underset{\sim}{p} \text{ at } B\text{, where } B \text{ varies from } E(\beta=\infty) \text{ to } A\ (\beta=0)\text{, on path } AFDEB & \text{(d)} \end{cases} \qquad (7.32)$$

where β is the hyperbolic angle, always defined between two points $u_\lambda^{(0)}$, u_λ on $\mathcal{S}^-$. Since $\underset{\sim}{p}_0$ is in the accessible region, the corresponding point $u_\lambda^{(0)}$ belongs to $\mathcal{S}^-$. If $\underset{\sim}{p}$ for example lies at D in Figure 7.4, then the point on $\mathcal{S}^-$ taken to correspond to $\underset{\sim}{p}$ is that point actually corresponding to $\underset{\sim}{p}\, p_E^2/p^2$ which is the momentum at A . Thus

$$\cos\omega^+ = \begin{cases} \cosh\beta & |\underset{\sim}{p}| > p_E \\ -\cosh\beta & |\underset{\sim}{p}| < p_E . \end{cases} \qquad (7.33)$$

To obtain the value of the action along the generalised classical paths in momentum space we first note that

$$\lim_{\varepsilon\to 0}\left(-2\mu(E+i\varepsilon)\right)^{-1/2} = i/\rho_E \qquad (7.34)$$

so that the action along the shortest path between $\underset{\sim}{\rho}_0$ and $\underset{\sim}{\rho}$ is

$$S_E^+(\underset{\sim}{\rho},\underset{\sim}{\rho}_0) = \begin{cases} \Pi\beta & |\underset{\sim}{\rho}| > \rho_E \\ \Pi(\beta + i\pi) & |\underset{\sim}{\rho}| < \rho_E\,. \end{cases} \qquad (7.35)$$

For $|\underset{\sim}{\rho}| > \rho_E$ this agrees with equation (7.23) for the value of the action between two points in the accessible region. For $|\underset{\sim}{\rho}| < \rho_E$, with reference to Figure 7.4, the action from A to C is the sum of a real part corresponding to the action along the path AB plus an imaginary action $i\pi\Pi$ which comes from passing from B through the energy shell at E into the inaccessible region at C.

If we had considered the analytic continuation in energy to $E - i\varepsilon$, for $E, \varepsilon > 0$, then we would have obtained for ω^- the complex conjugate of terms in equation (7.32), and consequently, since

$$\lim_{\varepsilon\to 0}\left\{-2\mu(E-i\varepsilon)\right\}^{-1/2} = -i/\rho_E \qquad (7.36)$$

we have the result that:

$$S_E^-(\underset{\sim}{p},\underset{\sim}{p}_0) = [S_E^+(\underset{\sim}{p},\underset{\sim}{p}_0)]^* . \qquad (7.37)$$

Since $\omega^\pm$ increase by a multiple of 2π each time the momentum orbit is described, then the corresponding action functions $S_E^\pm(\underset{\sim}{p},\underset{\sim}{p}_0)$ increase by multiples of $\pm 2\pi i \Pi$. Hence if c denotes the number of complete orbits described, the values of $S_{cE}^+(\underset{\sim}{p},\underset{\sim}{p}_0)$ for $\underset{\sim}{p}$ and $\underset{\sim}{p}_0$ lying in each of the regions of momentum space can be given for all the possible generalised classical paths in table form as in Table 7.1. The analytic path length given in Table 7.1 is just the analytic continuation of the path length for the bound states. For energy $\underset{\sim}{E} = E - i\varepsilon$ the quantities in the table become their complex conjugates.

6) Time along the Complete Orbits

The generalised classical paths in momentum space, as we have seen, are made up from the hodographs of particles of the same positive energy E moving in an attractive and repulsive Coulomb potential. The properties of the action along one of these generalised

Table 7.1.

Region	Path (figure 7.4)	Analytic path length in symmetric representation.	Action $S^+_{cE}(\underset{\sim}{\rho}, \underset{\sim}{\rho_0})$
$\lvert\underset{\sim}{\rho}\rvert, \lvert\underset{\sim}{\rho_0}\rvert > P_E$ $(u_\lambda, u_\lambda^{(0)}$ on $\mathcal{S}^-)$	$A(\underset{\sim}{\rho_0})$ to $B(\underset{\sim}{\rho})$ $c = 0, 1, \ldots, \infty$	$2\pi c - i\beta$	$\sqcap\beta + 2\pi ci\sqcap$
	$A(\underset{\sim}{\rho_0})$ to $B(\underset{\sim}{\rho})$ via F, E ; $c = 1, 2, \ldots, \infty$.	$2\pi c + i\beta$	$-\sqcap\beta + 2\pi ci\sqcap$
$\lvert\underset{\sim}{\rho}\rvert, \lvert\underset{\sim}{\rho_0}\rvert < P_E$ $(u_\lambda, u_\lambda^{(0)}$ on $\mathcal{S}^+)$	$D(\underset{\sim}{\rho_0})$ to $C(\underset{\sim}{\rho})$ $c = 0, 1, \ldots, \infty$	$2\pi c + i\beta$	$-\sqcap\beta + 2\pi ci\sqcap$
	$D(\underset{\sim}{\rho_0})$ to $C(\underset{\sim}{\rho})$ via F, E ; $c = 1, 2, \ldots, \infty$.	$2\pi c - i\beta$	$\sqcap\beta + 2\pi ic\sqcap$
$\lvert\underset{\sim}{\rho_0}\rvert > P_E, \lvert\underset{\sim}{\rho}\rvert < P_E$ $(u_\lambda^{(0)}$ on $\mathcal{S}^-$, u_λ on $\mathcal{S}^+)$	$A(\underset{\sim}{\rho_0})$ to $C(\underset{\sim}{\rho})$ via E ; $c = 0, 1, \ldots \infty$	$\pi(2c+1) - i\beta$	$\sqcap\beta + \pi(2c+1)i\sqcap$
	$A(\underset{\sim}{\rho_0})$ to $C(\underset{\sim}{\rho})$ via F ; $c = 1, 2, \ldots, \infty$	$\pi(2c-1) + i\beta$	$-\sqcap\beta + \pi(2c-1)i\sqcap$
$\lvert\underset{\sim}{\rho_0}\rvert < P_E, \lvert\underset{\sim}{\rho}\rvert > P_E$ $(u_\lambda^{(0)}$ on $\mathcal{S}^+$, u_λ on $\mathcal{S}^-)$	$D(\underset{\sim}{\rho_0})$ to $B(\underset{\sim}{\rho})$ via E ; $c = 0, 1, \ldots, \infty$	$\pi(2c+1) + i\beta$	$-\sqcap\beta + \pi(2c+1)i\sqcap$
	$D(\underset{\sim}{\rho_0})$ to $B(\underset{\sim}{\rho})$ via F ; $c = 1, 2, \ldots, \infty$	$\pi(2c-1) - i\beta$	$\sqcap\beta + \pi(2c-1)i\sqcap$

classical paths are different to the properties of the action for each particular path. For example, with reference to Figure 7.4 again, the value of the action from A to C along the generalised classical path AEC is not the sum of the action evaluated along A to E (for attractive Coulomb scattering) and the action from E to C (for repulsive Coulomb scattering). In the latter case of course the total action is infinite which is not the case for the generalised classical path AEC. Similar properties of generalised classical paths arise when we consider the time along these paths.

For the bound states, if $\underset{\sim}{p}_0$ is taken to be the momentum at the perihelion of the elliptic orbit, then ω is just the eccentric anomaly at the point with momentum $\underset{\sim}{p}$ (Landau and Lifshitz, 1960; Györgyi, 1968). The time taken by the particle in moving from $\underset{\sim}{p}_0$ around the orbit is given by Kepler's equation:

$$\Omega t = \omega - \epsilon \sin\omega \qquad (7.38)$$

where $\Omega = (-2\mu E)^{3/2}/k\mu^2$ is the fundamental angular frequency and ϵ is the eccentricity. The period for a complete revolution of the orbit is given by

$$\left(\frac{\partial S}{\partial E}\right)_{\text{orbit}} = \frac{2\pi}{\Omega} \quad . \tag{7.39}$$

The analytic continuation of Ω and ϵ to positive energies are Ω' and ϵ' where

$$\left.\begin{array}{l} \Omega \rightarrow \pm i\Omega \\ \epsilon \rightarrow \epsilon' \end{array}\right\} \mathcal{E} = E \pm i\varepsilon, E > 0 \ . \tag{7.40}$$

$\Omega' = p_E^3/k\mu^2$ and ϵ' is real and greater than unity. For positive energies, we again choose $\underset{\sim}{p}_0$ to be the momentum at the perihelion and using equations (7.32) and (7.40), the analytic continuation of the Kepler equation (7.38) is

$$\Omega' t = \begin{cases} \epsilon' \sinh\beta - \beta & \text{(a)} \\ \mp i\pi - \epsilon' \sinh\beta - \beta & \text{(b)} \\ \mp i\pi + \epsilon' \sinh\beta + \beta & \text{(c)} \\ \mp 2i\pi - \epsilon' \sinh\beta + \beta & \text{(d)} \end{cases} \tag{7.41}$$

where the ranges of $\underset{\sim}{p}$ and β correspond to those of equation (7.32).

In the accessible region the time obeys Kepler's equation for attractive Coulomb scattering (Landau and Lifshitz, 1960, p.38). The time taken for a particle to pass from a point in the accessible region to a point in the inaccessible region is complex. The time between any two points in the inaccessible region $ECDF$ of Figure 7.4 is real, increases from $-\infty$ at F to $+\infty$ at E for clockwise motion and obeys Kepler's equation for the repulsive case. Thus the analytic continuation of the classical bound-state Kepler problem yields the classical solutions to both the attractive and repulsive scattering problem. The time along a generalised classical path (as for the action), has different properties to the time along the separate paths and in passing through the energy shell $p^2 = 2\mu E$ the particle makes a sudden jump to the past. The time to traverse the complete orbit is $\pm 2\pi i/\Omega'$, and follows also from the fact that the action around the complete orbit is $\pm 2\pi i \Pi$.

Finally, with respect to t, the particle does not move uniformly along a path in the symmetric space. However, as for the bound states, the path will be traced out uniformly with respect to the symmetric 'time' variable

τ of equation (7.6). We can obtain the value of $ds/d\tau$ and we obtain

$$\frac{ds}{d\tau} = \frac{P_E^3}{k\mu^2} = \text{constant} \tag{7.42}$$

and thus

$$\tau = \beta/\Omega' \quad . \tag{7.43}$$

With respect to τ, the classical theory is symmetric and time between events on the hyperboloid is unchanged when the positions are rotated by the same amount on the surface of the hyperboloid.

CHAPTER 8

THE RUTHERFORD SCATTERING IDENTITY

1) Introduction

To explain the Rutherford scattering identity as it applies to the scattering of an electron by a fixed proton we have chosen to obtain a complete correspondence identity and then to show that the scattering identity follows as a consequence of this. The relevant classical theory has already been discussed in the previous chapter and we shall obtain the kernel of the quantum-mechanical spectral operator in momentum representation and express it explicitly as a sum over the generalised classical paths - thus providing a complete correspondence identity.

The classical Rutherford formula for the angular differential cross section $\sigma(\Theta)$ for the system of electron and (infinite mass) proton is given by

$$\sigma(\Theta) = \frac{e^4}{16E^2 \sin^4(\Theta/2)} = \left\{ \frac{2\mu e^2}{|\underset{\sim}{p} - \underset{\sim}{p}_0|^2} \right\}^2 \qquad (8.1)$$

and concerns the initial and final values of the momentum in the neighbourhood of the energy shell

$$\frac{p^2}{2\mu} = \frac{p_0^2}{2\mu} = E \quad . \tag{8.2}$$

Thus we would expect the Rutherford scattering identity to follow from the properties of the complete correspondence identity close to the energy shell and this is the case.

The quantum-mechanical angular differential cross section is obtained from the spectral operator kernel in section 4 of this chapter. There is no need to consider the long-range distortion of the Coulomb potential separately as it appears automatically in the analysis. In the conventional derivation of the quantum-mechanical differential cross section (see, for example, Mott and Massey 1965, chap. 3 , § 2, or Rodberg and Thaler 1967, chap. 3 , §5) there appears to be no connection with the classical derivation of equation (8.1) except in the initial specification of the same Hamiltonian and the final identical result. However, by deriving the Rutherford formula from the spectral operator kernel, as we do, we can see how the identity arises. This derivation of the angular differential cross section is of general application and independent of the correspondence identity.

As well as providing a means of explaining the scattering identity, the complete correspondence identity also illustrates that the electron-proton system for positive energies can be described completely and exactly by a theory based on rays. Although the rays in this case are the generalised classical trajectories, they can be identified with the paths which correspond to the scattering of both positrons and electrons and as such they are simpler in conception than Feynman paths discussed in chapter 4.

2) The Spectral Operator

In terms of the Green operators $G_E^{\pm}$, discussed in chapter 3, the spectral operator I_E is given by

$$I_E = \delta(E-H) = \frac{G_E^- - G_E^+}{2\pi i} \quad (E \text{ real}). \quad (8.3)$$

For negative values of the energy the spectral operator of the hydrogen atom is zero everywhere except at the bound-state energy levels E_n, and is a sum over delta functions at these poles. For positive values of the energy, I_E is a well-defined analytic operator function of E, and is the projection operator onto the space of all states of energy E (see equation (3.46)). This space is of infinite dimension because the energy $E > 0$ is degenerate with respect to the azimuthal quantum number ℓ which has infinite range.

In momentum representation the kernel of I_E is thus given by

$$I_E(\underset{\sim}{p},\underset{\sim}{p}_0) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} \psi_{\ell m}(\underset{\sim}{p},E)\,\psi^{*}_{\ell m}(\underset{\sim}{p}_0,E) \tag{8.4}$$

where the momentum-space wave functions are solutions of the time-independent Schrödinger wave equation:

$$(E-H)\psi_{\ell m}(\underset{\sim}{p},E) \equiv \left(E-\frac{p^2}{2\mu}\right)\psi_{\ell m}(\underset{\sim}{p},E) + \frac{k}{2\pi^2\hbar}\int\frac{d^3p'\,\psi_{\ell m}(\underset{\sim}{p}',E)}{|\underset{\sim}{p}-\underset{\sim}{p}'|^2} = 0 \tag{8.5}$$

and are normalised as follows

$$\int d^3p\,\psi_{\ell m}(\underset{\sim}{p},E)\,\psi^{*}_{\ell' m'}(\underset{\sim}{p},E') = \delta(E-E')\,\delta_{\ell\ell'}\,\delta_{mm'}\,. \tag{8.6}$$

The kernel of the spectral operator as given in equation (8.4) is most conveniently evaluated by considering the quantum-mechanical problem in the symmetric representation discussed in chapter 7. The problem has been considered in this representation by Bander and Itzykson (1966b) **and in** IV. If $\psi(\underset{\sim}{p}, E)$ is any momentum wave function, not necessarily satisfying equation (8.5), then the equivalent wave function $\psi_s(u_\lambda, E)$ in the symmetric representation is defined by

$$\psi_s(u_\lambda, E) = A(p^2 - p_E^2)^2 \psi(\underset{\sim}{p}, E) \, , \; E > 0 \qquad (8.7)$$

where A is a constant to be determined by normalization.

Now $\mathcal{S}$, the Minkowski sphere on which the four-vector u_λ lies, consists of two sheets $\mathcal{S}^+$ and $\mathcal{S}^-$. These sheets are respectively the classically inaccessible and accessible regions for the attractive Coulomb potential. Quantum-mechanically, of course, no one sheet can be labelled inaccessible, but when we have to consider quantities on $\mathcal{S}$ defined on one sheet only we shall usually work with the sheet $\mathcal{S}^-$. The three-dimensional surface element $d\Omega$ of $\mathcal{S}$ is related to the volume element of momentum space by the relation

$$d^3p = \begin{cases} \dfrac{(p_E^2 - p^2)^3}{8\,p_E^3}\,d\Omega^+ & \text{on } \mathcal{S}^+ \\[2ex] \dfrac{(p^2 - p_E^2)^3}{8\,p_E^3}\,d\Omega^- & \text{on } \mathcal{S}^- . \end{cases} \tag{8.8}$$

The distance between two points in momentum space is related to the corresponding Minkowski distance by

$$|\underset{\sim}{p} - \underset{\sim}{p}_0|^2 = -\frac{(p^2 - p_E^2)(p_0^2 - p_E^2)(u_\lambda - u_\lambda^{(0)})^2}{4\,p_E^2} \tag{8.9}$$

where $u_\lambda^{(0)}$ and u_λ correspond to $\underset{\sim}{p}_0$ and $\underset{\sim}{p}$.

The form of Schrödinger's equation in the symmetric representation now becomes

$$(I - \eta Q)\,\psi_s(u_\lambda, E) = 0 \ . \tag{8.10}$$

The continuous variable

$$\eta = k\mu / p_E \hbar \tag{8.11}$$

is the analogue of the discrete quantum number n , and the integral operator Q is defined by

$$Q\psi_s(u_\lambda,E) = \epsilon(u_\lambda)\int_{\mathcal{S}} \frac{d\Omega'\,\psi_s(u'_\lambda,E)}{2\pi^2\,|(u_\lambda-u'_\lambda)^2|} \tag{8.12}$$

where

$$\epsilon(u_\lambda) = \begin{cases} -1 & ; \ u_\lambda \text{ on } \mathcal{S}^+ \\ 1 & ; \ u_\lambda \text{ on } \mathcal{S}^-. \end{cases} \tag{8.13}$$

Equation (8.10) is invariant with respect to rotations on the surface $\mathcal{S}$ and is the analogue of the $O(4)$ invariant Schrödinger equation (6.45) of the bound states.

In the symmetric representation we can define the kernel of the operator J_E (the analogue of J_ν for the bound states) as follows

$$J_E(u_\lambda,u_\lambda^{(0)}) = \frac{2\pi^2(p_E^2-p_0^2)^2(p^2-p_E^2)^2}{16\mu\,p_E^3}\,I_E(\underset{\sim}{p},\underset{\sim}{p_0}) \ . \tag{8.14}$$

This operator kernel, as opposed to the spectral operator kernel, is symmetric (equal to its transpose) in symmetric representation. It is the kernel of the operator $I_E(E-T)$ where T is the kinetic energy operator $T = p^2/2\mu$.

The kernel $J_E(u_\lambda, u_\lambda^{(0)})$ may be written in terms of the solutions of equation (8.10) as follows

$$J_E(u_\lambda, u_\lambda^{(0)}) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \psi_{\eta\ell m}(u_\lambda)\psi^*_{\eta\ell m}(u_\lambda^{(0)}) \qquad (8.15)$$

and the wave functions $\psi_{\eta\ell m}(u_\lambda)$ can be expressed in terms of hyperspherical harmonics $H_{\eta\ell m}(u_\lambda)$ that are defined on the sheet $\mathcal{S}^-$. In Bander and Itzykson (1966b) the spherical harmonics are defined on $\mathcal{S}^+$ and to convert to their convention we change the sign of u_λ. The wave functions $\psi_{\eta\ell m}(u_\lambda)$ for a given value of the energy E, ℓ and m may be related to the hyperspherical harmonics in two different ways depending on the sign of k. We have assumed so far that k is positive, corresponding to the attractive Coulomb potential, but there are solutions of equation (8.10) for both positive and negative values of k. These attractive and repulsive states are discussed by Bander and Itzykson and in terms of the hyperspherical harmonics on

$\mathcal{S}^-$ the attractive solutions of (8.10) may be written

$$\Psi_{\eta l m}(u_\lambda) = \text{constant} \times \begin{cases} -e^{-\pi\eta} H_{\eta l m}(-u_\lambda)\,; & u_\lambda \text{ on } \mathcal{S}^+ \\ H_{\eta l m}(u_\lambda)\,; & u_\lambda \text{ on } \mathcal{S}^- . \end{cases} \qquad (8.16)$$

Although the functions $H_{\eta l m}(u_\lambda)$ form a complete orthonormal set on the lower sheet $\mathcal{S}^-$, the wave functions $\Psi_{\eta l m}(u_\lambda)$ are not orthonormal or complete for the entire symmetric space $\mathcal{S}$. In order to obtain the constant (C say) in equation (8.16) we note that in terms of $H_{\eta l m}(u_\lambda)$ the momentum-space wave function $\Psi_{lm}(\underline{p}, E)$ normalized by equation (8.7) is given by (Roberts, private communication)

$$\Psi_{lm}(\underline{p}, E) = \left\{\frac{8\mu\eta p_E^3}{(1-e^{-2\pi\eta})\pi^2}\right\}^{1/2} \exp\left[i\left\{\arg\Gamma(l+1-i\eta) + (l+1)\pi\right\}\right]$$

$$\times \begin{cases} e^{-\pi\eta} H_{\eta l m}(-u_\lambda)\,; & u_\lambda \text{ on } \mathcal{S}^+ \\ H_{\eta l m}(u_\lambda)\,; & u_\lambda \text{ on } \mathcal{S}^- . \end{cases} \qquad (8.17)$$

From equations (8.7), (8.14) and (8.15) it can be seen that the value of A, to within a phase factor, relating $\psi_{\eta\ell m}(u_\lambda)$ and $\psi_{\ell m}(\rho, E)$ is

$$A = \frac{\pi}{\sqrt{\mu 8 \rho_E^3}} \quad . \tag{8.18}$$

It then follows from equation (8.7) with this value of A together with equation (8.17) that the value of C (to within a phase factor) is

$$C = \left(\frac{\eta}{1-e^{-2\pi\eta}}\right)^{1/2} \exp\left[i\left\{\arg\Gamma(\ell+1-i\eta) + (\ell+1)\pi\right\}\right] . \tag{8.19}$$

To evaluate the sum (8.15) we make use of the addition theorem for the hyperspherical harmonics on $\mathcal{S}^-$ (Bander and Itzykson 1966b) viz:

$$\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} H_{\eta\ell m}(u_\lambda) H^*_{\eta\ell m}(u_\lambda^{(0)}) = \frac{\eta \sin \eta\beta}{\sinh \beta} \tag{8.20}$$

where β is the hyperbolic angle defined on $\mathcal{S}^-$ by equation (7.21). The value of $J_{E,k}(u_\lambda, u_\lambda^{(0)})$, which is the kernel of the projection operator onto the states of positive energy E for the attractive Coulomb potential is thus:

$$J_{E,k}(u_\lambda, u_\lambda^{(0)}) = \frac{\mathcal{E}(\eta)\,\eta^2 \sin\eta\beta}{(1 - e^{-2\pi\eta})\sinh\beta} \tag{8.21}$$

where, using Figure 8.1 to define the regions I, II, III, IV, the function $\mathcal{E}(\eta)$ is given by

$$\mathcal{E}(\eta) = \begin{cases} 1 & \text{in I} \\ -e^{-\pi\eta} & \text{in II, IV} \\ e^{-2\pi\eta} & \text{in III}\,. \end{cases} \tag{8.22}$$

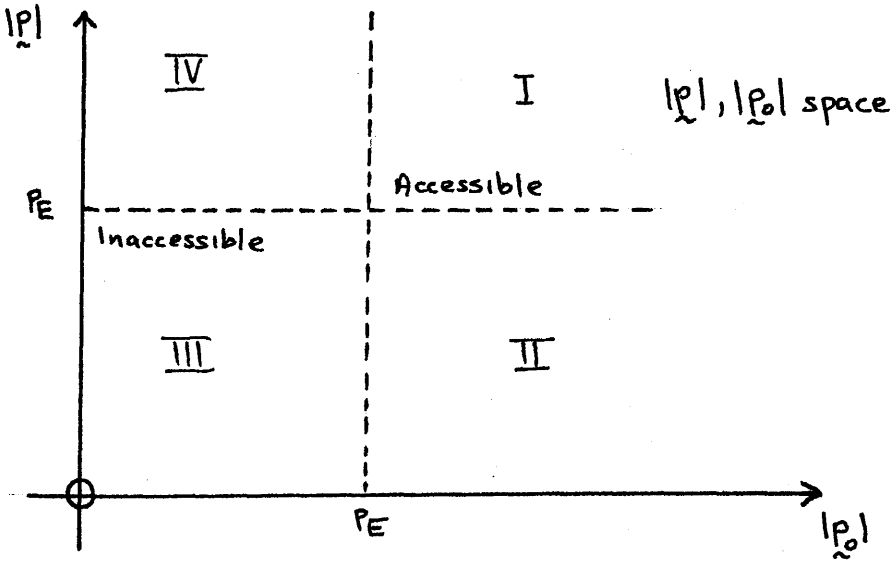

Figure 8.1. The four regions of $|\underset{\sim}{p}|, |\underset{\sim}{p}_0|$ space.

The value of the spectral operator kernel in momentum space can now be obtained via equation (8.14) and we have

$$I_{E,k}(\underset{\sim}{p},\underset{\sim}{p_0}) = \frac{\mathcal{E}(\eta)\,8\mu^3 p_E k^2}{\pi^2\hbar^2(p^2-p_E^2)^2(p_0^2-p_E^2)^2}\,\frac{\sin\eta\beta}{(1-e^{-2\pi\eta})\sinh\beta} \qquad (8.23)$$

where β is again always defined on $\mathcal{S}^-$. If $\underset{\sim}{p}$ (or $\underset{\sim}{p_0}$) is in the classically inaccessible region it must be replaced by $\underset{\sim}{p}\, p_E^2/p^2$ (or $\underset{\sim}{p_0}\, p_E^2/p_0^2$) to obtain the corresponding point on $\mathcal{S}^-$.

3) A Complete Correspondence Identity

As we have already mentioned in chapter 7 the classical paths that occur in attractive Coulomb scattering are insufficient to provide a complete correspondence identity and we have to consider the generalised classical paths. There is an infinite number of such paths leading from $\underset{\sim}{p_0}$ to $\underset{\sim}{p}$ or alternatively from $u_\lambda^{(0)}$ to u_λ and the spectral operator kernel $I_{E,k}(\underset{\sim}{p},\underset{\sim}{p_0})$ and the kernel $J_{E,k}(u_\lambda, u_\lambda^{(0)})$ for $E>0$ can then be expressed respectively as a sum over them.

Before doing this we may note that the properties of the energy spectrum and the spectral operators for positive and negative energies are determined from the different properties of the action functions. For negative energies the form of the spectral operator is determined by the sum $\sum_{c} \sin \{ S_{cE}(\underset{\sim}{\rho}, \underset{\sim}{\rho}_0)/\hbar \}$. For complete orbits i.e. when $\underset{\sim}{\rho} = \underset{\sim}{\rho}_0$, the sum over classical paths consists of sums of exponential terms of the form $\sum_{c=0}^{\infty} \exp \frac{ic}{\hbar}[S_E]$ where $[S_E]$ is the value of the action for one orbit. This is a geometric progression with each term having the same magnitude and is not convergent except as a generalised function. Destructive interference reduces the sum (when combined with its complex conjugate) to zero, unless the value of $[S_E]$ is given by the Bohr-Sommerfeld condition, and then constructive interference builds up the discrete spectrum.

For the positive energy case, the value of $[S_E]$ is $\pm 2\pi i \Pi$, as we saw in chapter 7, and if we consider the sum $\sum_{c=0}^{\infty} \exp \frac{ic[S_E]}{\hbar}$, where $[S_E] = 2\pi i \Pi$, then we obtain

$$\sum_{c=0}^{\infty} \exp \frac{ic[S_E]}{\hbar} = \sum_{c=0}^{\infty} \exp\left(-\frac{2\pi c \sqcap}{\hbar}\right) = \sum_{c=0}^{\infty} \exp -2\pi c\eta$$

$$= (1 - \exp -2\pi\eta)^{-1} . \qquad (8.24)$$

The series converges, and the sum is non-zero for all positive energies. The spectrum is thus continuous. The factor $(1 - \exp -2\pi\eta)^{-1}$ appears in the expressions (8.21) and (8.23) and equation (8.24) involving the sum over c provides the key to expressing the kernels as sums over generalised classical paths. First of all we note that the sum $\sum_{c=0}^{\infty} \exp \frac{ic[S_E]}{\hbar}$ where $[S_E]$ is $-2\pi i \sqcap$, diverges and we have to be selective over which paths to include in the complete correspondence identity. In Table 8.1 we have labelled the various paths attractive or repulsive according to whether the analytic path length has negative or positive imaginary part. We have had to do this because it is only in terms of the attractive paths that we can obtain a complete correspondence identity for the attractive Coulomb potential.

With reference to Table 8.1 and **Figure 7.4 the**

Table 8.1

Region.	Path (see figure 7.4).	Analytic path length in symmetric representation	$\exp \frac{i}{\hbar} S^{+}_{cE}(\underset{\sim}{p}, \underset{\sim}{p}_0)$.	sine of the analytic path length.	Potential.
$\lvert\underset{\sim}{p}\rvert, \lvert\underset{\sim}{p}_0\rvert > p_E$ $(u_\lambda, u_\lambda^{(0)}$ on $\mathcal{S}^-)$	$A(\underset{\sim}{p}_0)$ to $B(\underset{\sim}{p})$ $c = 0, 1, \ldots, \infty$.	$2\pi c - i\beta$	$\exp(i\eta\beta - 2\pi c\eta)$	$-i \sinh\beta$	attractive
	$A(\underset{\sim}{p}_0)$ to $B(\underset{\sim}{p})$ via F, E; $c = 1, 2, \ldots \infty$.	$2\pi c + i\beta$	$\exp(-i\eta\beta - 2\pi c\eta)$	$i \sinh\beta$	repulsive
$\lvert\underset{\sim}{p}\rvert, \lvert\underset{\sim}{p}_0\rvert < p_E$ $(u_\lambda, u_\lambda^{(0)}$ on $\mathcal{S}^+)$	$D(\underset{\sim}{p}_0)$ to $C(\underset{\sim}{p})$ $c = 0, 1, \ldots, \infty$.	$2\pi c + i\beta$	$\exp(-i\eta\beta - 2\pi c\eta)$	$i \sinh\beta$	repulsive
	$D(\underset{\sim}{p}_0)$ to $C(\underset{\sim}{p})$ via F, E; $c = 1, 2, \ldots, \infty$.	$2\pi c - i\beta$	$\exp(i\eta\beta - 2\pi c\eta)$	$-i \sinh\beta$	attractive
$\lvert\underset{\sim}{p}_0\rvert > p_E, \lvert\underset{\sim}{p}\rvert < p_E$ $(u_\lambda^{(0)}$ on $\mathcal{S}^-$, u_λ on $\mathcal{S}^+)$	$A(\underset{\sim}{p}_0)$ to $C(\underset{\sim}{p})$ via E; $c = 0, 1, \ldots, \infty$	$\pi(2c+1) - i\beta$	$\exp\{i\eta\beta - \pi(2c+1)\eta\}$	$i \sinh\beta$	attractive
	$A(\underset{\sim}{p}_0)$ to $C(\underset{\sim}{p})$ via F; $c = 1, 2, \ldots \infty$.	$\pi(2c-1) + i\beta$	$\exp\{-i\eta\beta - \pi(2c-1)\eta\}$	$-i \sinh\beta$	repulsive
$\lvert\underset{\sim}{p}_0\rvert < p_E, \lvert\underset{\sim}{p}\rvert > p_E$ $(u_\lambda^{(0)}$ on $\mathcal{S}^+$, u_λ on $\mathcal{S}^-)$	$D(\underset{\sim}{p}_0)$ to $B(\underset{\sim}{p})$ via E; $c = 0, 1, \ldots, \infty$.	$\pi(2c+1) + i\beta$	$\exp\{-i\eta\beta - \pi(2c+1)\eta\}$	$-i \sinh\beta$	repulsive
	$D(\underset{\sim}{p}_0)$ to $B(\underset{\sim}{p})$ via F; $c = 1, \ldots \infty$.	$\pi(2c-1) - i\beta$	$\exp\{i\eta\beta - \pi(2c-1)\eta\}$	$i \sinh\beta$	attractive

kernel of the operator $J_{E,k}$ of equation (8.21) can now be expressed as a sum over generalised classical paths as

$$J_{E,k}(u_\lambda,u_\lambda^{(0)}) = \eta^2 \sum_{\text{attractive } c} \frac{\exp\{i/\hbar\, S^{+}_{cE}(u_\lambda,u_\lambda^{(0)})\} - \exp\{-i/\hbar\, S^{-}_{cE}(u_\lambda,u_\lambda^{(0)})\}}{2i\sin(\text{analytic path length})} \,. \qquad (8.25)$$

The remaining paths, labelled repulsive, which do not contribute to this sum do contribute to the kernel of $J_{E,-k}$ of the repulsive potential (corresponding to the scattering of positrons). We have

$$J_{E,-k}(u_\lambda,u_\lambda^{(0)}) = \eta^2 \sum_{\text{repulsive } c} \frac{\exp\{i/\hbar\, S^{+}_{cE}(u_\lambda,u_\lambda^{(0)})\} - \exp\{-\frac{i}{\hbar} S^{-}_{cE}(u_\lambda,u_\lambda^{(0)})\}}{2i\sin(\text{analytic path length})} \,. \qquad (8.26)$$

The kernel of $J_{E,k} + J_{E,-k}$ is thus the sum of the expressions (8.25) and (8.26) and is

$$J_{E,k}(u_\lambda,u_\lambda^{(0)}) + J_{E,-k}(u_\lambda,u_\lambda^{(0)})$$

$$= \eta^2 \sum_{\text{all } c} \exp \frac{\{i/\hbar\, S^{+}_{cE}(u_\lambda,u_\lambda^{(0)})\} - \exp\{-i/\hbar\, S^{-}_{cE}(u_\lambda,u_\lambda^{(0)})\}}{2i\sin(\text{analytic path length.})} \qquad (8.27)$$

In momentum representation, since the classical action functions $S^{\pm}_{cE}(\underset{\sim}{p}, \underset{\sim}{p}_0)$ and $S^{\pm}_{cE}(u_\lambda, u^{(0)}_\lambda)$ are respectively the same, the spectral operator kernel for both potentials is thus given by

$$I_{E,\pm k}(\underset{\sim}{p}, \underset{\sim}{p}_0) = \frac{8\mu^3 p_E k^2}{\pi^2 \hbar^2 (p^2 - p_E^2)^2 (p_0^2 - p_E^2)^2}$$

$$\times \sum_{\substack{\text{attractive } c \\ \text{or repulsive } c}} \frac{\exp\left\{\frac{i}{\hbar} S^{+}_{cE}(\underset{\sim}{p}, \underset{\sim}{p}_0)\right\} - \exp\left\{-\frac{i}{\hbar} S^{-}_{cE}(\underset{\sim}{p}, \underset{\sim}{p}_0)\right\}}{2i \sin(\text{analytic path length})} \qquad (8.28)$$

and their sum by

$$I_{E,k}(\underset{\sim}{p}, \underset{\sim}{p}_0) + I_{E,-k}(\underset{\sim}{p}, \underset{\sim}{p}_0) = \frac{8\mu^3 p_E k^2}{\pi^2 \hbar^2 (p^2 - p_E^2)^2 (p_0^2 - p_E^2)^2}$$

$$\times \sum_{\text{all } c} \frac{\exp\left\{i/\hbar\, S^{+}_{cE}(\underset{\sim}{p}, \underset{\sim}{p}_0)\right\} - \exp\left\{-i/\hbar\, S^{-}_{cE}(\underset{\sim}{p}, \underset{\sim}{p}_0)\right\}}{2i \sin(\text{analytic path length})} . \qquad (8.29)$$

Now, the analytic path length of the equations (8.28) and (8.29) can be evaluated in terms of the momenta in the usual way with β positive by equation (7.21).

The form of equation (8.29) is identical to equation (6.59) for the bound states, since for the bound states $S_{cE}^{\pm}$ are identical as there is no cut in the action function for $E<0$. There are no bound states for k negative and thus equation (8.29) is valid for all real energies E and values of the momenta $\underset{\sim}{p}$ and $\underset{\sim}{p}_0$ except for a number of special singular points. It thus provides a complete correspondence identity for all real energies and does not require the definition of attractive and repulsive paths. However if we accept the definition of 'attractive' and 'repulsive' as applied to the generalised classical paths we can regard the expansions (8.25), (8.26) and (8.28) as valid complete correspondence identities. It should be noted that the attractive generalised classical paths, for example, are made up from the classical paths for both attractive and repulsive scattering and cannot be related solely to the classical paths of the attractive potential.

4) The Rutherford Scattering Identity

For values of $\underset{\sim}{p}$ and $\underset{\sim}{p}_0$ in the classically accessible region of momentum space the spectral operator kernel $I_{E,k}(\underset{\sim}{p},\underset{\sim}{p}_0)$ of equation (8.28) may be written in an analogous way to that of equation (6.60) for the bound states, namely

$$I_{E,k}(\underset{\sim}{p},\underset{\sim}{p}_0) = [\rho_E(\underset{\wedge}{p},\underset{\wedge}{p}_0)]^{1/2} \sum_{\text{attractive } c} \frac{\exp\{{}^{i}/_{\hbar}\, S^{+}_{cE}(\underset{\sim}{p},\underset{\sim}{p}_0)\} - \exp\{{}^{-i}/_{\hbar}\, S^{-}_{cE}(\underset{\sim}{p},\underset{\sim}{p}_0)\}}{2i\hbar^2} \quad (8.30)$$

where the 'density factor' $\rho_E(\underset{\sim}{p},\underset{\sim}{p}_0)$ is given by

$$\rho_E(\underset{\sim}{p},\underset{\sim}{p}_0) = \frac{16\,\mu^6 k^4}{\pi^4(p^2-2\mu E)^2(p_0^2-2\mu E)^2|\underset{\sim}{p}-\underset{\sim}{p}_0|^2(4\mu^2E^2+p^2p_0^2-4\mu E\,\underline{p}\cdot\underline{p}_0)}\,. \quad (8.31)$$

This density factor, as a function of energy, is identical to the corresponding factor for the bound states (see equation (6.61)). The factor for $E < 0$, we saw, was identical to the equivalent factor obtained by Gutzwiller (1967) using the phase-integral approximation in momentum representation for the Coulomb Green function. In the phase-integral approximation the physical interpretation of $\rho_E(\underset{\sim}{p},\underset{\sim}{p}_0)$ is that it is a measure of the density of classical paths leaving $\underset{\sim}{p}_0$ that reach $\underset{\sim}{p}$. We shall assume that $\rho_E(\underset{\sim}{p},\underset{\sim}{p}_0)$ for positive energies is also indicative of the density of classical paths. If we investigate $\rho_E(\underset{\sim}{p}, \underset{\sim}{p}_0)$ near the energy shell we see that it becomes singular, and in terms of the classical angular differential cross section $\sigma(\Theta)$ given by equation (8.1) it can be expressed as follows

$$\rho_E(\underset{\sim}{p}, \underset{\sim}{p}_0) \sim \frac{\sigma(\Theta)\ 4\mu^4 k^2}{\pi^4 p_E^2 (p^2 - p_E^2)^2 (p_0^2 - p_E^2)^2} \ . \qquad (8.32)$$

This indicates that all classical trajectories start and finish on the energy shell and that the dependence on scattering angle of $\rho_E(\underset{\sim}{p}, \underset{\sim}{p}_0)$ is the same as that of the angular differential cross section, which is not unexpected. It is because the factor $\rho_E(\underset{\sim}{p}, \underset{\sim}{p}_0)$ (and hence the quantum-mechanical spectral operator kernel $I_{E,k}(\underset{\sim}{p}, \underset{\sim}{p}_0)$) near the energy shell can be expressed in terms of the classical angular differential cross section that the Rutherford scattering identity arises as we shall now show.

Near the energy shell, the spectral operator kernel may now be written in terms of $\sigma(\Theta)$, for $|\underset{\sim}{p}|, |\underset{\sim}{p}_0| > p_E$, as

$$I_{E,k}(\underset{\sim}{\rho},\underset{\sim}{\rho}_0) \sim \frac{(\sigma(\Theta))^{1/2} 2\mu^2 k}{\pi^2 p_E (p^2 - p_E^2)(p_0^2 - p_E^2)} \cdot \sum_{\substack{\text{attractive} \\ c}} \frac{\exp\left\{\frac{i}{\hbar} S^+_{cE}(\underset{\sim}{\rho},\underset{\sim}{\rho}_0)\right\} - \exp\left\{\frac{-i}{\hbar} S^-_{cE}(\underset{\sim}{\rho},\underset{\sim}{\rho}_0)\right\}}{2i\hbar^2} \,.$$

$$\sim \frac{(\sigma(\Theta))^{1/2} 2\mu^2 k}{\pi^2 p_E (p^2 - p_E^2)(p_0^2 - p_E^2)} \cdot \frac{e^{i\eta\beta} - e^{-i\eta\beta}}{(1 - e^{-2\pi\eta})\, 2i\hbar^2} \,. \tag{8.33}$$

Since the asymptotic form, for large β , of $\cosh\beta$ is $\frac{1}{2} e^{\beta}$, it follows from equation (7.21) that

$$\cosh\beta \sim \frac{1}{2} e^{\beta} \sim \frac{E\,|\underset{\sim}{\rho} - \underset{\sim}{\rho}_0|^2}{\mu(T-E)(T_0 - E)} \tag{8.34}$$

so that

$$e^{i\eta\beta} \sim \left\{ \frac{2E\,|\underset{\sim}{\rho} - \underset{\sim}{\rho}_0|^2}{\mu(T-E)(T_0 - E)} \right\}^{i\eta} \,. \tag{8.35}$$

Regarding $I_{E,k}(\underset{\sim}{\rho},\underset{\sim}{\rho}_0)$ as the sum of two terms $I^+_{E,k}(\underset{\sim}{\rho},\underset{\sim}{\rho}_0) + I^-_{E,k}(\underset{\sim}{\rho},\underset{\sim}{\rho}_0)$ where $I^-_{E,k}(\underset{\sim}{\rho},\underset{\sim}{\rho}_0)$ is just $[I^+_{E,k}(\underset{\sim}{\rho},\underset{\sim}{\rho}_0)]^*$, we may now write $I^+_{E,k}(\underset{\sim}{\rho},\underset{\sim}{\rho}_0)$ near the energy shell in the form

$$I^{+}_{E,k}(\underset{\sim}{p},\underset{\sim}{p}_0) = \frac{8\mu p_E P_1^2 (x_1 x_2)^{i\eta-1}(x_3 x_4)^{-i\eta-1}}{i\pi^2(1 - e^{-2\pi\eta})} \qquad (8.36)$$

where

$$\left.\begin{aligned} \eta &= P_1/p_E \\ x_1 &= 4p_E^2 \\ x_2 &= |\underset{\sim}{p}-\underset{\sim}{p}_0|^2 = 2\mu k/\sigma(\Theta)^{1/2} \\ x_3 &= p_0^2 - p_E^2 \\ x_4 &= p^2 - p_E^2 \quad . \end{aligned}\right\} \qquad (8.37)$$

The Rutherford scattering identity is seen to arise when we evaluate the quantum-mechanical angular differential cross section from the spectral operator. The elaborate evaluation is carried out in detail in appendix D and here we shall only point out the important steps.

First of all we evaluate the evolution operator $U(\tau)$ from the spectral operator by a Fourier transformation as discussed in chapter 3. For our purposes we are interested in the value of

$$U_\tau(\underset{\sim}{p},\underset{\sim}{p}_0) = \int_{-\infty}^{\infty} dE\left(I^{+}_{E,k}(\underset{\sim}{p},\underset{\sim}{p}_0) + I^{-}_{E,k}(\underset{\sim}{p},\underset{\sim}{p}_0)\right)\exp\left(-\frac{iE\tau}{\hbar}\right) \qquad (8.38)$$

for large values of τ and β. Carrying out the integration over energy leads to the result

$$U_\tau(\underline{p},\underline{p}_0) = \frac{8 i p_m P_1^2 (x_1 x_2)^{i\eta_m - 1}}{\pi^{1/2}\{\exp(\pi\eta_m) - \exp(-\pi\eta_m)\}} \cdot \left(\frac{p^2 - p_0^2}{2}\right)^{-2i\eta_m - 1} \left\{\frac{(p^2 - p_0^2)\tau}{8\mu\hbar}\right\}^{i\eta_m + \frac{1}{2}}$$

$$\times \exp\left\{\frac{-i(p^2 + p_0^2)\tau}{4\mu\hbar}\right\} \frac{\underline{J}_{i\eta_m + \frac{1}{2}}\{(p^2 - p_0^2)\tau/4\mu\hbar\}}{\Gamma(1 + i\eta_m)} \qquad (8.39)$$

where the subscript m refers to the mean values of the quantities near to T and T_0 (which for large β are almost equal but have to be treated separately in the analysis). The expression (8.39) containing the term x_2 thus relates the evolution operator kernel for large times τ and large β directly to the classical quantity $\sigma(\Theta)$.

In terms of the evolution operator kernel for large times τ the probability P of scattering into unit solid angle is given by

$$\frac{\partial P}{\partial \Omega} = \int_0^\infty p^2 dp \, |U_\tau(\underline{p},\underline{p}_0)|^2 \quad . \qquad (8.40)$$

On carrying out this integration, the value of $\partial P/\partial \Omega$ on the energy shell is

$$\frac{\partial P}{\partial \Omega} = \frac{\sigma(\Theta)\tau p_E}{8\hbar^3 \mu \pi^3} . \tag{8.41}$$

The quantum-mechanical angular differential cross section $\sigma_{q.m.}(\Theta)$ is related to $\partial P/\partial \Omega$ by

$$\sigma_{q.m.}(\Theta) = 1/j\tau \; \partial P/\partial \Omega \tag{8.42}$$

where $j = p_E/\mu(2\pi\hbar)^3$ is the flux of the incident wave. We thus see that the value of $\sigma_{q.m.}(\Theta)$ is given by

$$\sigma_{q.m.}(\Theta) = \sigma(\Theta) \tag{8.43}$$

which is the Rutherford Scattering identity.

Tracing the derivation of the identity back from equation (8.43), we see that the identity arises, as we have said, because the quantum-mechanical spectral operator kernel as given in equation (8.36) may be expressed in terms of the classical angular differential cross section $\sigma(\Theta)$. That $\sigma(\Theta)$ occurs in this equation to the correct power is a consequence of the fact that near the energy shell, $\rho_E(\underset{\sim}{p}, \underset{\sim}{p}_0)$, although becoming singular, is also directly proportional to $\sigma(\Theta)$.

CHAPTER 9

CONCLUDING REMARKS

1) On the explanation of the Identities

The aim of this thesis has been primarily to explain the three correspondence identities that exist for the system of proton and electron. This has been achieved by obtaining a complete correspondence identity for the system and showing how each of the identities follows as a consequence of this. To provide a complete correspondence identity we have expressed the kernel of the quantum-mechanical spectral operator in momentum representation for all real values of the energy explicitly as a sum over paths of terms involving the classical action for the path.

From the form of the complete correspondence identity for negative values of the energy we have been able to explain for the first time the Bohr-Sommerfeld identity. It is well known that the Bohr-Sommerfeld conditions can be derived from the W.K.B. method and also from the phase-integral approximation: "The Bohr formula is obtained without gimmickry", Gutzwiller (1967), but no satisfactory explanation of the Bohr-Sommerfeld identity has ever been given: "The question why these quantum conditions give nevertheless the correct energy values for several important cases, such as the hydrogen atom or the linear oscillator is a purely mathematical problem whose discussion would lead us too far astray", Jammer (1966). We have seen that the question has been more one of obtaining a representation in which a ray theory is valid and describes exactly the behaviour of matter waves, than one purely of mathematics.

As well as obtaining a complete correspondence identity in momentum representation we saw that it was also possible to provide such an identity in the related symmetric representation. From the $O(4)$ dynamical symmetry properties exhibited by the classical- and quantum-mechanical solutions of the Coulomb problem in this representation we were able to explain the Fock identity. The $O(4)$ symmetry properties were useful in the derivation of the complete correspondence identity for the operator J_ν, but to what extent the presence of such dynamical symmetry is essential to the existence of correspondence identities is as yet unknown.

For positive energies the $O(1,3)$ symmetry properties were also useful in obtaining the kernel of the operator $\mathcal{J}_E$ and in providing a complete correspondence identity. Equally important in this derivation was the analytic continuation of the paths and action functions, through which we were able to obtain precisely the quantal barrier penetration in momentum space. The explanation of the Rutherford scattering identity, as given, is perhaps rather lengthy and mathematical. Nevertheless the origin of the identity can be traced back to the fact that the spectral operator kernel near the energy shell in momentum representation may be expressed in terms of the classical differential cross section in such a way that the quantal differential cross section, when derived from the spectral operator kernel, is identical to the classical result. This derivation is of general application and provides an alternative method of obtaining a differential cross section. It is particularly useful for the Coulomb interaction since the long range distortion of the incident wave (interpreted first of all by Gordon 1928) does not have to be considered explicitly. It is interesting to note that even when the distortion is deliberately not taken into account as in the first Born approximation for the differential cross section, the Rutherford formula is still obtained, although the phase of the scattering amplitude is then given incorrectly (see for example Burhop 1961, Wu and Ohmura 1962). The long-range effects of the Coulomb potential are implicit in the kernel of the spectral operator.

2) On the Complete Correspondence Identity

One very important feature of the work done in this thesis is the fact that we have shown that a ray theory does exist for the system of proton and electron which describes completely and exactly the behaviour of matter waves. Whether this is necessarily the case for other systems and there does always exist some operator and and a representation for which we can obtain a complete correspondence identity is just not known. For the system in question we ought to note the following points concerning the existence of the complete correspondence identity.

The existence seems to depend crucially on the choice of representation. We were not able to obtain a complete correspondence identity in position representation, for example, even though for positive energies it did seem the more natural choice as opposed to momentum representation. We were able to provide a complete correspondence identity only in momentum and the related symmetric representations.

Secondly the choice of operator is also important. We were not able to provide an expansion in terms of classical paths for either the Green functions or evolution operator kernel and only for the spectral operator kernel could we obtain a complete correspondence identity. Yet, for the free particle we were able to express all the operator kernels just mentioned in terms of sums over classical paths.

Finally, there were correspondence identities associated with the system. Whether this last remark has any bearing on the existence of a complete correspondence identity again is not known, but it seems reasonable to suppose that correspondence identities are consequences of a more general relation between the theories of classical and quantum mechanics, as is given, for example, by a complete correspondence identity. For the electron-proton system it was the three identities which stimulated the search for such a complete correspondence identity in the first place.

We should also note the differences in the form of the complete correspondence identity for negative and positive energies. For the bound states the spectral operator kernel is expressed as a sum over classical paths; for the continuum we have to consider generalised classical paths. For the bound states all classical paths are included in the expansion, whilst for positive energy states the expansion includes only those generalised classical paths associated with the particular potential under consideration. In the sense that we have labelled the generalised classical paths 'attractive' or 'repulsive', we have to label all the classical paths for the bound states 'attractive'. Each set of generalised classical trajectories, whether it is labelled attractive or repulsive, includes paths which are built up out of the classical trajectories of both the repulsive and attractive Coulomb potential. Thus for positive energies, the quantum-mechanical solution for one potential is intimately related to the classical solutions of both types of potential.

In contrast to the bound states the Fock identity no longer holds for positive energies. For the attractive potential the classical microcanonical momentum distribution $\rho_E^{c.m}(\underset{\sim}{p})$ normalised to unit inward flux is given by (Banks, private communication)

$$\rho_E^{c.m}(\underset{\sim}{p}) = \frac{64\pi k^3 \mu^4}{p_E^2 (p^2 - p_E^2)^4} \times \begin{cases} 1 & \text{for } |\underset{\sim}{p}| > p_E \\ 0 & \text{for } |\underset{\sim}{p}| < p_E \end{cases} \qquad (9.1)$$

whereas the quantal distribution, having the same normalization in the classical limit is

$$\rho_E^{q.m.}(\underset{\sim}{p}) = \frac{64\pi k^3 \mu^4}{p_E^2 (p^2 - p_E^2)^4 (1 - e^{-2\pi\eta})} \times \begin{cases} 1 & \text{for } |\underset{\sim}{p}| > p_E \\ e^{-2\pi\eta} & \text{for } |\underset{\sim}{p}| < p_E . \end{cases} \qquad (9.2)$$

That the identity does not hold is really to be expected since the region of momentum space $|\underset{\sim}{p}| < p_E$ is classically inaccessible. However in the classically accessible region the two distributions differ by the factor $(1 - e^{-2\pi\eta})^{-1}$. This factor, as we saw in chapter 8, arises from the quantal barrier penetration in momentum space. In the classical limit as $\eta \to \infty$ the two distributions nevertheless become equal.

3) Extensions of the Theory

By means of the complete correspondence identity for negative values of the energy we have thus provided a model of the hydrogen atom based on classical electron orbits. The model differs from the Bohr-Sommerfeld model of the hydrogen atom in several respects. First of all the electron orbits are those in momentum and symmetric space as opposed to the elliptic orbits in the Bohr-Sommerfeld model. Secondly, for a given energy level, the model includes a statistical distribution of orbits consistent with this energy, whereas the Bohr-Sommerfeld model includes only those with particular eccentricities and restricted orientations associated with the quantum numbers ℓ and m. The model also leads to the same physical results as modern non-relativistic quantum theory and can be generalised to positive energies. However, unlike the Bohr-Sommerfeld model, we cannot account for the quantization of ℓ and m in classical terms, and this would seem a worthwhile problem to consider.

More ambitious problems to consider are those which if solved could explain the difficulties encountered in providing a complete correspondence identity. We should expect, for the Coulomb interaction, that if we chose to evaluate the spectral operator kernel by means of path summation then we should have to consider Feynman path summation and not just sums over classical paths. As we have seen summing over only the classical paths is completely adequate in momentum and the related symmetric representations. Thus, why do the Feynman paths reduce to the classical paths in these representations? Also, why is this not the case for the Green functions or evolution operator kernels? Perhaps if these questions can be answered we may be able to provide criteria whereby for a given operator and a given potential we could decide whether a representation existed in which a complete correspondence identity was possible. If this is the case we may well find ourselves discovering new correspondence identities as well as explaining those already known.

Appendix A

The Green functions $G_E^{\pm}(x,x_0)$ for the continuous spectrum are given by

$$G_E^{\pm}(x,x_0) = \int_{\substack{\text{continuous}\\ \text{spectrum}}} dE' \, \frac{\psi_{E'}(x)\,\psi_{E'}^{*}(x_0)}{(E - E' \pm i\varepsilon)} \qquad (A.1)$$

For the free particle the normalised wave functions are

$$\psi_E^{\pm}(x) = \left(\frac{1}{2\pi\hbar}\sqrt{\frac{m}{2E}}\right)^{1/2} \exp \pm \frac{i}{\hbar}(2mE)^{1/2}x \quad . \qquad (A.2)$$

Thus substituting in equation (A.1) we have

$$G_E^{\pm}(x,x_0) = \int_0^{\infty} \frac{dE'}{2\pi\hbar}\left(\frac{m}{2E'}\right)^{1/2} \frac{\exp i/\hbar\,(2mE')^{1/2}(x-x_0)}{(E-E' \pm i\varepsilon)}$$

$$+ \int_0^{\infty} \frac{dE'}{2\pi\hbar}\left(\frac{m}{2E'}\right)^{1/2} \frac{\exp -i/\hbar\,(2mE')^{1/2}(x-x_0)}{(E-E' \pm i\varepsilon)} \quad . \qquad (A.3)$$

With the change of variable, $p^2 = 2mE'$, we have for $G_E^{\pm}(x,x_0)$:

$$G_E^+(x,x_0) = \int_0^\infty \frac{dp}{2\pi\hbar} \cdot \frac{\exp \frac{ip}{\hbar}(x-x_0)}{(E+i\varepsilon - p^2/2m)} + \int_0^\infty \frac{dp}{2\pi\hbar} \cdot \frac{\exp -\frac{ip}{\hbar}(x-x_0)}{(E+i\varepsilon - p^2/2m)}$$

$$= \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \frac{\exp i/\hbar \, p(x-x_0)}{(E+i\varepsilon - p^2/2m)} \quad . \qquad (A.4)$$

Regarding p as a complex variable, we see that the integrand has poles whenever $p^2 = 2mE + i\varepsilon$ as shown in the Figure A.1.

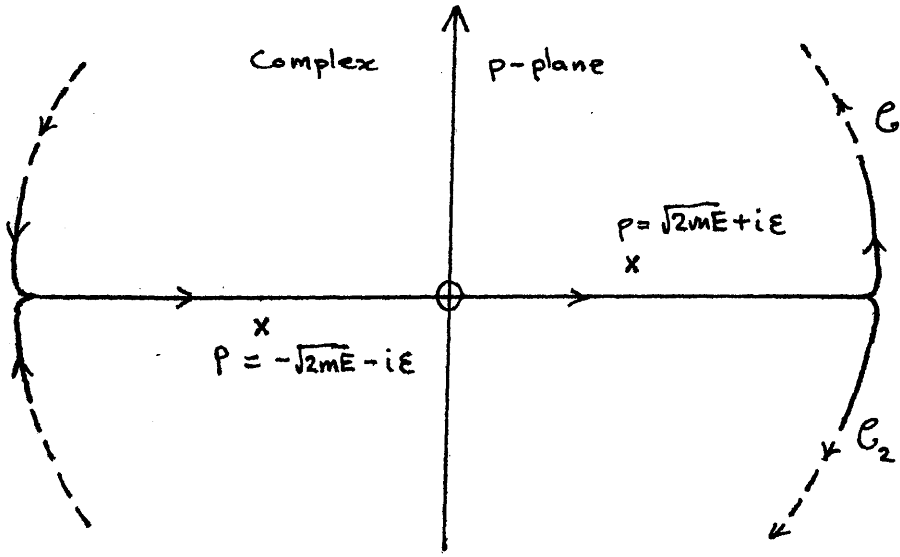

Figure A.1. Diagram showing the poles $p = \pm\sqrt{2mE} \pm i\varepsilon$ and the two contours $\mathcal{C}_1$ and $\mathcal{C}_2$.

If $x > x_0$, then the integrand of equation (A.4) tends to zero when evaluated along a large semicircle in the upper half-plane. Integrating over the contour $\mathcal{C}_1$ we obtain the result

$$\int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\, \frac{\exp i\, p/\hbar\,(x-x_0)}{(E+i\varepsilon-p^2/2m)} = \oint_{\mathcal{C}_1} \frac{dp}{2\pi\hbar}\, \frac{\exp i/\hbar\, p(x-x_0)}{(E-p^2/2m)}$$

$$= 2\pi i \times (\text{Residue at } p=\sqrt{2mE}+i\varepsilon)$$

$$= \frac{1}{i\hbar}\left(\frac{m}{2E}\right)^{1/2} \exp \frac{i}{\hbar}(2mE)^{1/2}(x-x_0). \qquad (A.5)$$

For $x < x_0$, we integrate over the contour $\mathcal{C}_2$ and obtain

$$\int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\, \frac{\exp i\, p/\hbar\,(x-x_0)}{(E+i\varepsilon-p^2/2m)} = \oint_{\mathcal{C}_2} \frac{dp}{2\pi\hbar}\, \frac{\exp i/\hbar\, p(x-x_0)}{(E-p^2/2m)}$$

$$= -2\pi i \times (\text{Residue at } p=-\sqrt{2mE}-i\varepsilon)$$

$$= \frac{1}{i\hbar}\left(\frac{m}{2E}\right)^{1/2} \exp \frac{i}{\hbar}(2mE)^{1/2}(x_0-x). \qquad (A.6)$$

Thus for all values of x, x_0, we obtain for the Green function

$$G_E^+(x,x_0) = \frac{1}{i\hbar}\left(\frac{m}{2E}\right)^{1/2} \exp \frac{i}{\hbar}(2mE)^{1/2}|x-x_0| \qquad (A.7)$$

and consequently, since $G_E^-(x,x_0) = [G_E^+(x,x_0)]^*$ we have also

$$G_E^-(x,x_0) = -\frac{1}{i\hbar}\left(\frac{m}{2E}\right)^{1/2} \exp -\frac{i}{\hbar}(2mE)^{1/2}|x-x_0| . \qquad (A.8)$$

Appendix B

We assume that the Lagrangian $L(\dot{x}, x, t)$ describing the system is a quadratic function of the variables $\dot{x}$, x so that

$$L = a(t)\dot{x}^2 + b(t)\dot{x}x + c(t)x^2 + d(t)\dot{x} + e(t)x + f(t) \, . \qquad \text{(B.1)}$$

We are interested in evaluating the path integral

$$U(x,t;x_0,t_0) = \int_{\Omega} \exp\left[\frac{i}{\hbar}\int_{t_0}^{t} dt' L(\dot{x},x,t')\right] d\left[x(t')\right] \qquad \text{(B.2)}$$

over all paths in Ω which go from (x_0, t_0) to (x,t) .

Let $\bar{x}(t')$ be the classical path between the specified end points. Along this path the value of the action is an extremum. For any other path, we can represent x in terms of $\bar{x}$ and a new variable y :

$$x = \bar{x} + y \quad . \qquad \text{(B.3)}$$

A point on the path is defined now in terms of the deviation $y(t')$ from the classical path as shown in Figure B.1. Since, for each given time t' in the interval $(t - t_0)$

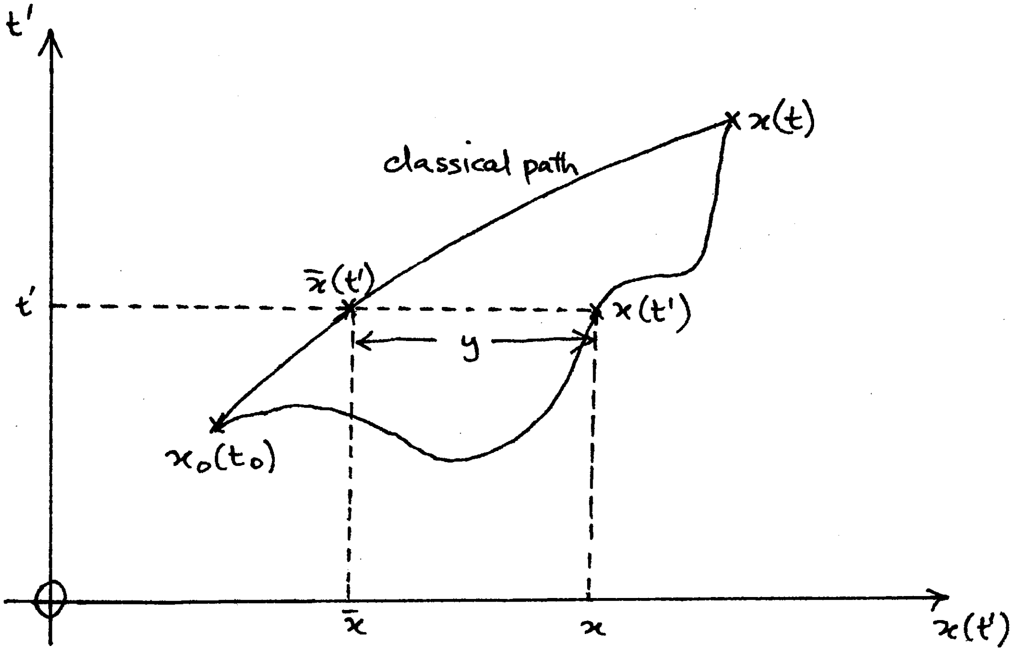

Figure B.1. The point $x(t')$ is given in terms of $\bar{x}(t')$ and its deviation from the classical path.

the variables x and y differ by the constant $\bar{x}$, then we have

$$d[x(t')] = d[y(t')] \quad . \tag{B.4}$$

The action along a path $x(t')$ in Ω between $x_0(t_0)$ and $x(t)$ is given by

$$S[x(t')] = S[\bar{x}(t') + y(t')]$$

$$= \int_{t_0}^{t} \left[a(t')\left(\dot{\bar{x}}^2 + 2\dot{\bar{x}}\dot{y} + \dot{y}^2\right) + \dots \quad \dots \right] dt' . \qquad (B.5)$$

Now since the value of the action along $\bar{x}(t')$ is stationary, then in the expression (B.5) only the terms that are of second order in $y, \dot{y}$ remain, together with the action for the classical path, so that

$$S[x(t')] = S_{cl}(x,t;x_0,t_0) + \int_{t_0}^{t} \left[a(t')\dot{y}^2 + b(t')\dot{y}y + c(t')y^2 \right] dt' . \qquad (B.6)$$

The path integration by virtue of equation (B.4) does not depend upon the classical path, so the kernel can be written

$$U(x,t;x_0,t_0) = e^{i/\hbar\, S_{cl}(x,t;x_0,t_0)} \int_0^0 \exp\left[\frac{i}{\hbar} \int_{t_0}^{t} \left[a(t')\dot{y}^2 + b(t')\dot{y}y + c(t')y^2 \right] dt' \right] d[y(t')] . \qquad (B.7)$$

Since all paths $y(t')$ start from and return to the point $y = 0$, the integral over paths can only be a function of the times (t, t_0) of the end points and the kernel is thus given by the classical path:

$$U(x,t;x_0,t_0) = F(t,t_0) \exp i/\hbar\, S_{cl}(x,t;x_0,t_0) . \qquad (B.8)$$

Appendix C

We have the following operator equation:

$$(E-H) = \left(E-\frac{p^2}{2\mu}\right)\left(I-\nu Q\right) . \qquad (C.1)$$

Taking the inverse of both sides we obtain

$$(E-H)^{-1} = (I-\nu Q)^{-1}\left(E-p^2/2\mu\right)^{-1}. \qquad (C.2)$$

Now by definition

$$\delta(E-H) = \frac{1}{2\pi i}\lim_{\varepsilon\to 0}\left((E-H-i\varepsilon)^{-1}-(E-H+i\varepsilon)^{-1}\right) . \qquad (C.3)$$

Since the operator $(E - p^2/2\mu)$ is never zero for $E<0$, we may use equation (C.2) with (C.3), noting that $E \pm i\varepsilon$ corresponds to $\nu \pm i\nu_I$ (where ε, ν_I are small) and we have

$$\delta(E-H) = \frac{1}{2\pi i}\lim_{\nu_I\to 0}\left\{(I-(\nu-i\nu_I)Q)^{-1}-(I-(\nu+i\nu_I)Q)^{-1}\right\}$$

$$\times\left(E-p^2/2\mu\right)^{-1}. \qquad (C.4)$$

The operator Q is a positive definite operator whose norm is bounded in symmetric space, so equation (C.4) may be expressed as

$$\delta(E-H) = \lim_{\nu_I \to 0} \frac{1}{2\pi i} \left\{ (I - \nu Q + i\nu_I)^{-1} - (I - \nu Q - i\nu_I)^{-1} \right\}$$

$$\times \, (E - p^2/2\mu)^{-1}. \qquad \text{(C.5)}$$

Using the definition in equation (C.3), we may rewrite the right-hand side of equation (C.5) and obtain the required result:

$$\delta(E-H) = -\,\delta(I - \nu Q)(E - p^2/2\mu)^{-1}.$$

Appendix D

The form of $I^{+}_{E,k}(\underset{\sim}{p},\underset{\sim}{p}_0)$ near the energy shell is

$$I^{+}_{E,k}(\underset{\sim}{p},\underset{\sim}{p}_0) = \frac{8\mu p_E P_1^2 (x_1x_2)^{i\eta-1}(x_3x_4)^{-i\eta-1}}{i\pi^2(1-e^{-2\pi\eta})} \qquad (D.1)$$

where

$$\left.\begin{aligned} \eta &= P_1/p_E \\ x_1 &= 4p_E^2 \\ x_2 &= |\underset{\sim}{p}-\underset{\sim}{p}_0|^2 \\ x_3 &= p_0^2 - p_E^2 \\ x_4 &= p^2 - p_E^2 \; . \end{aligned}\right\} \qquad (D.2)$$

In evaluating the evolution operator kernel $U_\tau(\underset{\sim}{p},\underset{\sim}{p}_0)$ for large τ and β given by

$$U_\tau(\underset{\sim}{p},\underset{\sim}{p}_0) = \int_{-\infty}^{\infty} dE\,\left(I^{+}_{E,k}(\underset{\sim}{p},\underset{\sim}{p}_0) + I^{-}_{E,k}(\underset{\sim}{p},\underset{\sim}{p}_0)\right) \exp -\frac{iE\tau}{\hbar} \qquad (D.3)$$

we note, by the Riemann-Lebesgue Lemma, that the only contributions will arise from the singularities in

$I_{E,k}^{\pm}(\underset{\sim}{\rho},\underset{\sim}{\rho_0})$. These occur when E takes on the values $T_0 = \rho_0^2/2\mu$, $T = \rho^2/2\mu$. Without loss of generality we assume that $T > T_0$ and investigate the singularities of $I_E^+(\underset{\sim}{\rho},\underset{\sim}{\rho_0})$ as the energy E ranges from $-\infty$ to ∞ along the real axis. For negative energies there can be no contribution to the scattering as the wave functions are bounded.

If $\underset{\sim}{\rho}, \underset{\sim}{\rho_0}$ lie in the accessible region, then by taking the branch cuts of $\log(T-E)$ in the complex E plane to run from T to $T-i\infty$, we can define the phase of x_4 , on the real axis, to be zero to the left and $-\pi$ to the right of the branch point. Similarly we can define the phases of x_3 on either side of the corresponding branch point to be 0 and $-\pi$, so that I_E^+ is uniquely defined for all regions of momentum space in accordance with equation (8.23). Because of the factor $\exp(-iE\tau/\hbar)$ in equation (D.3), the contour must be closed in the lower half plane to ensure convergence.

For $I_E^-(\underset{\sim}{\rho},\underset{\sim}{\rho_0})$ the singularities again arise at the same points but the branch cuts are now from T to $T+i\infty$ and T_0 to $T_0+i\infty$. Again the contour has to be closed in the lower half plane, and thus for large positive τ

$$\int_{-\infty}^{\infty} dE \, I^{-}_{E,k}(\underset{\sim}{\rho},\underset{\sim}{\rho_0}) \exp\left(-\frac{iE\tau}{\hbar}\right) = 0 . \qquad (D.4)$$

Thus

$$U_\tau(\underset{\sim}{\rho},\underset{\sim}{\rho_0}) = \int_{\mathcal{C}} \frac{dE \, 8\mu P_1^2 P_E (x_1 x_2)^{i\eta-1}(x_3 x_4)^{-i\eta-1} \exp(-iE\tau/\hbar)}{i\pi^2(1-e^{-2\pi\eta})} \qquad (D.5)$$

where the contour $\mathcal{C}$ is as shown in the Figure D.1.

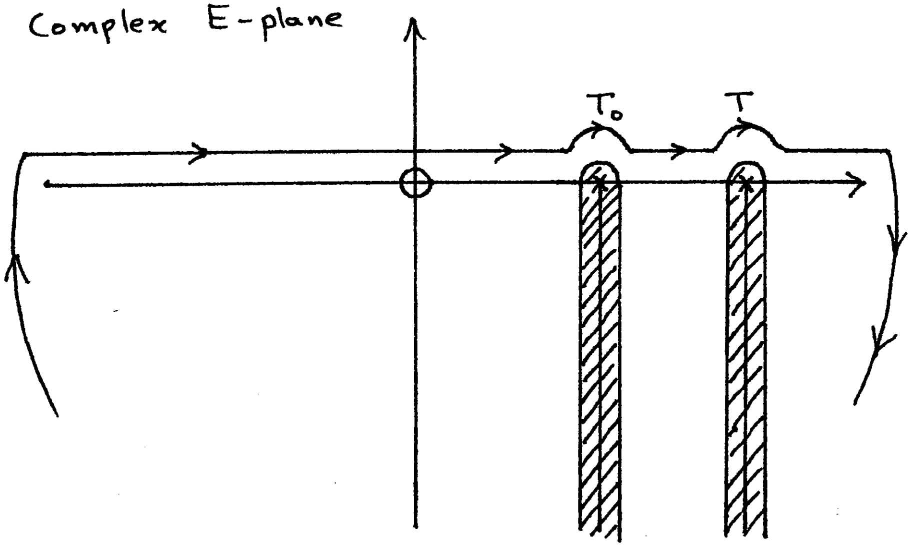

Figure D.1. The contour $\mathcal{C}$.

The terms in the integrand which are regular near the singular points may be considered constant and taken outside the integral. Since we are considering only large values of β then T and T_0 are approximately equal and we may label the mean quantities with the same subscript m. So we can write

$$U_\tau(\underset{\sim}{\rho},\underset{\sim}{\rho_0}) = \frac{8\mu P_m P_1^2 (x_1 x_2)^{i\eta_m - 1}\,\mathcal{J}}{i\pi^2\{1-\exp(-2\pi\eta_m)\}} \tag{D.6}$$

where

$$\mathcal{J} = \int_{\mathcal{C}} dE \exp\left(-\frac{iE\tau}{\hbar}\right)(x_3 x_4)^{-i\eta_m - 1} \tag{D.7}$$

To evaluate this latter integral we make the substitution $y = \{(p^2 + p_0^2) - 2p_E^2\}/(p^2 - p_0^2)$ and obtain

$$\mathcal{J} = \left(\frac{p^2 - p_0^2}{2}\right)^{2i\eta_m - 1} \frac{1}{2\mu} \exp\left\{\frac{-i(p^2+p_0^2)\tau}{4\mu\hbar}\right\} \mathcal{J}' \tag{D.8}$$

where $\mathcal{J}'$ is the integral

$$\mathcal{J}' = \int_{\mathcal{C}'} dy\, e^{i\alpha y}(y^2 - 1)^{\nu - \frac{1}{2}} \tag{D.9}$$

with

$$\alpha = \frac{(p^2 - p_0^2)\tau}{4\mu\hbar} \tag{D.10}$$

$$\nu = -i\eta_m - \frac{1}{2} \tag{D.11}$$

and $\mathcal{C}'$ is the contour shown in Figure D.2.

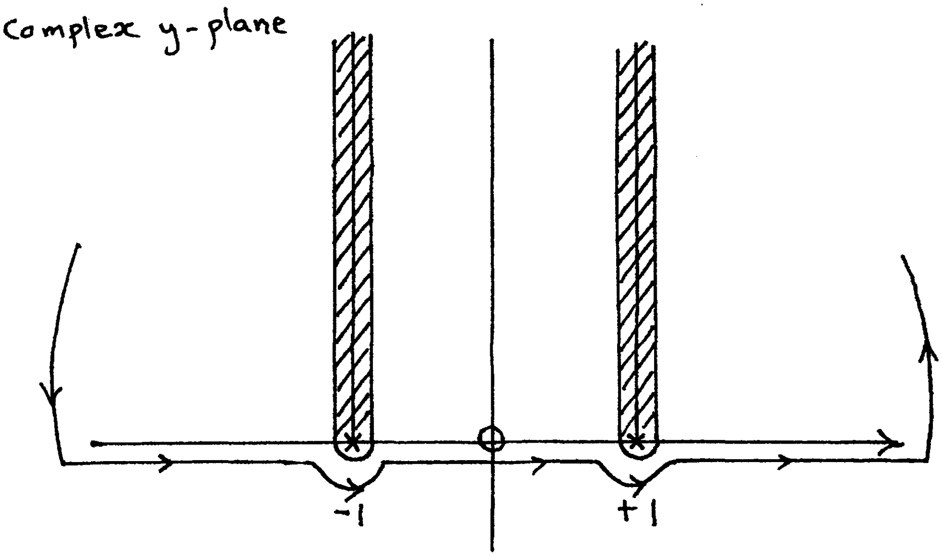

Figure D.2. Contour $\mathcal{C}'$ for the integral of equation (D.9).

With this contour, $\mathcal{J}'$ is just Hankel's integral for the Bessel function $J_{-\nu}(\alpha)$ given by (Watson 1966, chap. VI)

$$J_{-\nu}(\alpha) = \frac{\Gamma(\frac{1}{2}-\nu)(\frac{1}{2}\alpha)^{\nu} e^{i\pi\nu} g'}{2\pi i\,\Gamma(\frac{1}{2})} . \qquad (D.12)$$

It now follows that the kernel of the evolution operator for large τ is

$$U_\tau(\underset{\sim}{p}, \underset{\sim}{p}_0) = \frac{i\, 8 p_m P_1^2 (x_1 x_2)^{i\eta_m - 1}}{\pi^{1/2}\{\exp(\pi\eta_m) - \exp(-\pi\eta_m)\}} \left(\frac{p^2 - p_0^2}{2}\right)^{-2i\eta_m - 1} \left\{\frac{(p^2 - p_0^2)\tau}{8\mu\hbar}\right\}^{i\eta_m + \frac{1}{2}}$$

$$\times \exp\left\{\frac{i(p^2 + p_0^2)\tau}{4\mu\hbar}\right\} \frac{J_{i\eta_m + \frac{1}{2}}\{(p^2 - p_0^2)\tau/4\mu\hbar\}}{\Gamma(1 + i\eta_m)} \qquad (D.13)$$

and

$$|U_\tau(\underset{\sim}{p}, \underset{\sim}{p}_0)|^2 = \frac{64 P_m^2 P_1^4 x_1^{-2} x_2^{-2}}{\pi(\exp(\pi\eta_m) - \exp(-\pi\eta_m))^2} \left(\frac{p^2 - p_0^2}{2}\right)^{-2} \left(\frac{p^2 - p_0^2}{8\mu\hbar}\right)\tau$$

$$\times \frac{J_{i\eta_m + \frac{1}{2}}(\alpha)\, J_{-i\eta_m + \frac{1}{2}}(\alpha)}{\pi\eta_m \{\sinh(\pi\eta_m)\}^{-1}}$$

$$= \frac{\eta_m^3 \tau}{32\pi^2 \sinh(\pi\eta_m) P_m^2 \mu\hbar} \; \frac{1}{\sin^4\frac{\Theta}{2}} \; \frac{1}{p^2 - p_0^2} J_{i\eta_m + \frac{1}{2}}(\alpha) J_{-i\eta_m + \frac{1}{2}}(\alpha) \qquad (D.14)$$

where Θ is the scattering angle.

For large times τ the value of $|U_\tau(\underset{\sim}{p}, \underset{\sim}{p_0})|^2$ as a function of p^2 is small except near p_0^2 . The probability of scattering into unit solid angle is given by

$$\frac{\partial P}{\partial \Omega} = \int_0^\infty p^2 dp \, |U_\tau(\underset{\sim}{p}, \underset{\sim}{p_0})|^2$$

$$= \frac{\eta_m^3 \, \tau \, \operatorname{cosec}^4 \frac{1}{2}\Theta}{32 \mu \hbar \pi^2 \sinh(\pi\eta_m) p_m^2} \int_0^\infty \frac{p^2 dp}{p^2 - p_0^2} J_{i\eta_m+\frac{1}{2}}(\alpha) \, J_{-i\eta_m+\frac{1}{2}}(\alpha) . \qquad (D.15)$$

Noting that the only significant contribution to the integral arises near $p^2 = p_0^2$, we shift the origin to p_0^2 and obtain

$$\frac{\partial P}{\partial \Omega} = \frac{\eta_m^3 \, \tau \, \operatorname{cosec}^4 \frac{1}{2}\Theta}{32 \mu \hbar \pi^2 \sinh(\pi\eta_m) p_m} \int_0 \frac{d(p^2 - p_0^2)}{p^2 - p_0^2} J_{i\eta_m+\frac{1}{2}}(\alpha) J_{-i\eta_m+\frac{1}{2}}(\alpha)$$

$$= \frac{\eta_m^3 \, \tau \, \operatorname{cosec}^4 \frac{1}{2}\Theta}{32 \mu \hbar \pi^2 \sinh(\pi\eta_m) p_m} \cdot \frac{\sinh \pi\eta_m}{\pi\eta_m} \qquad (D.16)$$

which on the energy shell becomes $k^2 \mu \tau \operatorname{cosec}^4 \Theta/2 \,/\, \hbar^3 p_E^3 \pi^3 32$. The identity then follows as given in chapter 8.

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Abstract. The complete quantum-dynamical solutions for a free particle moving in one dimension and for a free particle moving on a ring are obtained in terms of classical path sums. The propagators and Green operator kernels, and, in particular, the kernel of the spectral operator $I_E = \delta(E-H)$ are expressed explicitly in this way. Relations between quantum and classical mechanics which hold for low quantum numbers and relatively small values of the classical action are discussed. They are the correspondence identities.

1. Introduction

We consider when and how the solutions of a quantum-mechanical problem with time-independent Hamiltonian may be obtained directly from the solution of the equivalent classical problem. The correspondence limit $\hbar \to 0$ is well known, but in the words of Schrödinger (1928), "The Hamiltonian analogy of mechanics to optics is an analogy to geometrical optics, since to the paths of the representative points in configuration space there corresponds, on the optical side, the light ray, which is only rigorously defined in terms of geometrical optics. The undulatory elaboration of the optical picture leads to the surrender of the idea of the path of the system as soon as the dimensions of the path are not great in comparison with the wavelength". However, in this and later papers we shall discuss several important simple physical systems for which the ray picture is valid for arbitrary wavelength, provided that an appropriate representation is chosen. For such problems we are able to obtain a complete quantum-dynamical solution in terms of sums over classical paths. These sums are of the same general form as the Feynman path sums, but are simpler in conception and analysis. From this general solution we obtain particular relations between classical and quantum mechanics which are valid even for low quantum numbers and for relatively small values of the action. These are the correspondence identities.

In this paper we shall restrict ourselves to the simplest examples of a system with a continuous and with a discrete energy spectrum, choosing the free particle moving in one dimension and the free particle with periodic boundary conditions, that is, the particle on a ring. The comparatively simple analysis is a useful introduction to the more difficult theory of the Coulomb potential. Because of the divergent properties of the kernels of some of the operators, generalized functions are used freely (Lighthill 1960, Messiah 1965, Kurşunoğlu 1962).

As is well known, the solution of a quantum-mechanical problem may be expressed in terms of the evolution operator (Messiah 1965, p. 310) or propagator (Kurşunoğlu 1962, p. 152), or in terms of the Green operators $G_E^{\pm}$ (Newton 1966, p. 178). We shall also make use of the 'spectral operator' given by

$$I_E = \delta(E-H) \tag{1}$$

which provides a solution of the dynamical problem with Hamiltonian H through the resolution of the identity. Each of these operators will be obtained as sums over classical paths for the simple systems above.

In related work, Garrod (1966) considers the spectral operator but not in terms of the classical path sums, whereas Gutzwiller (1967) expresses Green functions in terms of classical paths, but does not consider the spectral operator.

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2. Operators

The development of a quantum-mechanical system in time is given by a unitary transformation from the state $\psi(t_0)$ at time t_0 to the state $\psi(t)$ at another time t. Thus

$$\psi(t) = U(t, t_0)\psi(t_0) \qquad \text{all } t_0, t \tag{2}$$

where U is the evolution operator. As defined here, the evolution operator is two-sided and relates the state at time t_0 to both earlier and later states $\psi(t)$. Formally U may be expressed in terms of the time-independent Hamiltonian H as

$$U(t, t_0) = \exp\left\{\frac{-\mathrm{i}H(t-t_0)}{\hbar}\right\}. \tag{3}$$

The usual forward evolution operator $U^+(t, t_0)$, which relates $\psi(t_0)$ to the wave function at a later time t, is defined in terms of $U(t, t_0)$ by the equations

$$\begin{aligned} U^+(t,t_0) &= U(t,t_0), & t &> t_0 \\ &= 0 & t &< t_0. \end{aligned} \tag{4}$$

The kernel of U^+ is the propagator. The backward evolution operator is similarly defined by the equations

$$\begin{aligned} U^-(t,t_0) &= 0, & t &> t_0 \\ &= U(t,t_0), & t &< t_0. \end{aligned} \tag{5}$$

So that

$$U(t,t_0) = U^+(t,t_0)+U^-(t,t_0) \tag{6}$$

and

$$U^-(t,t_0) = [U^+(t_0,t)]^\dagger. \tag{7}$$

The Green operators are obtained by transforming the forward and backward evolution operators from time representation to energy representation by Fourier analysis. Using factors of the form $(2\pi\hbar)^{-1/2}\exp(\mathrm{i}Et/\hbar)$ to preserve normalization, we have

$$U^+(E,E_0) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\mathrm{d}t\int_{-\infty}^{\infty}\mathrm{d}t_0\,\epsilon(t-t_0)\exp\left(\frac{\mathrm{i}Et}{\hbar}\right)\exp\left\{-\frac{\mathrm{i}H(t-t_0)}{\hbar}\right\}\exp\left(-\frac{\mathrm{i}E_0t_0}{\hbar}\right) \tag{8}$$

where $\epsilon(t-t_0)$ is the Heaviside unit function. The integration gives

$$\begin{aligned} U^+(E,E_0) &= \delta(E-E_0)\frac{\mathrm{i}\hbar}{E-H+\mathrm{i}\epsilon} \\ &= \mathrm{i}\hbar\delta(E-E_0)G_E{}^+. \end{aligned} \tag{9}$$

Similarly

$$\begin{aligned} U^-(E,E_0) &= -\delta(E-E_0)\frac{\mathrm{i}\hbar}{E-H-\mathrm{i}\epsilon} \\ &= -\mathrm{i}\hbar\delta(E-E_0)G_E{}^- \\ &= -\mathrm{i}\hbar\delta(E-E_0)(G_E{}^+)^\dagger. \end{aligned} \tag{10}$$

On carrying out the transformation to energy representation of the two-sided evolution operator we obtain

$$
\begin{aligned}
U(E, E_0) &= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \mathrm{d}t_0 \int_{-\infty}^{\infty} \mathrm{d}t \exp\left\{-\frac{\mathrm{i}}{\hbar}(E_0-H)t_0\right\} \exp\left\{\frac{\mathrm{i}}{\hbar}(E-H)t\right\} \\
&= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \mathrm{d}t_0 \int_{-\infty}^{\infty} \mathrm{d}\tau \exp\left\{\frac{\mathrm{i}}{\hbar}(E-E_0)t_0\right\} \exp\left\{\frac{\mathrm{i}}{\hbar}(E-H)\tau\right\} \\
&= 2\pi\hbar\delta(E-E_0)\delta(E-H) \\
&= 2\pi\hbar\delta(E-E_0)I_E \qquad (11)
\end{aligned}
$$

where I_E is the spectral operator. It follows from the Fourier transform of equation (6) that

$$I_E = \frac{1}{2\pi\mathrm{i}}(G_E{}^{-} - G_E{}^{+}). \qquad (12)$$

Thus, at the νth energy level E_ν of the discrete spectrum, the form of the spectral operator is given by the residue of $(E-H)^{-1}$, and in the continuous spectrum it is given by the discontinuity across the cut in the complex plane. In each case, the spectral operator has the form of a projection operator.

This leads to an alternative treatment of the spectral operator. Any analytic function $f(H)$ of the Hamiltonian H can be expressed in terms of the projection operators P_ν onto the subspaces of eigenstates belonging to discrete energy levels E_ν, and the projection operators P_E onto the subspaces belonging to the continuous spectrum $\mathscr{S}$:

$$f(H) = \sum_\nu P_\nu f(E_\nu) + \int_{\mathscr{S}} \mathrm{d}E'\, P_{E'} f(E'). \qquad (13)$$

If we suppose that the same relations apply to generalized functions of H we obtain (Schönberg 1951)

$$
\begin{aligned}
I_E = \delta(E-H) &= \sum_\nu P_\nu \delta(E-E_\nu) + \int_{\mathscr{S}} \mathrm{d}E'\, P_{E'}\delta(E'-E) \\
&= \sum_\nu P_\nu \delta(E-E_\nu) + \mathscr{E}_{\mathscr{S}}(E) P_E \qquad (14)
\end{aligned}
$$

where $\mathscr{E}_{\mathscr{S}}(E) = 1$ when E is in the continuous spectrum and zero otherwise. This equation expresses the spectral operator explicitly in terms of projection operators. Care must be taken to ensure that the projection operator P_E is correctly normalized.

Thus a knowledge of the spectral operator enables us to perform a resolution of the identity operator, and to diagonalize the Hamiltonian.

From equation (14) it follows that

$$\int_{-\infty}^{\infty} I_E\, \mathrm{d}E = I \qquad \text{(resolution of the identity)} \qquad (15a)$$

$$HI_E = EI_E \qquad \text{(specification of Hamiltonian).} \qquad (15b)$$

These properties can be used to define the spectral operator. It should be noted that the integral in equation (15*a*) is taken over the entire real axis.

3. Free particle in one dimension

A theory based on rays or classical paths is entirely adequate for the treatment of waves in a homogeneous medium, or free particles in quantum mechanics, provided that a phase is associated with each ray or classical path between two points in space–time. Thus the original de Broglie relations between wave number and momentum, and between frequency and energy, are valid for arbitrary values of the classical action, and these relations are, thereby, correspondence identities. They follow from the more general relations between the kernel $U(x, t; x_0, t_0)$ of the evolution operator and the classical action $S_c(x, t; x_0, t_0)$. Here we restrict ourselves to motion in one dimension between the initial position x_0 at time t_0 and the final position x at time t.

It follows directly from either the Feynman theory of non-relativistic quantum mechanics (Feynman and Hibbs 1965, p. 42) or the Schrödinger theory in momentum representation that the kernel of $U^+(t, t_0)$ is

$$U^+(x, t; x_0, t_0) = \mathscr{E}(t-t_0)\left\{\frac{m}{2\pi \mathrm{i}\hbar(t-t_0)}\right\}^{1/2} \exp\left\{\frac{\mathrm{i}m(x-x_0)^2}{2\hbar(t-t_0)}\right\}. \tag{16}$$

The action $S_c(x, t; x_0, t_0)$, in position–time representation, for the classical path between the initial point $\mathrm{A}(x_0, t_0)$ and final point $\mathrm{B}(x, t)$ is given by

$$S_c(x, t; x_0, t_0) = \int_{\mathrm{A}}^{\mathrm{B}} L\,\mathrm{d}t' = \frac{m}{2}\frac{(x-x_0)^2}{t-t_0}. \tag{17}$$

Thus

$$U^+(x, t; x_0, t_0) = \epsilon(t-t_0) C \exp\frac{\mathrm{i}}{\hbar} S_c(x, t; x_0, t_0); \tag{18}$$

the external factor C is a product of a normalization factor and a constant phase factor. By transforming to energy representation (Feynman and Hibbs 1965, p. 357) we find the usual outgoing wave form of the Green function:

$$G_E{}^+(x, x_0) = \frac{1}{\mathrm{i}\hbar}\left(\frac{m}{2E}\right)^{1/2} \exp\left\{\frac{\mathrm{i}}{\hbar}|x-x_0|(2mE)^{1/2}\right\}. \tag{19}$$

On carrying out the integration, care must be taken with the choice of square roots.

The classical action $S_E(x, x_0)$ in energy (time-independent) representation is obtained from the classical action $S_c(x, t; x_0, t_0)$ by adding the difference between the final and initial values of the generating function for the canonical transformation from time to energy representation:

$$S_E(x, x_0) = S_c(x, t; x_0, t_0) + Et - E_0 t_0 \tag{20}$$

$$= \int_{\mathrm{A}}^{\mathrm{B}} p\,\mathrm{d}x \tag{21}$$

$$= |p(x-x_0)|$$

$$= (2mE)^{1/2}|x-x_0|. \tag{22}$$

Therefore

$$G_E{}^+(x, x_0) = \frac{1}{\mathrm{i}\hbar}\left(\frac{m}{2E}\right)^{1/2} \exp\left\{\frac{\mathrm{i}}{\hbar} S_E(x, x_0)\right\}. \tag{23}$$

Using equation (10), we find that

$$G_E{}^-(x, x_0) = -\frac{1}{\mathrm{i}\hbar}\left(\frac{m}{2E}\right)^{1/2} \exp\left\{-\frac{\mathrm{i}}{\hbar} S_E(x, x_0)\right\}$$

$$= -\frac{1}{\mathrm{i}\hbar}\left(\frac{m}{2E}\right)^{1/2} \exp\left\{-\frac{\mathrm{i}}{\hbar}|x-x_0|\right\}(2mE)^{1/2}. \tag{24}$$

Now, from equation (12), we obtain the spectral operator in terms of the classical path:

$$I_E(x, x_0) = \epsilon(E)\frac{1}{\pi\hbar}\left(\frac{m}{2E}\right)^{1/2} \cos\left\{\frac{1}{\hbar} S_E(x, x_0)\right\}. \tag{25}$$

For negative E, the Green functions G_E^+ and G_E^- are equal; the spectral operator must be defined for all real E, and hence the need for $\epsilon(E)$. Since I_E is a Hermitian operator, the wave form must be real. For $E > 0$ equation (25) can also be obtained directly as a projection onto the eigenspace of the energy E in the continuous spectrum.

4. Particle on a ring

A particle moving along a line with periodic boundary conditions is equivalent to a particle moving on a ring, which is a more convenient picture for our purposes (figure 1).

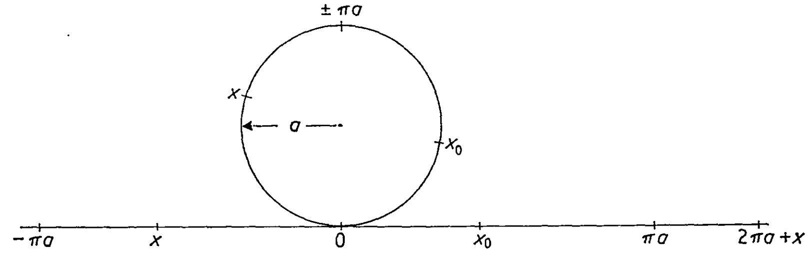

Figure 1. Illustration of the connection between the ring and the straight line. The point x on the ring is identified with the points $x+2\pi ca$ on the straight line.

The distance around the ring is denoted by x, where $|x| < \pi a$ and a is the radius of the ring. For any time interval $\tau \neq 0$ the particle may move along an infinite number of classical paths c between two points x_0 and x on the ring. Each of these paths corresponds to a path between the points x_0 and $2\pi ca+x$ on an infinite straight line, where c is a positive or negative integer. In this way we relate the problem of a particle on a ring to that of a particle on a line, which, as in the previous section, is without periodic boundary conditions. The magnitude and sign of the integer c, the classical path index, defines the number of times that the particle passes around the ring in a positive or negative sense. Evidently the velocity of the particle will be high for large values of $|c|$. There are also an infinite number of classical paths for a given energy E; in this case the velocities are all the same. The connection between the paths on the ring and the paths on the straight line is made by coiling the line onto itself and identifying all points on the line that were originally $2\pi ca$ apart.

The classical action $S_c(x, t; x_0, t_0)$ for a particular path c on the ring is the action for the equivalent path between (x_0, t_0) and $(x+2\pi ca, t)$ on the line, and the same applies for the action $S_{cE}(x, x_0)$ in energy representation. Therefore

$$S_c(x, t; x_0, t_0) = S^{\mathrm{SL}}(x+2\pi ca, t; x_0, t_0) = \frac{m}{2}\frac{(x-x_0+2\pi ca)^2}{t-t_0} \tag{26}$$

and

$$S_{cE}(x, x_0) = S_E^{\mathrm{SL}}(x+2\pi ca, x_0) = (2mE)^{1/2}|x-x_0+2\pi ca| \tag{27}$$

where the superscript SL refers to the straight line. In considering the motion between x_0 and x on the ring we must take into account all the classical paths labelled by the index c and corresponding values of the action. Thus, the presence of alternative classical paths between two points x_0 and x is the basic distinction between the motion on a ring and the motion along a straight line.

We have chosen to study a particle on a ring because it is the simplest dynamical system with a discrete quantum-mechanical spectrum. It is tempting to identify the various classical paths c with the discrete levels ν, but in fact no such identification is possible. We shall show that sums over classical paths are quite distinct from the expansion in eigenstates of the energy, and in some respects are more useful. We shall use the device of coiling the line upon itself to solve the equivalent quantum-mechanical problem of a particle on a ring. Consider any wave packet $\psi(x_0, t_0)$ on the ring at time t_0, which is zero and has zero derivative at $x_0 = \pm a\pi$. For times $t > t_0$ the corresponding wave packet $\psi^{\mathrm{SL}}(x_0, t_0)$ on the straight line, which is originally confined to the region $|x| < \pi a$, will move into regions where $|x| > \pi a$, and this motion will be determined by the evolution operator $U^{\mathrm{SL}+}(t, t_0)$ so that

$$\psi^{\mathrm{SL}}(t) = U^{\mathrm{SL}+}(t; t_0)\psi^{\mathrm{SL}}(t_0). \tag{28}$$

The value of the amplitude on the ring is obtained by the interference (constructive and destructive) of each of the segments of the wave packet between $(2c-1)\pi a$ and $(2c+1)\pi a$ on the straight line for every value of the integer c:

$$\left.\begin{aligned}\psi(x, t) &= \sum_c \psi^{\mathrm{SL}}(x+2\pi ca, t)\\ &= \sum_c U^{\mathrm{SL}+}(t, t_0)\psi(x_0, t_0)\end{aligned}\right\}|x|,\ |x_0| < \pi a. \tag{29}$$

Therefore, for the corresponding kernels,

$$\begin{aligned}U^+(x, t; x_0, t_0) &= \sum_c U^{\mathrm{SL}+}(x+2\pi ca, t; x_0, t_0) &(30)\\ &= \epsilon(t-t_0)\sum_c \left\{\frac{m}{2\pi \mathrm{i}\hbar(t-t_0)}\right\}^{1/2} \exp\left\{\frac{\mathrm{i}}{\hbar} S^{\mathrm{SL}}(x+2\pi ca, t; x_0, t_0)\right\}\\ &= \epsilon(t-t_0)\sum_c \left\{\frac{m}{2\pi \mathrm{i}\hbar(t-t_0)}\right\}^{1/2} \exp\left\{\frac{\mathrm{i}}{\hbar} S_c(x, t; x_0, t_0)\right\} &(31)\\ &= \epsilon(t-t_0)\sum_c \left\{\frac{m}{2\pi \mathrm{i}\hbar(t-t_0)}\right\}^{1/2} \exp\left\{\frac{\mathrm{i}}{\hbar}\frac{m}{2}\frac{(x-x_0+2\pi ca)^2}{t-t_0}\right\}. &(32)\end{aligned}$$

This kernel, as it stands, is divergent almost everywhere and must be treated as a generalized function of x_0.

On carrying out the transformation to energy representation we obtain the outgoing wave form of the Green function:

$$\begin{aligned}G_E^+(x, x_0) &= \sum_c \frac{1}{\mathrm{i}\hbar}\left(\frac{m}{2E}\right)^{1/2} \exp\left\{\frac{\mathrm{i}}{\hbar}|x-x_0+2\pi ca|(2mE)^{1/2}\right\}\\ &= \sum_c \frac{1}{\mathrm{i}\hbar}\left(\frac{m}{2E}\right)^{1/2} \exp\left\{\frac{\mathrm{i}}{\hbar} S_{cE}(x, x_0)\right\}. \end{aligned}\tag{33}$$

As before, from equation (10) it follows that

$$G_E^-(x, x_0) = \sum_c -\frac{1}{\mathrm{i}\hbar}\left(\frac{m}{2E}\right)^{1/2} \exp\left\{-\frac{\mathrm{i}}{\hbar} S_{cE}(x, x_0)\right\} \tag{34}$$

and from equation (12)

$$I_E(x, x_0) = \epsilon(E)\frac{1}{\pi\hbar}\left(\frac{m}{2E}\right)^{1/2} \sum_c \cos\frac{S_{cE}(x, x_0)}{\hbar}. \tag{35}$$

Equations (31), (33), (34) and (35) give the respective kernels, in position representation, explicitly in terms of sums over the various classical paths c on the ring between the points x_0 and x.

We can carry out the summation over c in equation (33) and obtain the Green function $G_E^+(x, x_0)$ as a simple generalized function which possesses the desired properties of the corresponding Green function obtained as sums over the quantum states ν. In doing so we appeal to Abel's theorem (Whittaker and Watson 1962, p. 57) and assume that E is complex with small positive imaginary part, so that

$$E = E_{\mathrm{R}}+\mathrm{i}\epsilon, \qquad \epsilon > 0. \tag{36}$$

$G_E{}^+(x, x_0)$ is now the sum

$$\sum_c \frac{1}{\mathrm{i}\hbar}\left(\frac{m}{2E}\right)^{1/2} \exp\left\{\frac{\mathrm{i}}{\hbar}\,|x-x_0+2\pi ca|(2mE)^{1/2}\right\} \tag{37}$$

for complex E. For $x > x_0$,

$$G_E{}^+(x, x_0) = \frac{1}{\mathrm{i}\hbar}\left(\frac{m}{2E}\right)^{1/2}\left[\sum_{c=0}^{\infty} \exp\left\{\frac{\mathrm{i}}{\hbar}(x-x_0+2\pi ca)(2mE)^{1/2}\right\}\right.$$

$$\left. + \sum_{c=1}^{\infty} \exp\left\{\frac{\mathrm{i}}{\hbar}(x_0-x+2\pi ca)(2mE)^{1/2}\right\}\right]. \tag{38}$$

Summing the geometric series we obtain

$$G_E{}^+(x, x_0) = \frac{1}{\hbar}\left(\frac{m}{2E}\right)^{1/2}\frac{\cos\{(x-x_0-\pi a)(2mE)^{1/2}/\hbar\}}{\sin\{\pi a(2mE)^{1/2}/\hbar\}}, \qquad x > x_0. \tag{39}$$

By the same process, for $x < x_0$,

$$G_E{}^+(x, x_0) = \frac{1}{\hbar}\left(\frac{m}{2E}\right)^{1/2}\frac{\cos\{(x-x_0+\pi a)(2mE)^{1/2}/\hbar\}}{\sin\{\pi a(2mE)^{1/2}/\hbar\}}, \qquad x < x_0. \tag{40}$$

The Green function $G_E{}^+(x, x_0)$ for all x is then

$$G_E{}^+(x, x_0) = \lim_{\epsilon\to 0}\frac{1}{\hbar}\left(\frac{m}{2E}\right)^{1/2}\frac{\cos\{(\pi a-|x-x_0|)(2mE)^{1/2}/\hbar\}}{\sin\{\pi a(2mE)^{1/2}/\hbar\}}. \tag{41}$$

Similarly

$$G_E{}^-(x, x_0) = \lim_{\epsilon\to 0}\frac{1}{\hbar}\left(\frac{m}{2E}\right)^{1/2}\frac{\cos\{(\pi a-|x-x_0|)(2mE)^{1/2}/\hbar\}}{\sin\{\pi a(2mE)^{1/2}/\hbar\}} \tag{42}$$

where

$$E = E_{\mathrm{R}} - \mathrm{i}\epsilon, \qquad \epsilon > 0. \tag{43}$$

It should be noted that $G_E{}^+(x, x_0)$ and $G_E{}^-(x, x_0)$, as given by equations (41) and (42), are functions of the complex variable E, defined only in the upper and lower half planes respectively. In the limit $\epsilon \to 0$ (i.e. on the real axis) this must not be forgotten. Bearing this in mind

$$I = \int_{-\infty}^{\infty} I_E(x, x_0)\,\mathrm{d}E = \frac{1}{2\pi\mathrm{i}}\oint_{\mathrm{C}} \frac{1}{\hbar}\left(\frac{m}{2E}\right)^{1/2}\frac{\cos\{(\pi a-|x-x_0|)(2mE)^{1/2}/\hbar\}}{\sin\{\pi a(2mE)^{1/2}/\hbar\}}\,\mathrm{d}E \tag{44}$$

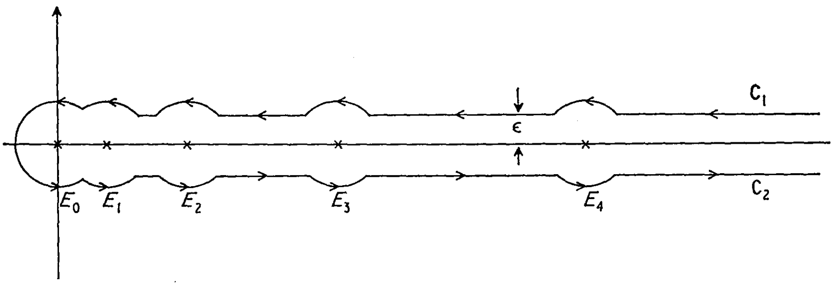

Figure 2. The contours C_1 and C_2 for integration of $I_E(x, x_0)$ in the complex E plane.

where C is the contour $\mathrm{C}_2+\mathrm{C}_1$ (figure 2) closed at infinity as $\epsilon \to 0$. The contributions to the integral arise from the various poles E_ν along the real positive axis. The Green functions

$G_E^{\pm}(x, x_0)$ have poles given by the zeros of $\sin\{\pi a(2mE)^{1/2}/\hbar\}$, and so the corresponding energy levels are given by

$$E_\nu = \frac{\nu^2\hbar^2}{2a^2m}, \qquad \text{for integer } \nu. \tag{45}$$

The appropriate residues R_ν are

$$R_\nu = \frac{1}{2\pi a}\left[\exp\left\{\frac{i\nu}{a}(x-x_0)\right\}+\exp\left\{-\frac{i\nu}{a}(x-x_0)\right\}\right] \tag{46}$$

which confirms the fact that the normalized eigenfunctions corresponding to the eigenvalues E_ν are just

$$\psi(x) = \frac{1}{(2\pi a)^{1/2}}\exp\left(\pm\frac{i\nu x}{a}\right), \qquad \text{integer } \nu. \tag{47}$$

Equations (47) and (46) illustrate the twofold degeneracy of the eigenvalue E_ν and show that the residue R_ν is just the kernel of the projection operator P_ν.

The spectral operator in equation (35) can also be used directly to obtain the kernels of the projection operators onto the eigenstates of the energy eigenvalues E_ν:

$$I_E(x, x_0) = \sum_c \epsilon(E)\frac{1}{\pi\hbar}\left(\frac{m}{2E}\right)^{1/2}\cos\left\{\frac{(x-x_0+2\pi ca)(2mE)^{1/2}}{\hbar}\right\}. \tag{48}$$

Expanding the cosine terms we obtain

$$I_E(x, x_0) = \epsilon(E)\frac{1}{\pi\hbar}\left(\frac{m}{2E}\right)^{1/2}\cos\left\{\frac{(2mE)^{1/2}(x-x_0)}{\hbar}\right\}\left\{1+\sum_{c=1}^{\infty}2\cos\frac{(2mE)^{1/2}2\pi ac}{\hbar}\right\}. \tag{49}$$

In terms of Dirac δ-functions (Lighthill 1960, p. 68)

$$1+2\sum_{c=1}^{\infty}\cos\frac{(2mE)^{1/2}2\pi ac}{\hbar} = \sum_{l=-\infty}^{\infty}\delta\left\{\frac{(2mE)^{1/2}a}{\hbar}-l\right\} \tag{50}$$

and equation (49) may now be written

$$I_E(x, x_0) = \mathscr{E}(E)\frac{1}{\pi\hbar}\left(\frac{m}{2E}\right)^{1/2}\cos\left\{\frac{(2mE)^{1/2}(x-x_0)}{\hbar}\right\}\sum_{l=-\infty}^{l=\infty}\delta\left\{\frac{(2mE)^{1/2}a}{\hbar}-l\right\} \tag{51}$$

where l is an integer. From the properties of the delta function we obtain

$$I_E(x, x_0) = \sum_{l=-\infty}^{l=\infty}\frac{1}{2\pi a}\exp\left\{\frac{il}{a}(x-x_0)\right\}\delta\left(E-\frac{l^2\hbar^2}{2a^2m}\right). \tag{52}$$

The integer l is just the quantum-mechanical label ν, and so

$$I_E(x, x_0) = \sum_{\nu=-\infty}^{\infty}\frac{1}{2\pi a}\exp\left\{\frac{i\nu}{a}(x-x_0)\right\}\delta(E-E_\nu). \tag{53}$$

From equation (14), the kernel of P_ν is given by

$$P_\nu(x, x_0) = \frac{1}{2\pi a}\left[\exp\left\{\frac{i\nu}{a}(x-x_0)\right\}+\exp\left\{-\frac{i\nu}{a}(x-x_0)\right\}\right] \tag{54}$$

which is the residue R_ν of equation (46).

5. Conclusion

In the previous two sections we have obtained a complete quantum-dynamical solution of the free-particle problem and of the problem of the particle on the ring in terms of classical paths. The classical path sums provide an alternative to sums over quantum states and to perturbation expansions, and are often more useful, as was shown in the derivation of the closed form of the Green functions $G_E^{\pm}(x, x_0)$ in equations (41) and (42). The relation between sums over quantum states and sums over classical paths is shown at its simplest in equation (50).

Clutton-Brock (1965) has suggested that propagators might be obtained in terms of classical action functions for arbitrary potentials. However, his analysis is based on Feynman-type path summations in phase space, and implicitly requires the steps in the coordinates and conjugate momenta to tend to zero simultaneously, violating the uncertainty principle. Counter examples to his results may be found. Nevertheless, the general form that is suggested is clearly valid for some interesting particular cases, provided one takes into account the multiplicity of the classical paths between two points.

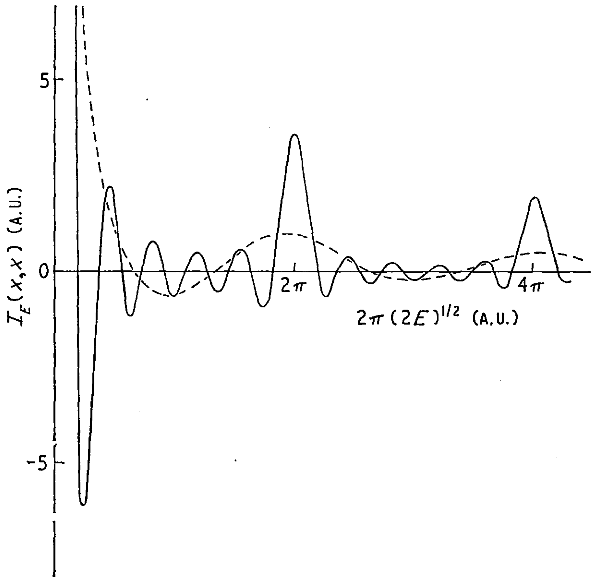

Figure 3. Partial summation of equation (35) for $I_E(x, x)$ (atomic units) against $2\pi(2E)^{1/2}$ (atomic units), $a = 1$. The curve -------- is the partial summation for three paths, and the curve ——— for eleven paths.

Finally, in the case of the particle on a ring, the classical path treatment of the spectral operator shows how the spectrum is formed from the amplitudes of the classical paths by constructive interference at the energy levels E_ν and by destructive interference elsewhere. The onset of such interference is shown by partial summation of equation (35) for $I_E(x, x_0)$ in figure 3.

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Correspondence identities
II. The Bohr–Sommerfeld identity for the hydrogen atom

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Abstract. The Bohr–Sommerfeld identity between the hydrogen energy levels given by the old quantum theory and the actual energy levels is explained. The quantum-dynamical solution of the hydrogen-like problem is obtained for bound states in terms of sums over classical paths using the symmetric representation of Fock. The classical analogue of the Fock theory of the hydrogen atom is discussed. Schwinger's expression for the Green function is obtained in a new form.

1. Introduction

The correspondence principle of Bohr relates quantum phenomena to classical mechanics in the limit as $\hbar/A \to 0$, as the dynamical action variables A become large in comparison with Planck's constant. However, for particular potentials of physical importance some of these relations hold even for low quantum numbers and for relatively small values of the action. These are the correspondence identities.

There are correspondence identities for free particles, as described in the previous paper (Norcliffe and Percival 1968, to be referred to as I), and for systems of harmonic oscillators, as described by Feynman (Feynman and Hibbs 1965). For the Coulomb potential, the following identities are known:

(i) *The Rutherford scattering identity.* The quantum-mechanical and classical angular differential cross sections for the scattering of a charged particle by a fixed charge are the same (see Mott and Massey 1965, p. 53).

(ii) *The Bohr–Sommerfeld identity.* The old quantum theory, which postulated that only those orbits occur for which the action around the classical path of a periodic system is a multiple of $2\pi\hbar$, gives the correct energy levels of the hydrogen atom and hydrogenic ions.

(iii) *The Fock identity.* It was shown by Fock (1935) that the electron momentum distribution for any energy level E_n of the hydrogen atom has the form, with the usual notation,

$$\rho(\boldsymbol{p}) = \frac{1}{n^2}\sum_{l,m} \psi^*_{nlm}(\boldsymbol{p})\psi_{nlm}(\boldsymbol{p})$$
$$= \frac{\text{constant}}{(p^2+p_n{}^2)^4}$$

provided that every quantum-mechanical state of that level has the same probability. It follows from the correspondence principle that, for any n, the above momentum distribution is the same as that of a classical electron in an H atom of energy E_n, provided that every region of classical phase space at that energy has the same probability. This is the classical microcanonical distribution (Landau and Lifshitz 1958, p. 12).

The first two identities were important in the early development of atomic physics: Rutherford was able to study the structure of atoms without the need for minor quantum corrections to his scattering formulae; Bohr and Sommerfeld were able to study transitions between low levels of the H atom, whereas their theory has general validity only in the limit of high quantum numbers. For neither of these identities does there appear to be any obvious connection between the usual classical- and quantum-mechanical theories.

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The Fock identity was obtained as a consequence of the O(4) dynamical symmetry of the hydrogen atom (Fock 1935, see also Bander and Itzykson 1966 and §§ 2 and 3 of this paper). We shall here show that the Bohr–Sommerfeld identity follows from O(4) symmetry, and in a following paper that the Rutherford identity also has its origin in dynamical symmetry.

For the bound states we further obtain a more general relation between the classical and quantum mechanics of the H atom, in which the spectral operator (see I), and thus also the projection operators onto the bound states of each level of the atom, are obtained as sums over classical paths. Thus a solution of the quantum bound-state dynamical problem is obtained in terms of a solution of the corresponding classical problem. At the same time we show that for the hydrogen atom in symmetric representation, and in momentum representation, a 'ray' treatment completely and exactly describes the behaviour of matter waves.

This paper deals entirely with bound states, a subsequent paper with scattering states. As in the previous paper, generalized functions are used extensively.

Gutzwiller (1967) has approached the subject of this paper: he obtained correspondence identities from the poles of an approximate Coulomb Green function which was obtained by classical path summation. However, he did not obtain the complete destructive interference between classical paths at other negative energies, and did not relate the identities to the symmetric representation.

2. Classical Fock theory

The symmetric representation for bound quantum states of hydrogenic systems has been described in the literature by Fock (1935) and more recently by Kurşunoğlu (1962) and by Bander and Itzykson (1966). The corresponding classical theory for elliptic orbits follows similar lines. Let us consider a particle of mass μ in the field of a central potential

$$V(r) = -\frac{k}{r} = -\frac{Ze^2}{r} \tag{1}$$

and moving in an elliptic orbit with energy

$$E = -\frac{p_E{}^2}{2\mu}. \tag{2}$$

The energy equation for the particle is

$$E = \frac{p^2}{2\mu} - \frac{k}{r}. \tag{3}$$

It follows from the virial theorem in both classical and quantum mechanics that $p_E{}^2$ is the mean square momentum of a particle in a bound state of energy E. The classical theory of the Kepler problem (Sommerfeld 1952) is simpler in momentum representation, in which the orbit is a circle, than in position representation, in which it is an ellipse. If ϵ is the eccentricity of the ellipse, then the radius of the circle is $p_E(1-\epsilon^2)^{-1/2}$ and the centre is at a distance $p_E\epsilon(1-\epsilon^2)^{-1/2}$ from the origin, which is enclosed by the circle.

The Fock theory gives further simplification. The momentum is first represented by the vector $\boldsymbol{p} = (p_1, p_2, p_3, 0)$ in a four-dimensional space. The scaled momentum vector is then $\boldsymbol{p}/p_E$. In the symmetric representation the classical state of the system is represented by the unit 4-vector $\boldsymbol{u}$ obtained by projecting $\boldsymbol{p}/p_E$ onto the unit hypersphere (centred at the origin) from the 'north pole' given by $\boldsymbol{n} = (0, 0, 0, 1)$. The vector $\boldsymbol{u}$ is given in terms of the momentum 4-vector by the equation

$$\boldsymbol{u} = \frac{2p_E\boldsymbol{p} + (p^2 - p_E{}^2)\boldsymbol{n}}{p^2 + p_E{}^2}. \tag{4}$$

Two examples of the projection are shown in figure 1, restricted to three dimensions for simplicity.

To formulate the classical-dynamical problem in symmetric representation we must obtain the energy equation and the stationary action principle. The vectors $\boldsymbol{u}$ and $\boldsymbol{p}$ are related by a coordinate transformation. The corresponding canonical transformation from momentum to symmetric representation is generated by the function $\psi'(\alpha, \theta, \phi; x, y, z)$, where (α, θ, ϕ) are the new coordinates and $(-x, -y, -z)$ the old momenta (Corben and Stehle 1966, p. 177). The action function $S_{cE}(\boldsymbol{u}, \boldsymbol{u}_0)$ in the symmetric representation is then given in terms of the energy–momentum action function by the equation

$$S_{cE}(\boldsymbol{u}, \boldsymbol{u}_0) = S_{cE}(\boldsymbol{p}, \boldsymbol{p}_0) - [\psi']_{\mathrm{A}}^{\mathrm{B}} + [\boldsymbol{r} \cdot \boldsymbol{p}]_{\mathrm{A}}^{\mathrm{B}} \tag{5}$$

where A and B are the initial and final points of the motion. The generating function ψ' has the form

$$\begin{aligned} \psi' &= f_1(\alpha, \theta, \phi)x + f_2(\alpha, \theta, \phi)y + f_3(\alpha, \theta, \phi)z \\ &= \boldsymbol{f}(\alpha, \theta, \phi) \cdot \boldsymbol{r}. \end{aligned} \tag{6}$$

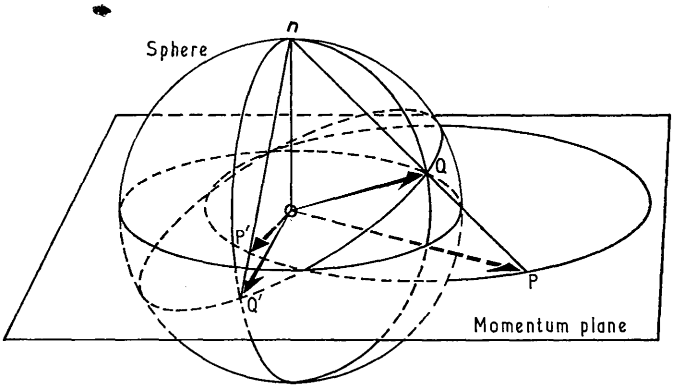

Figure 1. Two examples of the stereographic projection. The points P, P′ on the scaled momentum circle become the points Q, Q′ on the sphere.

Unless otherwise stated, all vectors have fourth component zero. The angles α, θ, ϕ are polar coordinates of u on the hypersphere (Fock 1935). By the general theory of canonical transformations

$$\begin{aligned} \boldsymbol{p} &= \frac{p_E}{1-\cos\alpha}(\sin\alpha\sin\theta\cos\phi, \sin\alpha\sin\theta\sin\phi, \sin\alpha\cos\theta, 0) \\ &= \boldsymbol{f}(\alpha, \theta, \phi) \\ &= \frac{p_E \sin\alpha}{1-\cos\alpha}\hat{\boldsymbol{p}}. \end{aligned} \tag{7}$$

It should be noted that p_x, p_y, p_z in the momentum (initial) representation are the generalized coordinates and $-x$, $-y$, $-z$ the generalized momenta; in the symmetric (final) representation the generalized coordinates and momenta are α, θ, ϕ and p_α, p_θ, p_ϕ, respectively. By the transformation theory

$$p_\alpha = -\frac{\partial(\psi')}{\partial\alpha} \tag{8}$$

and similarly for the other angular variables. It is simpler to work with a vector form for the hyperspherical momentum. As the line element ds on the hypersphere is

$$\mathrm{d}\boldsymbol{s} = \mathrm{d}\alpha\hat{\boldsymbol{\alpha}} + \sin\alpha\,\mathrm{d}\theta\hat{\boldsymbol{\theta}} + \sin\alpha\sin\theta\,\mathrm{d}\phi\hat{\boldsymbol{\phi}} \tag{9}$$

we find that we can preserve the symmetry by defining the hyperspherical momentum $\boldsymbol{p}_u$ to be

$$\boldsymbol{p}_u = p_\alpha \hat{\boldsymbol{\alpha}} + \frac{p_\theta \hat{\boldsymbol{\theta}}}{\sin\alpha} + \frac{p_\phi \hat{\boldsymbol{\phi}}}{\sin\alpha \sin\theta} \tag{10}$$

$$= -(1-\boldsymbol{u}\boldsymbol{u}.)\nabla_u \left(\frac{p_E \boldsymbol{u}\,.\,\boldsymbol{r}}{1-\cos\alpha}\right), \qquad (r \text{ constant}). \tag{11}$$

The second equality is obtained from the canonical transformation; the factor $(1-\boldsymbol{u}\boldsymbol{u}.)$ removes components parallel to $\boldsymbol{u}$. From equation (11)

$$\boldsymbol{p}_u = -\frac{p_E \boldsymbol{r}}{1-\cos\alpha} + \frac{p_E \boldsymbol{u}\,.\,\boldsymbol{r}}{(1-\cos\alpha)^2}\{(1-\cos\alpha)\boldsymbol{u} + \sin\alpha\,\hat{\boldsymbol{\alpha}}$$

$$= -\frac{p_E \boldsymbol{r}}{1-\cos\alpha} + \frac{p_E \boldsymbol{u}\,.\,\boldsymbol{r}}{(1-\cos\alpha)^2}(\boldsymbol{u}-\boldsymbol{n}) \tag{12}$$

where, from the geometry (figure 2),

$$\hat{\boldsymbol{\alpha}} = -\boldsymbol{n}\sin\alpha + \hat{\boldsymbol{p}}\cos\alpha.$$

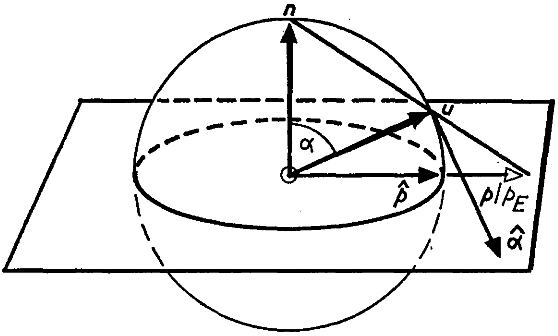

Figure 2. Illustration of the connection between the unit vectors $\boldsymbol{n}$, $\boldsymbol{u}$, $\hat{\boldsymbol{p}}$ and $\hat{\boldsymbol{\alpha}}$.

To obtain the energy (Hamilton–Jacobi) equation in symmetric representation, we express $\boldsymbol{r}$ in terms of $\boldsymbol{u}$ and $\boldsymbol{p}_u$ by taking the scalar product of equation (12) with $\boldsymbol{n}$:

$$\boldsymbol{p}_u\,.\,\boldsymbol{n} = -\frac{p_E \boldsymbol{u}\,.\,\boldsymbol{r}}{1-\cos\alpha} = p_\alpha \sin\alpha \tag{13}$$

$$\boldsymbol{r} = \frac{1}{p_E}\{\boldsymbol{p}_u(1-\cos\alpha) - \boldsymbol{p}_u\,.\,\boldsymbol{n}(\boldsymbol{n}-\boldsymbol{u})\} \tag{14}$$

$$r = \frac{1-\cos\alpha}{p_E}|\boldsymbol{p}_u|. \tag{15}$$

The energy equation in momentum representation is

$$E = \frac{p^2}{2\mu} - \frac{k}{r} \tag{16}$$

and therefore, using equation (15), the energy equation in symmetric representation is

$$E = \frac{p_E{}^2(1+\cos\alpha)}{2\mu(1-\cos\alpha)} - \frac{k p_E}{(1-\cos\alpha)|\boldsymbol{p}_u|}$$

$$= -\frac{k p_E}{2|\boldsymbol{p}_u|}$$

$$= -\frac{k p_E}{2(p_\alpha{}^2 + p_\theta{}^2/\sin^2\alpha + p_\phi{}^2/\sin^2\alpha\sin^2\theta)^{1/2}}. \tag{17}$$

The symmetry of this equation on the hypersphere is evident. It should be noted that the magnitude p_u of $\mathbf{p}_u$ is a function of energy alone. The explicit energy dependence of the above transformation introduces no great difficulty into the theory. All that we require is that the new Hamiltonian should be a function of p_u alone, giving

$$\dot{\alpha} = \frac{\partial}{\partial p_\alpha} f(p_u) \tag{18}$$

and similarly for the other angles. Then the line element ds given by equation (9) is in the direction of $\mathbf{p}_u$. The stationary action principle now becomes

$$\begin{aligned} 0 &= \Delta \int \mathbf{p}_u \,.\, \mathrm{d}\mathbf{s} \\ &= p_u \Delta \int \mathrm{d}s. \end{aligned} \tag{19}$$

The path on the hypersphere is therefore a geodesic, that is, a great circle.

This result can also be obtained directly from the circular orbits in momentum space by projecting onto the hypersphere (see Györgyi 1967). As in the case of the particle on a ring in I, there is an infinite number of classical paths c between the initial point $\mathbf{u}_0$ and the final point $\mathbf{u}$ on the hypersphere for a given energy E. As before, the index c will be used to determine the number of times that the particle cycles around its elliptic orbit in position space before reaching its final position.

In the symmetric representation the classical action for the path c on the hypersphere is thus given by

$$\begin{aligned} S_{cE}(\mathbf{u}, \mathbf{u}_0) &= \int_{\text{path } c} p_u \, \mathrm{d}s \\ &= -\frac{kp_E s_c(\mathbf{u}, \mathbf{u}_0)}{2E} \\ &= \frac{\mu k|\omega + 2\pi c|}{(-2\mu E)^{1/2}}, \qquad c = 0, \pm 1, \pm 2 \ldots \end{aligned} \tag{20}$$

where $s_c(\mathbf{u}, \mathbf{u}_0)$ is the path length and ω is the corresponding angle between the initial and final points on the sphere, so that

$$\cos\omega = \mathbf{u} \,.\, \mathbf{u}_0, \qquad (0 \leqslant \omega \leqslant \pi). \tag{21}$$

The value of the action function remains unchanged under a canonical transformation which is only a coordinate transformation (see equations (5), (6) and (7), or Corben and Stehle (1966, p. 178)), and therefore

$$S_{cE}(\mathbf{u}, \mathbf{u}_0) = S_{cE}(\mathbf{p}, \mathbf{p}_0) = \frac{\mu k|\omega + 2\pi c|}{(-2\mu E)^{1/2}}. \tag{22}$$

From equation (4)

$$\mathbf{u} \,.\, \mathbf{u}_0 = \frac{4p_E^2 \mathbf{p} \cdot \mathbf{p}_0 + (p^2 - p_E^2)(p_0^2 - p_E^2)}{(p^2 + p_E^2)(p_0^2 + p_E^2)} \tag{23}$$

so that in terms of momenta

$$\omega = \cos^{-1}\left\{\frac{4p_E^2 \mathbf{p} \cdot \mathbf{p}_0 + (p^2 - p_E^2)(p_0^2 - p_E^2)}{(p^2 + p_E^2)(p_0^2 + p_E^2)}\right\}. \tag{24}$$

The value of $S_{cE}(\mathbf{p}, \mathbf{p}_0)$ can be obtained directly from first principles. It is shown by Györgyi (1967), for example, that for a given orbit the path length on the hypersphere is the magnitude of the difference between the initial and final values of the eccentric anomaly w. Using appropriate axes, the parametric equations of the orbit are

$$x = a(\cos w - \epsilon)$$

$$y = a(1-\epsilon^2)^{1/2} \sin w \tag{25}$$

$$t = \left(\frac{\mu a^3}{k}\right)^{1/2} (w - \epsilon \sin w) \tag{26}$$

where a is the semi-major axis of the elliptic orbit.

Using w as the independent variable, we have

$$\boldsymbol{p} = \mu \frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}w} \frac{\mathrm{d}w}{\mathrm{d}t} \tag{27}$$

and therefore the classical action is

$$\begin{aligned} S_{cE}(\boldsymbol{p}, \boldsymbol{p}_0) &= \int_{\mathrm{A}}^{\mathrm{B}} -\boldsymbol{r} \,.\, \mathrm{d}\boldsymbol{p}' \\ &= \frac{\mu k |w - w_0|}{(-2\mu E)^{1/2}} \end{aligned} \tag{28}$$

where

$$|w - w_0| = |\omega + 2\pi c|. \tag{29}$$

3. Quantum-mechanical Fock theory

For the elements of the quantum theory of the symmetric representation, the reader is referred to the references quoted in the previous section. As in the classical theory the transformation to symmetric representation is obtained by projecting the normalized momentum $\boldsymbol{p}/p_E$ onto the hypersphere.

We wish to transform the Green operators, and follow Schwinger (1964) and the above classical theory in choosing an arbitrary negative real value for the energy E, in contrast to Fock, who chose E to be an energy level of the hydrogen atom. For convenience we label our wave functions with the energy E.

If $\psi(\boldsymbol{p}, E)$ is a momentum wave function and $\mathscr{S}$ represents the transformation to symmetric representation, then we define the equivalent symmetric wave function $\psi_{\mathrm{s}}(\boldsymbol{u}, E)$ by

$$\begin{aligned} \psi_{\mathrm{s}}(\boldsymbol{u}, E) &= \mathscr{S}\psi(\boldsymbol{p}, E) \\ &= \frac{\pi}{\sqrt{8}} p_E^{-5/2} (p_E^2 + p^2)^2 \psi(\boldsymbol{p}, E). \end{aligned} \tag{30}$$

The factor in equation (30) is chosen so that if $\psi(\boldsymbol{p}, E)$ is a solution of the Schrödinger equation belonging to energy E, then

$$\begin{aligned} \int \frac{\mathrm{d}\Omega}{2\pi^2} |\psi_{\mathrm{s}}(\boldsymbol{u}, E)|^2 &= \int \mathrm{d}^3p \frac{p_E^2 + p^2}{2p_E^2} |\psi(\boldsymbol{p}, E)|^2 \\ &= \int \mathrm{d}^3p |\psi(\boldsymbol{p}, E)|^2 \\ &= 1. \end{aligned} \tag{31}$$

If $L(\boldsymbol{p}, \boldsymbol{p}_0)$ is the kernel of an integral operator L in momentum representation and $L(\boldsymbol{u}, \boldsymbol{u}_0)$ is the kernel in symmetric representation, then for any $\psi(\boldsymbol{p}, E)$ we have

$$\begin{aligned} \int \frac{\mathrm{d}\Omega_0}{2\pi^2} L(\boldsymbol{u}, \boldsymbol{u}_0) \psi_{\mathrm{s}}(\boldsymbol{u}_0, E) &= \mathscr{S} \int \mathrm{d}^3p_0 \, L(\boldsymbol{p}, \boldsymbol{p}_0) \psi(\boldsymbol{p}_0, E) \\ &= \int \frac{\mathrm{d}\Omega_0}{2\pi^2} \frac{(p_E^2 + p^2)^2 (p_E^2 + p_0^2)}{8p_E^3} 2\pi^2 L(\boldsymbol{p}, \boldsymbol{p}_0) \psi_{\mathrm{s}}(\boldsymbol{u}_0, E). \end{aligned} \tag{32}$$

Noting that both sides are functions of $\boldsymbol{u}$, we have

$$L(\boldsymbol{u}, \boldsymbol{u}_0) = \frac{2\pi^2(p_E{}^2+p^2)^2(p_E{}^2+p_0{}^2)L(\boldsymbol{p},\boldsymbol{p}_0)}{8p_E{}^3}. \tag{33}$$

A symmetric kernel in one representation is not a symmetric kernel in the other.

Let H be the Hamiltonian of the hydrogen atom. Then by Fock's theory, and with a view to obtaining the Green function, we have

$$(E-H)\psi(\boldsymbol{p}, E) = \left(E-\frac{p^2}{2\mu}\right)\psi(\boldsymbol{p}, E)+\frac{k}{2\pi^2\hbar}\int\frac{\mathrm{d}^3p_0\psi(\boldsymbol{p}_0, E)}{|\boldsymbol{p}-\boldsymbol{p}_0|^2} \tag{34}$$

which in symmetric representation reduces via equation (4) to

$$(E-H)\psi_{\mathrm{s}}(\boldsymbol{u}, E) = \left(E-\frac{p^2}{2\mu}\right)(I-\nu Q)\psi_{\mathrm{s}}(\boldsymbol{u}, E) \tag{35}$$

where

$$\nu = \frac{k\mu}{p_E\hbar} \tag{36}$$

$$Q\psi_{\mathrm{s}}(\boldsymbol{u}, E) = \int\frac{\mathrm{d}\Omega_0}{2\pi^2}\frac{\psi_{\mathrm{s}}(\boldsymbol{u}_0, E)}{|\boldsymbol{u}-\boldsymbol{u}_0|^2}. \tag{37}$$

Assuming we can construct analytic functions of both sides of equation (35), in particular the inverse, we have

$$\begin{aligned}(E-H)^{-1} &= \left\{\left(E-\frac{p^2}{2\mu}\right)(I-\nu Q)\right\}^{-1}\\ &= (I-\nu Q)^{-1}\left(E-\frac{p^2}{2\mu}\right)^{-1}.\end{aligned} \tag{38}$$

The Green operator $(E-H)^{-1}$ is not uniquely defined when E is on the real axis, and as usual we define

$$G_E{}^{\pm} = \lim_{\nu_{\mathrm{I}}\to 0}\{I-(\nu\pm \mathrm{i}\nu_{\mathrm{I}})Q\}^{-1}\left(E-\frac{p^2}{2\mu}\right)^{-1}. \tag{39}$$

The spectral operator is thus given by

$$\begin{aligned}I_E = \delta(E-H) &= \lim_{\nu_{\mathrm{I}}\to 0}\left[\frac{\{I-(\nu-\mathrm{i}\nu_{\mathrm{I}})Q\}^{-1}-\{I-(\nu+\mathrm{i}\nu_{\mathrm{I}})Q\}^{-1}}{2\pi\mathrm{i}}\right]\left(E-\frac{p^2}{2\mu}\right)^{-1}\\ &= J_\nu\left(E-\frac{p^2}{2\mu}\right)^{-1}.\end{aligned} \tag{40}$$

4. The kernels of $(I-\nu Q)^{-1}$ and of the spectral operator

As in Schwinger's (1964) theory of the Coulomb Green function, it follows directly from Fock's (1935) work that if $\psi_n(\boldsymbol{u}, E)$ is a hyperspherical harmonic of order n, and P_n is the projection operator onto the nth harmonics, then

$$Q\psi_n(\boldsymbol{u}, E) = n^{-1}\psi_n(\boldsymbol{u}, E)$$

$$Q = \sum_{n=1}^{\infty} n^{-1}P_n \tag{41}$$

and

$$(I-\nu Q)^{-1} = \sum_{n=1}^{\infty}\frac{P_n}{1-\nu/n}. \tag{42}$$

It should be noted that the stereographic projection used by Schwinger, and in this paper, depends on E and not on the E_n belonging to a hyperspherical harmonic as with Fock. The functions in momentum space corresponding to these harmonics are therefore scaled hydrogen atom wave functions. They form a complete but not orthogonal set of functions in momentum space.

The kernel of $(I-\nu Q)^{-1}$ in symmetric representation is:

$$\sum_{n=1}^{\infty}\frac{n^2}{n-\nu}\frac{\sin n\omega}{\sin\omega}=\sum_{n=1}^{\infty}\frac{n\sin n\omega}{\sin\omega}+\nu\sum_{n=1}^{\infty}\frac{\sin n\omega}{\sin\omega}+\frac{\nu^2 A}{\sin\omega} \tag{43}$$

where

$$A=\sum_{n=1}^{\infty}\frac{\sin n\omega}{n-\nu}. \tag{44}$$

All terms of equation (43) must be considered as generalized functions. The first two terms are strongly divergent, but are eventually removed from the analysis. The term with A has singularities at $\nu = 1, 2, 3, \ldots$, which are the poles of the Green function, which is not uniquely defined unless the sign of ν_{I} (the imaginary part of ν) is defined. Suppose that $A^{\pm}$ corresponds to $\pm\nu_{\mathrm{I}}$, where $\nu_{\mathrm{I}} > 0$. Then

$$A^{+}=\frac{1}{2\mathrm{i}}(B_{+}-B_{-})$$

where

$$B_{\pm}=\sum_{n=1}^{\infty}\frac{\exp(\pm\mathrm{i}n\omega)}{n-\nu}. \tag{45}$$

For convergence of $B_{\pm}$ we make ω slightly complex:

$$\begin{aligned}B_{+}&=\sum_{n=1}^{\infty}\frac{\exp\{\mathrm{i}n(\omega+\mathrm{i}\epsilon)\}}{n-\nu},\qquad \epsilon>0\\&=\exp\{\mathrm{i}\nu(\omega+\mathrm{i}\epsilon)\}\sum_{n=1}^{\infty}\mathrm{i}\int_{-\infty+\mathrm{i}\epsilon}^{\omega+\mathrm{i}\epsilon}d\omega'\exp\{\mathrm{i}(n-\nu)\omega'\}\\&=\exp\{\mathrm{i}\nu(\omega+\mathrm{i}\epsilon)\}\mathrm{i}\int_{-\infty+\mathrm{i}\epsilon}^{\omega+\mathrm{i}\epsilon}d\omega'\frac{\exp\{\mathrm{i}(1-\nu)\omega'\}}{1-\exp(\mathrm{i}\omega')}.\end{aligned} \tag{46}$$

Since $B_{-}(\omega^{*},\nu)=\{B_{+}(\omega,\nu^{*})\}^{*}$, we have

$$\begin{aligned}A^{+}(\nu)&=\frac{1}{2}\int_{-\infty+\mathrm{i}\epsilon}^{\omega+\mathrm{i}\epsilon}d\omega'\frac{\exp\{\mathrm{i}(1-\nu)\omega'\}}{1-\exp(\mathrm{i}\omega')}\exp\{\mathrm{i}\nu(\omega+\mathrm{i}\epsilon)\}\\&\quad-\frac{1}{2}\int_{\omega-\mathrm{i}\epsilon}^{\infty-\mathrm{i}\epsilon}d\omega'\frac{\exp\{-\mathrm{i}(1-\nu)\omega'\}}{1-\exp(-\mathrm{i}\omega')}\exp\{-\mathrm{i}\nu(\omega-\mathrm{i}\epsilon)\}\\&=-\frac{1}{4\mathrm{i}}\int_{-\infty+\mathrm{i}\epsilon}^{\omega+\mathrm{i}\epsilon}d\omega'\frac{\exp\{\mathrm{i}(\frac{1}{2}-\nu)\omega'\}}{\sin\frac{1}{2}\omega'}\exp\{\mathrm{i}\nu(\omega+\mathrm{i}\epsilon)\}\\&\quad-\frac{1}{4\mathrm{i}}\int_{\omega-\mathrm{i}\epsilon}^{\infty-\mathrm{i}\epsilon}d\omega'\frac{\exp\{-\mathrm{i}(\frac{1}{2}-\nu)\omega'\}}{\sin\frac{1}{2}\omega'}\exp\{-\mathrm{i}\nu(\omega-\mathrm{i}\epsilon)\}.\end{aligned} \tag{47}$$

The poles of each integrand lie at $\omega' = 2\pi c$, where c is an integer, and we shall find that the residues correspond to contributions from classical paths, but unfortunately the contours are incomplete. For this reason we are unable to obtain the exact Coulomb Green functions as sums over classical paths†, unlike the particle on a ring of I.

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† Gutzwiller (1967) has obtained approximate Green functions in this way, however.

However, the Green functions can be combined to form the spectral operator I_E, and for the corresponding operator J_ν in the symmetric representation the contours are complete.

Using the relation $A^-(\nu^*) = \{A^+(\nu)\}^*$ with equations (40) and (43) and remembering that the argument of A^- must have a negative imaginary part, we have

$$\begin{aligned}\frac{\sin\omega}{\nu^2}J_\nu(\boldsymbol{u},\boldsymbol{u}_0) &= \lim_{\nu_{\mathrm{I}}\to 0}\frac{1}{2\pi\mathrm{i}}\{A^-(\nu^*)-A^+(\nu)\}\\ &= -\lim_{\nu_{\mathrm{I}}\to 0}\left[+\frac{1}{8\pi}\exp\{-\mathrm{i}\nu^*(\omega-\mathrm{i}\epsilon)\}\int_{-\infty-\mathrm{i}\epsilon}^{\omega-\mathrm{i}\epsilon}\mathrm{d}\omega'\frac{\exp\{-\mathrm{i}(\frac{1}{2}-\nu^*)\omega'\}}{\sin\frac{1}{2}\omega'}\right.\\ &\quad+\frac{1}{8\pi}\exp\{\mathrm{i}\nu^*(\omega+\mathrm{i}\epsilon)\}\int_{\omega+\mathrm{i}\epsilon}^{\infty+\mathrm{i}\epsilon}\mathrm{d}\omega'\frac{\exp\{\mathrm{i}(\frac{1}{2}-\nu^*)\omega'\}}{\sin\frac{1}{2}\omega'}\\ &\quad+\frac{1}{8\pi}\exp\{\mathrm{i}\nu(\omega+\mathrm{i}\epsilon)\}\int_{-\infty+\mathrm{i}\epsilon}^{\omega+\mathrm{i}\epsilon}\mathrm{d}\omega'\frac{\exp\{\mathrm{i}(\frac{1}{2}-\nu)\omega'\}}{\sin\frac{1}{2}\omega'}\\ &\quad\left.+\frac{1}{8\pi}\exp\{-\mathrm{i}\nu(\omega-\mathrm{i}\epsilon)\}\int_{\omega-\mathrm{i}\epsilon}^{\infty-\mathrm{i}\epsilon}\mathrm{d}\omega'\frac{\exp\{-\mathrm{i}(\frac{1}{2}-\nu)\omega'\}}{\sin\frac{1}{2}\omega'}\right]. \qquad (48)\end{aligned}$$

The first and fourth terms may be combined together to give a single contour: the functions are slightly different, but become the same as $\nu_{\mathrm{I}} \to 0$. The same applies to the second and third terms, giving

$$\begin{aligned}\frac{\sin\omega}{\nu^2}J_\nu(\boldsymbol{u},\boldsymbol{u}_0) &= -\frac{\exp(-\mathrm{i}\nu\omega)}{8\pi}\int_{\mathrm{C}_1}\mathrm{d}\omega'\frac{\exp\{-\mathrm{i}(\frac{1}{2}-\nu)\omega'\}}{\sin\frac{1}{2}\omega'}\\ &\quad+\frac{\exp(\mathrm{i}\nu\omega)}{8\pi}\int_{\mathrm{C}_2}\mathrm{d}\omega'\frac{\exp\{\mathrm{i}(\frac{1}{2}-\nu)\omega'\}}{\sin\frac{1}{2}\omega'} \qquad (49)\end{aligned}$$

where the contours C_1 and C_2 are illustrated in figure 3.

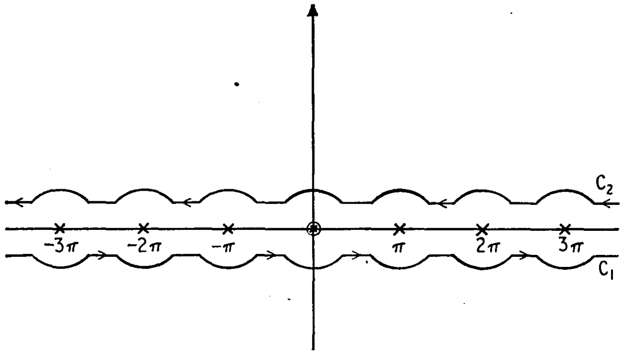

Figure 3. The contours C_1 and C_2 in the complex ω plane over which the integrations are taken.

For $\nu < 0$ the semicircles which may be used to complete the contours enclose no poles, so that

$$J_\nu = 0 \qquad (\nu < 0). \qquad (50)$$

For $\nu > 0$ the contours C_1 and C_2 may be completed by large semicircles in the positive and negative half-planes respectively. On summing over the residues at the poles, we obtain

$$J_\nu(\boldsymbol{u}, \boldsymbol{u}_0) = \frac{\nu^2}{\sin\omega}\epsilon(\nu) \sum_{c=-\infty}^{\infty} \sin\{\nu(2\pi c - \omega)\} \tag{51}$$

$$= -\nu^2\epsilon(\nu) \sum_{c=-\infty}^{\infty} \frac{\sin\{S_{cE}(\boldsymbol{u}, \boldsymbol{u}_0)/\hbar\}}{\sin\{s_c(\boldsymbol{u}, \boldsymbol{u}_0)\}}. \tag{52}$$

We have thus succeeded in obtaining the operator J_ν in symmetric representation, which is analogous to the operator I_E in momentum representation, in terms of sums over classical paths. The expression for the spectral operator in momentum representation is not so simple as it involves the path length on the hypersphere in terms of momenta:

$$I_E(\boldsymbol{p}, \boldsymbol{p}_0) = \frac{-8\mu^3 p_E k^2}{\pi^2\hbar^2(p^2+p_E{}^2)^2(p_0{}^2+p_E{}^2)^2} \sum_{c=-\infty}^{\infty} \frac{\sin\{S_{cE}(\boldsymbol{p}, \boldsymbol{p}_0)/\hbar\}}{\sin|\omega+2\pi c|}; \qquad E < 0 \tag{53}$$

where ω is given in terms of momenta by equation (24), and equation (22) may be used to obtain the action explicitly. The denominator is the square root of the density of classical paths from $\boldsymbol{p}_0$ (Gutzwiller 1967), as can be seen clearly in the symmetric representation.

Equation (51) may be summed using the generalized function expansion of Lighthill (1960, p. 68), giving

$$J_\nu(\boldsymbol{u}, \boldsymbol{u}_0) = -\epsilon(\nu)\nu^2 \frac{\sin\nu\omega}{\sin\omega} \sum_{n=-\infty}^{\infty} \delta(\nu - n) \tag{54}$$

and then transformed to momentum representation, giving the spectral operator in projection operator form (I, equation (14)):

$$I_E = \delta(E-H) = \sum_{n=1}^{\infty} \delta(E-E_n)P_n \qquad (E < 0) \tag{55}$$

where

$$P_n(\boldsymbol{p}, \boldsymbol{p}_0) = \frac{8p_E{}^5}{\pi^2(p^2+p_E{}^2)^2(p_0{}^2+p_E{}^2)^2} \frac{n\sin n\omega}{\sin\omega} \tag{56}$$

is the projection operator onto the nth subspace (Fock 1935). The analysis may be reversed to give equation (52) without using the complex variable theory, but we shall need the latter for the continuous spectrum.

5. Conclusion

The Bohr–Sommerfeld identity now follows from equation (54), which shows that for bound states ν is a positive integer (n), so that, by equation (20) and the definition of ν, the action once around an orbit when E is the energy of a bound state is

$$(S_E)_{\text{orbit}} = 2\pi n\hbar. \tag{57}$$

The left-hand side is independent of the representation as the initial and final points are the same.

The spectral operator has been expressed as a sum over classical paths, and this sum thereby enables us to obtain the dynamical solution of the hydrogen atom problem in terms of classical paths; but we have been unable to obtain the Green operators and the evolution operators in these terms, so that our theory is not so general as for the free particle of I.

The theory will be completed by a study of the continuous spectrum and the Rutherford scattering identity in a following paper.

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III. Classical paths and Rutherford scattering

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Abstract. In preparation for the derivation of correspondence identities for the Rutherford scattering problem, the relevant classical theory is developed. Convenient conventions for classical canonical transformations are introduced. Classical O(1, 3) symmetry properties are discussed. Classically accessible and inaccessible regions of momentum space are defined, and, for the latter, generalized classical paths and the corresponding action functions are obtained by analytic continuation.

1. Introduction

In this and the following paper the results of Norcliffe and Percival (1968, to be referred to as II) are generalized to include the states of positive energy, which represent the Rutherford scattering of an electron by a proton.

The original correspondence identities for the negative energy states, representing the bound hydrogen atom, were obtained in momentum representation and the related symmetric representation, and not in position representation. This appears to be a direct consequence of the accessibility of every region of momentum space to a bound electron of given negative energy E, which is confined in position space to a spherical region around the centre of the potential.

By contrast, an electron of given positive energy E can reach every position, but a large region of momentum space is inaccessible, as discussed in § 2. Nevertheless, we still find correspondence identities in the symmetric and momentum representations only. Inaccessibility in momentum space complicates the derivation of correspondence identities, so this paper is restricted to a treatment of the relevant classical theory. The quantum theory and correspondence identities are dealt with in the following paper (Norcliffe *et al.* 1969, to be referred to as IV).

Section 3 of this paper describes conventions and notations for classical canonical transformations which resemble those of quantal unitary transformations more closely than those of the standard texts. In the following section transformations and action functions for the position, momentum and symmetric respresentations are introduced. Although this treatment of Rutherford scattering is non-relativistic, much of the mathematics resembles that of the relativistic motion of a free particle. This is because the symmetry properties are the same: for each, the appropriate symmetry group is O(1, 3).

In § 5 generalized classical paths are introduced which pass through the inaccessible region of momentum space. Their properties are determined by analytic continuation from the usual physical classical paths. The action functions for the generalized paths are usually complex; through them the correspondence identities which relate classical and quantum mechanics are obtained, but the treatment of these relations is left to IV.

2. Classical trajectories

Consider a particle of mass μ and positive energy $E = p_E{}^2/2\mu$ moving in an attractive Coulomb potential

$$V(\mathbf{r}) = -\frac{k}{r} = -\frac{Ze^2}{r} \qquad k > 0. \tag{1}$$

The trajectory in position space is one branch of a hyperbola which has one focus at the origin. The momentum-space trajectory, or hodograph, is an arc of a circle whose radius is $p_E(\epsilon^2 - 1)^{-1/2} = k\mu/bp_E$, and whose centre is at a distance $\epsilon p_E(\epsilon^2 - 1)^{-1/2}$ from the origin. The eccentricity of the orbit is ϵ and b is the impact parameter. The tangents to the circular hodograph at the extremities of the arc intersect at the origin at an angle Θ which is the scattering angle, as shown in figure 1. The remaining arc of the circle is the hodograph of a particle having the same energy moving under the influence of a repulsive Coulomb potential $V(\boldsymbol{r}) = k/r$. In position space this corresponds to a trajectory which is the other branch of the same hyperbola. The two regions $|\boldsymbol{p}| \geqslant p_E$ and $|\boldsymbol{p}| \leqslant p_E$ of momentum space are thus classically inaccessible to a particle moving in a repulsive and an attractive Coulomb potential respectively.

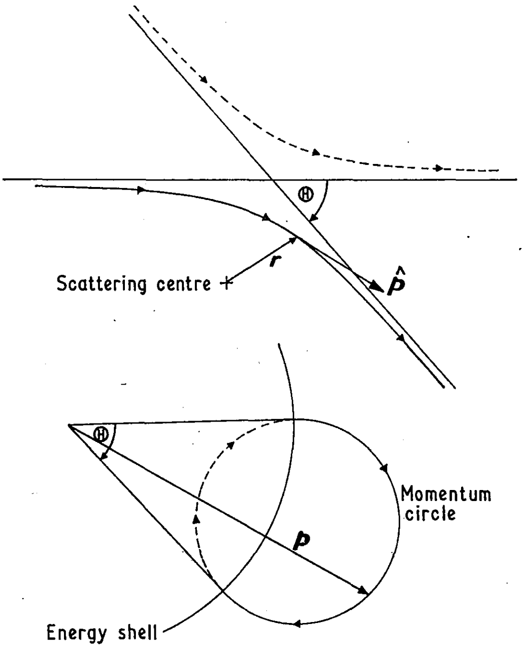

Figure 1. The hyperbolic trajectory in position space and the circular hodograph. The continuous curves are the trajectories for the attractive Coulomb potential and the dotted for the repulsive.

3. Classical canonical transformation theory

As described in textbooks on classical mechanics (e.g. Corben and Stehle 1960, Goldstein 1950), the state of a classical system with a finite number of degrees of freedom is represented by a point $P(q_i, p_i)$ in phase space and is defined by any complete set of canonical coordinates q_i and conjugate momenta p_i. The state at any time is determined by the state at any other time. The relation between different choices of q_i and conjugate p_i, which leave the form of Hamilton's equations invariant, is the subject of canonical transformation theory.

In this theory it is not usual, but it is convenient, to refer to a 'classical representation', which is given the name of the set of variables which play the role of the canonical coordinates. Canonical transformations are then transformations between different classical representations.

For example, in the position representation for a particle in a scalar potential field the coordinates x, y, z of the position vector $\boldsymbol{r}$ are the canonical coordinates. The conjugate momenta are p_x, p_y, p_z, but this need not be stated explicitly. In the momentum representation p_x, p_y, p_z are the canonical coordinates, and, by canonical transformation theory, $-x$, $-y$, $-z$ are the conjugate momenta.

The solution of a quantum-mechanical problem can be obtained from a knowledge of certain operators connecting initial and final quantal states, e.g. the evolution operator or propagator. Any representation may be used for the states, provided it is known how to transform from this representation to others. Analogously the solution of a classical-mechanical problem can be obtained from a knowledge of certain classical action functions S connecting initial and final classical states.

The usual classical action integral of time-dependent theory can be represented in position representation in a similar way to that given by Feynman and Hibbs (1965):

$$S(\boldsymbol{r}, t; \boldsymbol{r}_0, t_0) = \int_{\mathrm{P}(\boldsymbol{r}_0), t_0}^{\mathrm{P}(\boldsymbol{r}), t} L \, \mathrm{d}t' \tag{2}$$

where L is the Lagrangian evaluated along a classical path between $\boldsymbol{r}_0$ and $\boldsymbol{r}$ which is traversed by the particle from time t_0 to time t. The corresponding action function of time-independent theory is usually known as Hamilton's principal function, but we shall refer to it simply as the time-independent action:

$$S(\boldsymbol{r}, E; \boldsymbol{r}_0, E_0) = \int_{\mathrm{P}(\boldsymbol{r}_0), E_0}^{\mathrm{P}(\boldsymbol{r}), E} \boldsymbol{p} \, . \, \mathrm{d}\boldsymbol{r}'. \tag{3}$$

For a time-independent Hamiltonian the energy is conserved, one energy is redundant, and we write $S_E(\boldsymbol{r}, \boldsymbol{r}_0)$. As in quantum mechanics the second coordinate refers to the initial state.

Transformation to other representations is effected by generating functions which also have the dimensions of action. There are four standard types of transformation (Corben and Stehle 1960, § 59, Goldstein 1950, chap. 8), but only one of them, the 'direct' transformation, is equivalent to a unitary transformation of quantum mechanics. This is the one in which the generating function, here denoted by ϕ, is an explicit function of the canonical coordinates of both the original and final representation. The others are sometimes more convenient to use and consist of a direct transformation together with one or two of the special transformations which transpose the canonical coordinates and momenta.

A generating function of a direct transformation is analogous to a unitary transformation operator which effects a transformation in quantum mechanics. A classical action such as $S_E(\boldsymbol{r}, \boldsymbol{r}_0)$ is analogous to a quantal operator. In quantal transformations of operators the transformation operator appears twice: once for the initial and once for the final state. Similarly, in a transformation of a classical action $S_E(q, q_0)$ from q to $\bar{q}$ representation, the generating function ϕ appears twice:

$$S_E(\bar{q}, \bar{q}_0) = -\phi(\bar{q}, q) + S_E(q, q_0) + \phi(q_0, \bar{q}_0). \tag{4}$$

We note that the functional forms of $S_E(\bar{q}, \bar{q}_0)$ and $S_E(q, q_0)$ may be quite different, just as in the quantal transformation

$$X = U^{\dagger} X U \tag{5}$$

the functional forms of the kernels $X(\bar{q}, \bar{q}_0)$ and $X(q, q_0)$ may be quite different, despite the notation.

In a given classical representation the action function is defined by the initial and final canonical coordinates, together with the energy. The classical path defined by these coordinates may not be unique. Frequently there is a discrete set of classical paths. In these cases a further label $c = 0, 1, 2, \ldots$ is required to specify a particular classical path and the corresponding action function $S_{cE}(q, q_0)$.

Usually canonical transformations do not depend explicitly on energy or time. The new canonical coordinates and momenta are functions of the old ones and certain fixed parameters. The time variable remains unchanged. Such a transformation appears in § 4, and p_E is there a fixed parameter independent of the energy.

However, in the most general canonical transformations the time and energy appear on the same footing as the canonical coordinates and momenta, as shown in § 86 of the article by Synge (1960). For such transformations the new time variable can be a function of the old coordinates and momenta, and in § 6 such a transformation is considered in which the new coordinates are functions of the old coordinates and of the energy E.

The variable p_E is then energy dependent, and the new time variable is position dependent. This transformation and the previous energy-independent transformation must be carefully distinguished.

4. The symmetric representation

Since the correspondence identities are most directly expressed in symmetric representation (see §3 of IV), we choose this representation to solve the classical dynamical problem of the Coulomb potential. We then have the solution of the Coulomb scattering problem in each representation.

The symmetric representation has been discussed in the literature by Bander and Itzykson (1966), and others. Let u_λ ($\lambda = 0, 1, 2, 3$) denote a position vector in the four-dimensional Minkowski space with a metric whose signature is $(1, -1, -1, -1)$ (see Dirac 1958, p. 253).

The surface $\mathscr{S}$ of a unit sphere in this space has equation

$$u_\lambda u^\lambda = u_0{}^2 - u_1{}^2 - u_2{}^2 - u_3{}^2 = 1 \tag{6}$$

and consists of two sheets $\mathscr{S}^+$ and $\mathscr{S}^-$ defined by $u_0 \geqslant 1$ and $u_0 \leqslant -1$ respectively. In four-dimensional Euclidean space $\mathscr{S}$ is the surface of a rectangular hyperboloid. A point u_λ on $\mathscr{S}$ is associated with a point $\boldsymbol{p}$ in momentum space by projecting the scaled momentum 4-vector $(0, \boldsymbol{p}/p_E)$ from the point $(-1, 0, 0, 0)$ on $\mathscr{S}^-$, onto the surface $\mathscr{S}$. At first we choose p_E to be a fixed parameter. The projection is shown in figure 2, in three dimensions for simplicity. Explicitly,

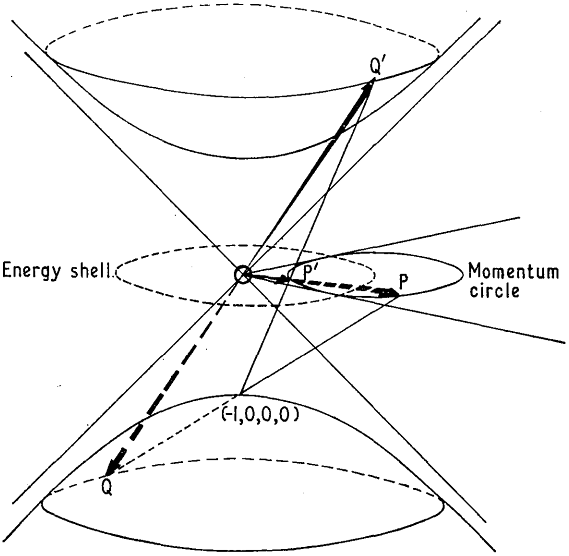

Figure 2. The stereographic projection. The points P and P′ in the scaled momentum space project onto the points Q and Q′ on the surface of the hyperboloid.

$$u_\lambda = (\cosh\alpha, \sinh\alpha\,\hat{\boldsymbol{p}}), \text{ where } \tanh\tfrac{1}{2}\alpha = p/p_E;$$
$$|\boldsymbol{p}| \leqslant p_E \tag{7a}$$
$$u_\lambda = -(\cosh\alpha, \sinh\alpha\,\hat{\boldsymbol{p}}), \text{ where } \tanh\tfrac{1}{2}\alpha = p_E/p;$$
$$|\boldsymbol{p}| \geqslant p_E. \tag{7b}$$

All points in the region of momentum space for which $|\boldsymbol{p}| \geqslant p_E$ are projected onto $\mathscr{S}^-$ and all those in the region $|\boldsymbol{p}| \leqslant p_E$ onto $\mathscr{S}^+$. Thus $\mathscr{S}^-$ and $\mathscr{S}^+$ are respectively the classically accessible regions of the attractive and repulsive Coulomb potentials in the symmetric representation.

If θ and ϕ are the usual polar angles defining the direction of the unit vector $\hat{\boldsymbol{p}}$, then α, θ, ϕ may be taken as the generalized coordinates of the particle in the symmetric representation. Let $p_\alpha, p_\theta, p_\phi$ be the canonical momenta conjugate to them. In the momentum representation the canonical coordinates for a given energy may be expressed solely in terms of the canonical coordinates in symmetric representation, viz. on $\mathscr{S}^-$:

$$\left.\begin{aligned} p_x &= p_E \coth \tfrac{1}{2}\alpha \sin\theta \cos\phi \\ p_y &= p_E \coth \tfrac{1}{2}\alpha \sin\theta \sin\phi \\ p_z &= p_E \coth \tfrac{1}{2}\alpha \cos\theta \end{aligned}\right\} \tag{8}$$

then the canonical transformation from symmetric to momentum representation† is a coordinate transformation. The generating function of a contact transformation appropriate to such a coordinate transformation is given by Corben and Stehle (1960, p. 178, equation (59.9)) and leaves the value of the classical action function unchanged, so that

$$S_E(u_\lambda, u_\lambda^{(0)}) = S_E(\boldsymbol{p}, \boldsymbol{p}_0) = \int_{\mathrm{P}(\alpha_0,\theta_0,\phi_0)}^{\mathrm{P}(\alpha,\theta,\phi)} (p_\alpha' \mathrm{d}\alpha' + p_\theta' \mathrm{d}\theta + p_\phi' \mathrm{d}\phi') \tag{9}$$

where P represents a classical state of the system. As was seen in II, the energy dependence of the transformation (8) introduces no great difficulty into the theory. The generating function ψ' (Corben and Stehle 1960, § 59) is given explicitly by

$$\psi'(\alpha,\theta,\phi; -x, -y, -z) = -\boldsymbol{r} \cdot \boldsymbol{p} = -p_E \coth \tfrac{1}{2}\alpha \, (x \sin\theta\cos\phi + y\sin\theta\sin\phi + z\cos\theta). \tag{10}$$

In symmetric representation the generalized momenta are given by

$$p_\alpha = \frac{\partial\psi'}{\partial\alpha} \text{ and similarly for } p_\theta, p_\phi. \tag{11}$$

By a method analogous to that of II we solve for $r = |\boldsymbol{r}|$ and find that

$$r = 2\sinh^2 \tfrac{1}{2}\alpha \, \frac{\Pi}{p_E} \tag{12}$$

where

$$\Pi = \left(p_\alpha^2 + \frac{p_\theta^2}{\sinh^2\alpha} + \frac{p_\phi^2}{\sinh^2\alpha \sin^2\theta}\right)^{1/2}. \tag{13}$$

Π is the analogue of the magnitude $|\boldsymbol{p}_u|$ of the hyperspherical momentum defined in II, equation (10).

Since the transformation from symmetric to momentum representation does not depend explicitly on time, the value of the Hamiltonian remains the same in either representation. For the attractive potential, the expression for the Hamiltonian in symmetric representation becomes

$$H(\boldsymbol{r},\boldsymbol{p}) = \frac{p^2}{2\mu} - \frac{k}{r} = \frac{p_E^2 \coth^2 \frac{1}{2}\alpha}{2\mu} - \frac{k p_E \operatorname{cosech}^2 \frac{1}{2}\alpha}{2\Pi}. \tag{14}$$

We can express the action integral in equation (9) along any path on $\mathscr{S}^-$ in a Lorentz-invariant form, which is the same thing as symmetry under the group O(1, 3). The element of distance along the path is

$$\mathrm{d}u_\lambda = \mathrm{d}\alpha \, \hat{\alpha}_\lambda + \sinh\alpha \, \mathrm{d}\theta \, \hat{\theta}_\lambda + \sinh\alpha \sin\theta \, \mathrm{d}\phi \, \hat{\phi}_\lambda \tag{15}$$

where $\hat{\alpha}_\lambda$, $\hat{\theta}_\lambda$, $\hat{\phi}_\lambda$ are mutually orthonormal vectors in the Minkowski space. The invariant

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† For convenience we choose the symmetric representation to be the initial representation in contrast with II.

distance s along the path is given by

$$\frac{\mathrm{d}s}{\mathrm{d}t} = \left(-\frac{\mathrm{d}u_\lambda}{\mathrm{d}t}\frac{\mathrm{d}u^\lambda}{\mathrm{d}t}\right)^{1/2}. \tag{16}$$

From equations (13), (14) and (15) together with Hamilton's equations

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = \frac{\partial H}{\partial p_\alpha}, \text{ etc.} \tag{17}$$

it follows that

$$\frac{\mathrm{d}s}{\mathrm{d}t} = \frac{kp_E \operatorname{cosech}^2 \tfrac{1}{2}\alpha}{2\Pi^2}. \tag{18}$$

The representation is symmetric only for the energy $E = p_E{}^2/2\mu$, and we limit our consideration to this particular energy. A representation which is symmetric for all positive energies is used in § 6.

For this energy, under the subsidiary condition $H(\boldsymbol{r}, \boldsymbol{p}) - E = 0$, we have from equation (14)

$$\Pi = \text{constant} = k\mu/p_E. \tag{19}$$

A 4-vector Π_λ can be defined as

$$\Pi_\lambda = \Pi\frac{\mathrm{d}u_\lambda}{\mathrm{d}s} = p_\alpha\hat{\alpha}_\lambda + \frac{p_\theta\hat{\theta}_\lambda}{\sinh\alpha} + \frac{p_\phi\hat{\phi}_\lambda}{\sinh\alpha\sin\theta}. \tag{20}$$

This is consistent with the definition of Π, since

$$\Pi^2 = -\Pi_\lambda\Pi^\lambda. \tag{21}$$

Hence

$$S_E(u_\lambda, u_\lambda{}^{(0)}) = -\int_{s_0}^{s} \Pi^\lambda \frac{\mathrm{d}u_\lambda}{\mathrm{d}s'}\mathrm{d}s' = \Pi\int_{s_0}^{s} \mathrm{d}s'. \tag{22}$$

The stationary action principle then implies that $\Delta \int_{s_0}^{s} \mathrm{d}s' = 0$, and the trajectories on $\mathscr{S}^-$ are thus geodesics. In this case they are the curves in which planes through the origin intersect $\mathscr{S}^-$, and in the Euclidean sense they are rectangular hyperbolae. They are analogous to the great circles on the unit hypersphere in the case of the discrete spectrum. In fact, if β is the Minkowski distance along a geodesic between the two points $u_\lambda{}^{(0)}$ and u_λ on $\mathscr{S}^-$, then

$$\cosh\beta = u_\lambda{}^{(0)}u^\lambda = 1 + \frac{E|\boldsymbol{p}-\boldsymbol{p}_0|^2}{\mu(T_0-E)(T-E)} \tag{23}$$

where the kinetic energies T and T_0 are

$$T = \frac{p^2}{2\mu}, \qquad T_0 = \frac{p_0{}^2}{2\mu}. \tag{24}$$

β is thus the hyperbolic angle between the two points on $\mathscr{S}^-$ and, as we shall see in the next section, is just the analytic continuation of the angle ω defined in equation (21) of II.

From equation (22) the action is thus

$$S_E(u_\lambda, u_\lambda{}^{(0)}) = \Pi\beta = S_E(\boldsymbol{p}, \boldsymbol{p}_0), \qquad |\boldsymbol{p}|, |\boldsymbol{p}_0| \geqslant p_E. \tag{25}$$

This result may be obtained from the Kepler theory using the parametrization by the eccentric anomaly (the ξ of Landau and Lifshitz 1960, § 15). β, as defined in equation (23), is just the difference in the eccentric anomalies corresponding to the points $\boldsymbol{p}_0$ and $\boldsymbol{p}$, as shown for bound states by Györgyi (1968). We obtain a similar result for the action between two points in the accessible region of the repulsive potential.

The correspondence identities depend critically on the properties of the action function as defined in equation (25). In quantum theory the electron has a finite probability of being in the classically inaccessible region and, at first sight, this appears to exclude all possibility of complete correspondence identities, because no classical paths reach this inaccessible region. However, this is not the case and we shall show how the classical path and the action function may be analytically continued into this region.

5. Paths through the inaccessible region

It is shown in II that, in the discrete spectrum $E < 0$, the kernel $I_E(\boldsymbol{p}, \boldsymbol{p}_0)$ of the spectral operator can be expressed as a sum over classical paths between $\boldsymbol{p}_0$ and $\boldsymbol{p}$, each path being characterized by the number c of times that the particle passes around the complete circular momentum orbit. The contribution from each path depends on the corresponding classical action $S_{cE}(\boldsymbol{p}, \boldsymbol{p}_0)$.

For the continuous spectrum $E > 0$ there is one physical path between $\boldsymbol{p}_0$ and $\boldsymbol{p}$ if they both lie in the accessible region and no path if either $\boldsymbol{p}_0$ or $\boldsymbol{p}$ are in the inaccessible region. Nevertheless, the kernel of the spectral operator $I_E(\boldsymbol{p}, \boldsymbol{p}_0)$ is non-zero in the latter region, so that a theory in terms of the usual classical paths is not possible.

A way out of this impasse is found by considering generalized classical paths which can pass through the inaccessible region. For positive energies we consider paths which pass around the momentum circle any number of times, as for classical paths of negative energy. Here they may pass into and out of the inaccessible region. Between any two points $\boldsymbol{p}_0$ and $\boldsymbol{p}$ within or without the classically accessible region, there is an infinite number of such paths, each path again being characterized by the number c of times that the particle passes around the complete momentum circle. The corresponding classical actions $S_{cE}(\boldsymbol{p}, \boldsymbol{p}_0)$ must then be defined for $E > 0$. Since the action for $E < 0$ is defined for arbitrary $\boldsymbol{p}$ and $\boldsymbol{p}_0$ we obtain the result for $E > 0$ by analytic continuation.

It is well known that quantal scattering Green functions and scattering amplitudes have a cut along the positive real axis in the complex energy plane. The same applies to the classical action function $S_{cE}(\boldsymbol{p}, \boldsymbol{p}_0)$, and for the same reason: that the kinetic energy is a quadratic function of the momentum. The value of ω, and hence of $S_{cE}(\boldsymbol{p}, \boldsymbol{p}_0)$ depends on whether we analytically continue above or below the cut, i.e. the two actions

$$S_{cE}^{(\pm)}(\boldsymbol{p},\boldsymbol{p}_0) = \lim_{\varepsilon\to 0} S_{c,E\pm i\varepsilon}(\boldsymbol{p},\boldsymbol{p}_0) \qquad (E, \varepsilon > 0) \tag{26}$$

are different. They are related to the two Green functions $G_E^{(\pm)}(\boldsymbol{p}, \boldsymbol{p}_0)$.

From II we know that for the attractive Coulomb potential the action along the shortest path between $\boldsymbol{p}_0$ and $\boldsymbol{p}$ for a negative energy $\mathscr{E}$ is given by

$$S_{0\mathscr{E}}(\boldsymbol{p},\boldsymbol{p}_0) = \frac{\mu k\omega}{(-2\mu\mathscr{E})^{1/2}} \tag{27}$$

where

$$\cos\omega = 1+\frac{\mathscr{E}|\boldsymbol{p}-\boldsymbol{p}_0|^2}{\mu(\mathscr{E}-T)(\mathscr{E}-T_0)} = z(\mathscr{E}) \tag{28}$$

so that when $\mathscr{E}$ is real and negative ω is real and lies between 0 and π; it is, in fact, the angle between the position vectors of the points on the hypersphere corresponding to $\boldsymbol{p}$ and $\boldsymbol{p}_0$. Now for positive energies we first suppose that $\boldsymbol{p}_0$ is fixed in the accessible region and we shall obtain ω from equation (28) for $\mathscr{E} = E+\mathrm{i}\varepsilon$, i.e. $\omega^+(E) = \lim_{\varepsilon\to 0}\omega(E+\mathrm{i}\varepsilon)$ where $E > 0$ and ε is small and positive, and for $\boldsymbol{p}$ on different parts of the momentum circle as shown in figure 3.

From equation (28) we have

$$\omega = \pm\mathrm{i}\ln\{z+(z^2-1)^{1/2}\} \tag{29}$$

which is a many-valued function of z. The function $z+(z^2-1)^{1/2}$ is itself a double-valued function of z and all its values are given on the Riemann surface consisting of two sheets R_1, R_2 joined by cuts from $-\infty$ to -1, and from $+1$ to $+\infty$. On R_1 we define $\mathrm{Im}(z^2-1)^{1/2} \geqslant 0$. Then $(z^2-1)^{1/2}$ is uniquely defined on the Riemann surface. On R_2, $(z^2-1)^{1/2}$ takes on values of opposite sign to those at the corresponding points on R_1. The argument of $z+(z^2-1)^{1/2}$ then varies continuously from 0 to 2π as z passes around the branch points ± 1 on the two sheets. If we now take an infinite set of such pairs of sheets joined in the usual way along the above cuts, then $\arg\{z+(z^2-1)^{1/2}\}$ takes on all real values on the Riemann surface thus obtained and from equation (29) ω is a single-valued function of z on this surface, given by

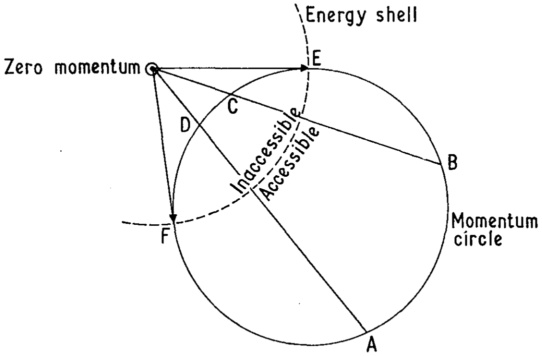

Figure 3. The different types of paths in momentum space. Between A and B we have the path in the accessible region and also AFDCEB which passess through the inaccessible region.

$$\omega = \arg\{z+(z^2-1)^{1/2}\} - \mathrm{i} \ln |z+(z^2-1)^{1/2}|. \tag{30}$$

When z is real and lies between -1 and $+1$ on R_1, ω is real and lies between 0 and π.

We now consider z as a function of $E+\mathrm{i}\varepsilon$ defined by equation (28), where $E > 0$ with $\boldsymbol{p}_0$ fixed at $\mathrm{A}(\boldsymbol{p}_0)$, say, and $\boldsymbol{p}$ varying around the momentum circle from A through E and F and back to A as in figure 3. By examination of the real and imaginary parts of z we find that z describes the contour shown in figure 4. Using equation (30) we find that the analytic continuation of ω for $\boldsymbol{p}_0$ fixed in the accessible region at A, when $\boldsymbol{p}$ lies on different

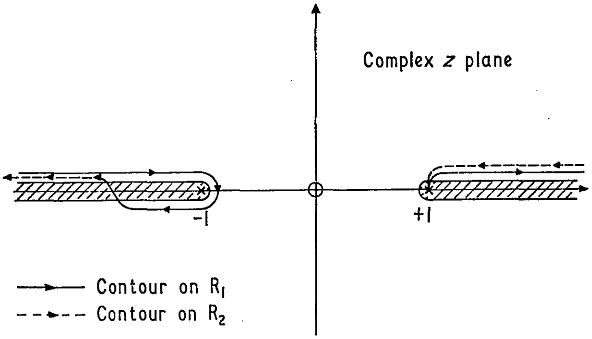

Figure 4. The path on the Riemann sheets R_1 and R_2, described by z defined in equation (28) for $\mathscr{E} = E+\mathrm{i}\varepsilon$ (E, $\varepsilon > 0$) and p_0 fixed in the accessible region, with $\boldsymbol{p}$ varying round the hodograph.

Table 1. **The analytic continuation of the path length and action function between two points p_0 and p on various segments of the hodograph, for energy $\mathscr{E} = E+i\epsilon$ $(E, \epsilon > 0)$**

Region	Path (figure 3)	Analytic path length in symmetric representation	Action $S_{cE}{}^{+}(\boldsymbol{p}, \boldsymbol{p}_0)$	$\exp \frac{i}{\hbar}$(action)	Sine of the analytic path length	Potential
$\lvert\boldsymbol{p}\rvert, \lvert\boldsymbol{p}_0\rvert > p_E$ $(u_\lambda, u_\lambda{}^{(0)}$ on $\mathscr{S}^-)$	A($\boldsymbol{p}_0$) to B($\boldsymbol{p}$) $c = 0, 1, \ldots, \infty$	$2\pi c - i\beta$	$\eta\beta\hbar + 2\pi i c\hbar\eta$	$\exp(i\eta\beta - 2\pi c\eta)$	$-i \sinh \beta$	attractive
	A($\boldsymbol{p}_0$) to B($\boldsymbol{p}$) via F, E $c = 1, 2, \ldots, \infty$	$2\pi c + i\beta$	$-\eta\beta\hbar + 2\pi i c\hbar\eta$	$\exp(-i\eta\beta - 2\pi c\eta)$	$i \sinh \beta$	repulsive
$\lvert\boldsymbol{p}\rvert, \lvert\boldsymbol{p}_0\rvert < p_E$ $(u_\lambda, u_\lambda{}^{(0)}$ on $\mathscr{S}^+)$	D($\boldsymbol{p}_0$) to C($\boldsymbol{p}$) $c = 0, 1, \ldots, \infty$	$2\pi c + i\beta$	$-\eta\beta\hbar + 2\pi i c\hbar\eta$	$\exp(-i\eta\beta - 2\Pi c\eta)$	$i \sinh \beta$	repulsive
	D($\boldsymbol{p}_0$) to C($\boldsymbol{p}$) via F, E $c = 1, 2, \ldots, \infty$	$2\pi c - i\beta$	$\eta\beta\hbar + 2\pi i c\hbar\eta$	$\exp(i\eta\beta - 2\pi c\eta)$	$-i \sinh \beta$	attractive
$\lvert\boldsymbol{p}_0\rvert > p_E$, $\lvert\boldsymbol{p}\rvert < p_E$ $(u_\lambda{}^{(0)}$ on $\mathscr{S}^-$, u_λ on $\mathscr{S}^+)$	A($\boldsymbol{p}_0$) to C($\boldsymbol{p}$) via E $c = 0, 1, \ldots, \infty$	$\pi(2c+1) - i\beta$	$\eta\beta\hbar + \pi(2c+1)i\hbar\eta$	$\exp\{i\eta\beta - \pi(2c+1)\eta\}$	$i \sinh \beta$	attractive
	A($\boldsymbol{p}_0$) to C($\boldsymbol{p}$) via F $c = 1, 2, \ldots, \infty$	$\pi(2c-1) + i\beta$	$-\eta\beta\hbar + \pi(2c-1)i\hbar\eta$	$\exp\{-i\eta\beta - \pi(2c-1)\eta\}$	$-i \sinh \beta$	repulsive
$\lvert\boldsymbol{p}_0\rvert < p_E$, $\lvert\boldsymbol{p}\rvert > p_E$ $(u_\lambda{}^{(0)}$ on $\mathscr{S}^+$, u_λ on $\mathscr{S}^-)$	D($\boldsymbol{p}_0$) to B($\boldsymbol{p}$) via E $c = 0, 1, \ldots, \infty$	$\pi(2c+1) + i\beta$	$-\eta\beta\hbar + \pi(2c+1)i\hbar\eta$	$\exp\{-i\eta\beta - \pi(2c+1)\eta\}$	$-i \sinh \beta$	repulsive
	D($\boldsymbol{p}_0$) to B($\boldsymbol{p}$) via F $c = 1, \ldots, \infty$	$\pi(2c-1) - i\beta$	$\eta\beta\hbar + \pi(2c-1)i\hbar\eta$	$\exp\{i\eta\beta - \pi(2c-1)\eta\}$	$i \sinh \beta$	attractive

For energy $\mathscr{E} = E - i\varepsilon$ the above quantities become their complex conjugate. A($\boldsymbol{p}_0$), etc., means that the momentum vector $\boldsymbol{p}_0$ is taken to be OA of figure 3. The last three columns are of use in IV.

arcs of the momentum circle, is given by (see figure 3)

$$\omega^+ = \begin{cases} -\mathrm{i}\beta, \text{ for } \boldsymbol{p} \text{ at B, where B varies from A}(\beta = 0) \\ \qquad \text{to E}(\beta = \infty) \text{ on path ABE} \qquad (a) \\ \pi - \mathrm{i}\beta, \text{ for } \boldsymbol{p} \text{ at C, where C varies from E}(\beta = \infty) \\ \qquad \text{to D}(\beta = 0) \text{ on path ABED} \qquad (b) \\ \pi + \mathrm{i}\beta, \text{ for } \boldsymbol{p} \text{ at C, where C varies from D}(\beta = 0) \\ \qquad \text{to E}(\beta = \infty) \text{ on path AFDE} \qquad (c) \\ 2\pi + \mathrm{i}\beta, \text{ for } \boldsymbol{p} \text{ at B, where B varies from E}(\beta = \infty) \\ \qquad \text{to A}(\beta = 0) \text{ on path AFDEB} \qquad (d) \end{cases} \tag{31}$$

where β is the hyperbolic angle, always defined between two points $u_\lambda^{(0)}$, u_λ on $\mathscr{S}^-$. The momentum $\boldsymbol{p}_0$ projects onto $u_\lambda^{(0)}$ and $\boldsymbol{p}$ projects onto u_λ if $|\boldsymbol{p}| > p_E$. It projects onto $-u_\lambda$ if $|\boldsymbol{p}| < p_E$, that is u_λ corresponds to the point $\boldsymbol{p}\, p_E^2/p^2$ in this case (see figure 2). Thus

$$\cos\omega^+ = \begin{cases} +\cosh\beta & |\boldsymbol{p}| > p_E \\ -\cosh\beta & |\boldsymbol{p}| < p_E. \end{cases} \tag{32}$$

Since

$$\lim_{\varepsilon\to 0} \{-2\mu(E+\mathrm{i}\varepsilon)\}^{-1/2} = \mathrm{i}(2\mu E)^{-1/2} = \frac{\mathrm{i}}{p_E} \tag{33}$$

the classical action along the shortest path between $\boldsymbol{p}_0$ and $\boldsymbol{p}$ is

$$S_E{}^+(\boldsymbol{p}, \boldsymbol{p}_0) = \begin{cases} \Pi\beta & \text{if } |\boldsymbol{p}| > p_E \\ \Pi(\beta + \mathrm{i}\pi) & \text{if } |\boldsymbol{p}| < p_E \end{cases} \tag{34}$$

where Π is defined in equation (19). For $|\boldsymbol{p}| > p_E$ this agrees with equation (25) for the action between two points in the accessible region. For $|\boldsymbol{p}| < p_E$, with reference to figure 3, the action from A to C is the sum of a normal real part, which is just the action along the physical path from A to B, plus an imaginary action $\mathrm{i}\pi\Pi$ which comes from passing from B through the energy shell at E into the inaccessible region at C.

For $\mathscr{E} = E - \mathrm{i}\varepsilon$ we find that

$$S_E{}^-(\boldsymbol{p}, \boldsymbol{p}_0) = [S_E{}^+(\boldsymbol{p}, \boldsymbol{p}_0)]^*. \tag{35}$$

From equations (31) we see that ω^+ increases by a multiple of 2π each time the complete momentum orbit is described, so that the action $S_E{}^\pm(\boldsymbol{p}, \boldsymbol{p}_0)$ increases by multiples of $\pm 2\pi\mathrm{i}\Pi$. Hence, if c denotes the number of complete orbits described, then the value of $S_{cE}{}^+(\boldsymbol{p}, \boldsymbol{p}_0)$ for $\boldsymbol{p}$ and $\boldsymbol{p}_0$ lying in each of the regions of momentum space is given for all the possible generalized paths in table 1, where $\eta = \Pi/\hbar$. This definition of η together with the last three columns of the table will be used in IV.

6. Time along the complete orbits

For the discrete spectrum, if $\boldsymbol{p}_0$ is taken to be the momentum at the perihelion of the elliptic orbit, then the angle w of equations (25)–(29) of II is just the eccentric anomaly at the point with momentum $\boldsymbol{p}$ (Landau and Lifshitz 1960, Györgyi 1968); the time taken by the particle in moving from $\boldsymbol{p}_0$ around the orbit is given by Kepler's equation

$$\Omega t = w - \epsilon \sin w \tag{36}$$

where $\Omega = (-2\mu\mathscr{E})^{3/2}/k\mu^2$ is the fundamental angular frequency and ϵ is the eccentricity of the elliptic orbit which is determined uniquely for a given energy $\mathscr{E} < 0$ and given momenta $\boldsymbol{p}_0$ and $\boldsymbol{p}$. The period for a complete revolution of the orbit is given by

$$\left(\frac{\partial S}{\partial \mathscr{E}}\right)_{\text{orbit}} = \frac{2\pi}{\Omega}. \tag{37}$$

The analytic continuation of Ω and ϵ to positive energies are Ω' and ϵ', where

$$\left.\begin{aligned} \Omega &\to \pm \mathrm{i}\Omega' \\ \epsilon &\to \epsilon' \end{aligned}\right\} \text{for } \mathscr{E} = E \pm \mathrm{i}\varepsilon, \qquad E > 0 \tag{38}$$

$\Omega' = p_E{}^3/k\mu^2$ and ϵ' is real and greater than unity.

For positive energy we may again choose $\boldsymbol{p}_0$ to be the momentum of the particle at the perihelion. Consequently, using equations (31) and (38), the analytic continuation of the Kepler equation (36) is

$$\Omega' t = \begin{cases} \epsilon' \sinh \beta - \beta & (a) \\ \mp \ \mathrm{i}\pi - \epsilon' \sinh \beta - \beta & (b) \\ \mp \ \mathrm{i}\pi + \epsilon' \sinh \beta + \beta & (c) \\ \mp 2\mathrm{i}\pi - \epsilon' \sinh \beta + \beta & (d). \end{cases} \tag{39}$$

The ranges of $\boldsymbol{p}$ and β in equations (39) correspond to those of equation (31).

We see that in the accessible region the time obeys Kepler's equation for the attractive hyperbolic orbit (Landau and Lifshitz 1960, p. 38). The time taken for a particle to pass from a point in the accessible region to a point in the inaccessible region is complex. However, the time between any two points in the inaccessible region ECDF of figure 3 is real, increases from $-\infty$ at F to $+\infty$ at E for clockwise motion and obeys Kepler's equation for the repulsive hyperbolic orbit.

In passing through the energy shell $p^2 = 2\mu E$ the particle thus picks up an action

$$S^{\pm}_{\text{shell}} = \pm \mathrm{i}\pi\Pi \tag{40}$$

and has made a sudden jump to the past. We note also that the time to traverse the complete hyperbolic orbit is $\pm 2\pi\mathrm{i}/\Omega'$, from equation (39), which agrees with the analytic continuation of equation (37). We have seen that the action around the complete momentum orbit is $\pm 2\pi\mathrm{i}\Pi$.

Thus the analytic continuation of the classical bound-state Kepler problem yields the classical solutions to both the attractive and repulsive scattering problem.

It will be noticed that the electron does not move uniformly along a path on the hyperboloid. When time t is introduced, the O(1, 3) Lorentz invariance is lost. This is because time is obtained by differentiation with respect to energy, and in the above representation O(1, 3) invariance holds only for the particular energy $E = p_E{}^2/2\mu$. A completely symmetric representation is obtained by a general transformation of the type described at the end of § 3. The coordinate transformation relating the symmetric representation to momentum representation still has the form of equation (8), but p_E is no longer an energy-independent parameter. It is given by $p_E{}^2 = 2\mu E$ for all energies E. The transformation is therefore explicitly energy-dependent. In this representation the new time τ is obtained from the theory of canonical transformations in extended phase space. It is

$$\tau = t - \frac{\boldsymbol{r} \cdot \boldsymbol{p}}{2E} = \frac{\beta}{\Omega'} \tag{41}$$

and corresponds to the new time obtained by Györgyi (1968) for bound states. The new theory is completely symmetric. Motion is uniform on the hypersphere with respect to the new time τ.

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Correspondence identities
IV. The Rutherford scattering identity

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Abstract. A complete correspondence identity is obtained for the electron–proton system, whereby the non-relativistic quantum dynamics of the system is obtained from solutions of the corresponding classical problem and their analytic continuation given by the authors in the previous paper. The kernels of the spectral operator $I_E = \delta(E-H)$ in momentum and symmetric representation are obtained as sums over classical action functions for all non-zero real energies E. A general derivation of a scattering cross section from a spectral operator is presented, and applied to this system: the long-range distortion appears naturally. By this means and alternatively in terms of transition operators it is shown how the correct quantum-mechanical differential scattering formula follows from classical Rutherford theory. Complete correspondence identities are discussed. Quantum-mechanical barrier penetration is obtained through analytic continuation of classical action functions. A model of the system based on classical electron orbits is an improvement on the Bohr–Sommerfeld model.

1. Introduction

Correspondence identities are described by Norcliffe and Percival (1968 a, b, to be referred to as I and II, respectively). The Rutherford scattering identity is a particular example: the quantum-mechanical and classical angular differential cross sections $\sigma(\Theta)$ for the scattering of a charged particle by a fixed charge are the same. For a system of electron and (infinite mass) proton the Rutherford formula is

$$\sigma(\Theta) = \frac{e^4}{16E^2\sin^4(\frac{1}{2}\Theta)} = \left\{\frac{2\mu e^2}{(\boldsymbol{p}-\boldsymbol{p}_0)^2}\right\}^2 \tag{1}$$

where E is the energy of the incident electron, μ is its mass and $\boldsymbol{p}_0$ and $\boldsymbol{p}$ its initial and final momenta. Because of this identity, as it applies to the scattering of alpha particles by nuclei, Rutherford was able to use classical mechanics to demonstrate the nuclear structure of the elements from the heaviest to the lightest, without the need for any small quantal corrections to his classical formulae. There appears to be no connection between the usual classical and quantal derivations of equation (1), except the initial specification of the same Hamiltonian and the final identical result (Landau and Lifshitz 1960, § 19, Mott and Massey 1965, chap. III, § 2); nor is there any obvious connection between this correspondence identity for the scattering states of the electron–proton system and the correspondence identities of II for the hydrogen atom bound states.

In this paper these correspondence identities are all shown to follow from a *complete correspondence identity*, whereby the quantum dynamics of electron and proton is completely determined from the classical dynamics for both positive and negative energies E. The classical paths in momentum representation, which are considered by Norcliffe *et al.* (1969, to be referred to as III) play the role of rays in the sense of geometrical optics.

The Rutherford scattering identity is concerned solely with relations close to the energy shell

$$p^2 = p_0{}^2 = E \tag{2}$$

and is thus much more restricted than the complete correspondence identity which is valid for arbitrary $\boldsymbol{p}_0$ and $\boldsymbol{p}$. Unfortunately, the complete correspondence identity is more complicated off the energy shell than on it (equation (26*c*)), and the derivation of the Rutherford scattering identity is not so straightforward as the derivation of the Bohr–Sommerfeld identity of II.

Off the energy shell the Rutherford identity requires the analytic continuation of classical paths in momentum space, given by III, into the classically inacessible region. The analytically continued paths are the usual classical paths for the scattering of positrons by protons. As before, the quantum-mechanical problem is solved by summing over an infinite number of classical paths in momentum space. For positive energies the complete set of paths corresponds to scattering of both positrons and electrons, and the choice of which path corresponds to which scattering process is a subtle one.

In momentum representation the scattering amplitudes and cross sections are conventionally obtained from the Green operators $G_E{}^{\pm}$, but the complete correspondence identity is obtained in terms of the spectral operator $I_E = \delta(E-H)$ of I and II. We therefore have to show how the Rutherford scattering formula (1) is derived from I_E. This is done first in § 4 directly. There is then no need to consider the long-range distortion of the Coulomb potential separately as in the conventional theory: it appears automatically in the analysis. The theory of the derivation of the scattering amplitude and cross section from the spectral operator is of general application and independent from the correspondence identity. In § 5 the scattering formula is derived from the spectral operator by an alternative more conventional route via the Green operators $G_E{}^{\pm}$ and transition operator $\mathbf{T}_E$ whose elements form the **T** matrix.

The classical and quantal momentum distributions are compared in § 3. In contrast with those for negative energy *E*, they are not identical.

2. The spectral operator

For positive energies *E* the Green operators $G_E{}^{\pm}$ are defined on either side of the right-hand cut in the complex *E* plane. In terms of $G_E{}^{\pm}$ the spectral operator I_E is obtained in I as

$$I_E = \delta(E-H) = \frac{G_E{}^{-} - G_E{}^{+}}{2\pi \mathrm{i}} \qquad (E\,\text{real}). \tag{3}$$

As shown in I, the evolution operator, and thus the solution of a quantum-dynamical problem with Hamiltonian *H*, can be obtained by Fourier transformation of the spectral operator.

For negative energies *E* the Green operators $G_E{}^{+}$ and $G_E{}^{-}$ are equal except when *E* is a bound-state energy E_n. The spectral operator I_E is thus zero for all negative energies except the poles E_n of $G_E{}^{\pm}$, and is a sum over delta functions at these poles (see I and II).

By contrast, for positive energies, I_E is a well-defined analytic operator function of *E*. It is then the projection operator onto the vector space of all states of energy *E*. The space is of infinite dimension because the energy level $E > 0$ is degenerate with respect to the azimuthal quantum number *l*, which has infinite range.

As in II, the correspondence identities depend on the representation. They may be derived in momentum-representation, or even more simply in symmetric representation. In the former the kernel of I_E is

$$I_E(\boldsymbol{p}, \boldsymbol{p}_0) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \psi_{lm}(\boldsymbol{p}, E)\psi^*_{lm}(\boldsymbol{p}_0, E). \tag{4}$$

The momentum-space wave functions $\psi_{lm}(\boldsymbol{p}, E)$ of energy *E* are normalized by the energy condition

$$\int \mathrm{d}^3p\, \psi^*_{lm}(\boldsymbol{p}, E)\psi_{l'm'}(\boldsymbol{p}, E') = \delta(E-E')\delta_{ll'}\delta_{mm'} \tag{5}$$

and are solutions of the Schrödinger equation

$$(E-H)\psi_{lm}(\boldsymbol{p}, E) \equiv \left(E - \frac{p^2}{2\mu}\right)\psi_{lm}(\boldsymbol{p}, E) + \frac{k}{2\pi^2\hbar}\int \mathrm{d}^3p'\, \frac{\psi_{lm}(\boldsymbol{p}', E)}{|\boldsymbol{p}-\boldsymbol{p}'|^2} = 0. \tag{6}$$

The kernel of the spectral operator is most conveniently evaluated in symmetric representation as used in III for the classical problem, which should be consulted for notation and definitions. For the quantum-mechanical problem the methods of Bander and Itzykson (1966) are used. If $\psi(\boldsymbol{p}, E)$ is an arbitrary momentum wave function, not necessarily the solution of the Schrödinger equation for any energy, as in II, then the equivalent wave function in symmetric representation $\psi_s(u_\lambda, E)$ is given by

$$\psi_s(u_\lambda, E) = A(p^2 - p_E^2)^2 \psi(\boldsymbol{p}, E) \qquad (E > 0) \tag{7}$$

where A is a constant to be determined by normalization.

The 4-vector u_λ lies on a Minkowski sphere $\mathscr{S}$, which consists of two sheets $\mathscr{S}^+$ and $\mathscr{S}^-$, which are respectively classically inaccessible and accessible, as shown in III. As $\mathscr{S}^-$ is classically accessible we shall usually work with this sheet when a choice is to be made. The three-dimensional surface element $\mathrm{d}\Omega$ of $\mathscr{S}$ is related to the volume element of momentum space by the relation

$$\mathrm{d}p^3 = \begin{Bmatrix} \dfrac{(p_E^2 - p^2)^3 \, \mathrm{d}\Omega^+}{8 p_E^3} \text{ on } \mathscr{S}^+ \\ \dfrac{(p^2 - p_E^2)^3 \, \mathrm{d}\Omega^-}{8 p_E^3} \text{ on } \mathscr{S}^- \end{Bmatrix}. \tag{8}$$

The distance between two points in momentum space is related to the corresponding Minkowski distance by

$$|\boldsymbol{p} - \boldsymbol{p}_0|^2 = -\frac{(p^2 - p_E^2)(p_0^2 - p_E^2)}{4 p_E^2} (u_\lambda - u_\lambda^{(0)})^2 \tag{9}$$

where $u_\lambda^{(0)}$ and u_λ correspond to $\boldsymbol{p}_0$ and $\boldsymbol{p}$.

In symmetric representation the Schrödinger equation (6) reduces to

$$(I - \eta Q)\psi_s(u_\lambda, E) = 0 \tag{10}$$

where the continuous variable

$$\eta = \frac{k\mu}{p_E \hbar} \tag{11}$$

is analogous to the discrete quantum number n. The operator Q is defined by

$$Q\psi_s(u_\lambda, E) = \epsilon(u_\lambda) \int_{\mathscr{S}} \frac{\mathrm{d}\Omega' \, \psi_s(u_\lambda', E)}{2\pi^2 |(u_\lambda - u_\lambda')^2|} \tag{12}$$

where

$$\epsilon(u_\lambda) = \begin{Bmatrix} -1; u_\lambda \text{ on } \mathscr{S}^+ \\ 1; u_\lambda \text{ on } \mathscr{S}^- \end{Bmatrix}. \tag{13}$$

As in II, we define the kernel of the operator J_E in symmetric representation to be

$$J_E(u_\lambda, u_\lambda^{(0)}) = \frac{2\pi^2 (p_E^2 - p_0^2)^2 (p^2 - p_E^2)^2}{2\mu \times 8 p_E^3} I_E(\boldsymbol{p}, \boldsymbol{p}_0). \tag{14}$$

Unlike the spectral operator, the kernel of J_E is symmetric (equal to its transpose) in symmetric representation. It is the kernel of the operator $I_E(E - T)$, where the kinetic energy operator $T = p^2/2\mu$.

The kernel $J_E(u_\lambda, u_\lambda^{(0)})$ is obtained as a projection operator from the solutions $\psi_{\eta l m}(u_\lambda)$ of the Schrödinger equation (10), which are related to the four-dimensional spherical harmonics thus:

$$J_E(u_\lambda, u_\lambda^{(0)}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \psi_{\eta l m}(u_\lambda) \psi^*_{\eta l m}(u_\lambda^{(0)}). \tag{15}$$

The functions $\psi_{\eta lm}(u_\lambda)$ are defined on both sheets of the Minkowski sphere, and are given by†

$$\psi_{\eta lm}(u_\lambda) = \text{const.} \times \begin{Bmatrix} -\mathrm{e}^{-\pi\eta} H_{\eta lm}(-u_\lambda), & u_\lambda \text{ on } \mathscr{S}^+ \\ H_{\eta lm}(u_\lambda), & u_\lambda \text{ on } \mathscr{S}^- \end{Bmatrix}. \tag{16}$$

The hyperspherical harmonics $H_{\eta lm}(u_\lambda)$ are defined on one sheet only. For convenience we choose this to be the lower classically accessible sheet $\mathscr{S}^-$. To convert to the convention of Bander and Itzykson, we simply change the sign of u_λ.

Although the hypergeometric functions $H_{\eta lm}(u_\lambda)$ form a complete orthonormal set on the lower sheet $\mathscr{S}^-$, the wave functions $\psi_{\eta lm}$ are not orthonormal or complete for the entire symmetric space $\mathscr{S} = \mathscr{S}^+ + \mathscr{S}^-$. In order to determine the external constant of equation (16), it is necessary to transform back to momentum representation and use the energy normalization of equation (5).

The addition theorem for the hyperspherical harmonics on $\mathscr{S}^-$ is (Bander and Itzykson 1966)

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{l} H_{\eta lm}(u_\lambda) H^*_{\eta lm}(u_\lambda^{(0)}) = \frac{\eta \sin \eta\beta}{\sinh \beta} \tag{17}$$

where β is the hyperbolic angle defined on $\mathscr{S}^-$ in III as

$$\cosh \beta = u_\lambda^{(0)} u^\lambda = 1 + \frac{E|\boldsymbol{p} - \boldsymbol{p}_0|^2}{\mu(T_0 - E)(T - E)}. \tag{18}$$

Using this addition theorem, the required kernel is obtained entirely in terms of trigonometric functions as

$$J_E(u_\lambda, u_\lambda^{(0)}) = \frac{\xi(\eta)\eta^2 \sin(\eta\beta)}{(1 - \mathrm{e}^{-2\pi\eta}) \sinh \beta}. \tag{19}$$

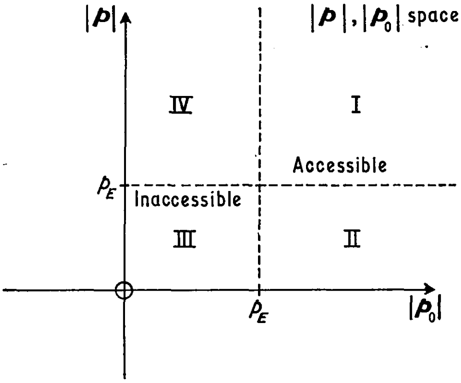

Figure 1. The four regions of $|\boldsymbol{p}|$, $|\boldsymbol{p}_0|$ space.

Using figure 1 to define the regions I, II, III, IV, the function $\xi(\eta)$ is

$$\xi(\eta) = \begin{Bmatrix} 1 \text{ in I} \\ -\mathrm{e}^{-\pi\eta} \text{ in II and IV} \\ \mathrm{e}^{-2\pi\eta} \text{ in III} \end{Bmatrix} \tag{20}$$

where η is given in equation (11).

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† There is a mistake in the sign of the exponential factor in the corresponding equation (36) of Bander and Itzykson (1966). In the classical limit $\eta \to \infty$ the relative probability of being on $\mathscr{S}^+$ tends to zero, as it should for an attractive potential (see III), and not for a repulsive potential as implied by their equation.

On transforming to momentum representation using equation (14), we obtain for the kernel of the spectral operator

$$I_E(\boldsymbol{p},\boldsymbol{p}_0) = \frac{\xi(\eta)8\mu^3 p_E k^2}{\pi^2\hbar^2(p^2-p_E{}^2)^2(p_0{}^2-p_E{}^2)^2(1-\mathrm{e}^{-2\pi\eta})}\,\frac{\sin(\eta\beta)}{\sinh\beta}. \tag{21}$$

The variable β is given by its principal value in the second part of equation (18), but if $\boldsymbol{p}$ is in the classically inaccessible region it must be replaced by $\boldsymbol{p}p_E{}^2/p^2$ as in III, equation (31). The case is similar for $\boldsymbol{p}_0$.

Equations (19) and (21) correspond to equations (51), (55) and (56) of II for the discrete spectrum. For completeness we note that the normalization constant A of equation (7), giving the momentum-space wave functions in terms of the hyperspherical harmonics, is

$$A = \left(\frac{16\mu\eta p_E{}^3}{1-\mathrm{e}^{-2\pi\eta}}\right)^{-1/2} \exp[-\mathrm{i}\{\arg\Gamma(l+1-\mathrm{i}\eta)+(l+1)\pi\}]. \tag{22}$$

3. Complete correspondence identity

Before obtaining a correspondence identity for the spectral operator when $E > 0$ it is instructive to contrast the relevant properties of classical paths and spectral operators for positive and negative energies, as in table 1.

Table 1

Negative energies, $E < 0$	Positive energies, $E > 0$
(*a*) All regions of momentum space are classically accessible.	(*a*) The region $p^2 < p_E{}^2$ of momentum space is inaccessible. This corresponds to the sheet $\mathscr{S}^+$ of the Minkowski sphere.
(*b*) There is an infinite number of classical paths between any two momenta $\boldsymbol{p}_0$ and $\boldsymbol{p}$.	(*b*) The number of classical paths is 0 or 1, unless we allow analytic continuation as in III, when it is infinite.
(*c*) The quantum-mechanical spectrum is discrete, the spectral operator a series of delta functions in E.	(*c*) The spectrum is continuous, the spectral operator an analytic function of E.
(*d*) The spectral operator $I_E(\boldsymbol{p},\boldsymbol{p}_0)$ can have non-zero values for all values of $\boldsymbol{p}$ and $\boldsymbol{p}_0$. By (*a*) and (*b*) these momenta can always be joined by an infinite number of classical paths.	(*d*) There is quantum-mechanical barrier penetration in momentum space into the classically inaccessible region, so that there are momenta $\boldsymbol{p}_0$ and $\boldsymbol{p}$ for which the spectral operator $I_E(\boldsymbol{p},\boldsymbol{p}_0)$ is non-zero; yet there are no classical paths in the normal sense joining $\boldsymbol{p}_0$ and $\boldsymbol{p}$.

From table 1(*d*) the normal classical paths cannot be used to provide a correspondence identity for positive energies. It was for this reason that the general theory of analytic classical paths was considered in III. There is an infinite number of analytic classical paths c joining any two momenta $\boldsymbol{p}_0$ and $\boldsymbol{p}$ whether the energy is positive or negative. To obtain a correspondence identity for positive energies, it is necessary to sum over these.

Surprisingly the contrasting properties of the spectrum and the spectral operators are obtained from the slightly different form of the action functions for positive and negative energies. For negative energies the spectral operator was obtained in II, equation (53), from the sum $\Sigma_c \sin\{S_{cE}(\boldsymbol{p},\boldsymbol{p}_0)/\hbar\}$. The important properties remain if we consider only the diagonal elements, for which $\boldsymbol{p} = \boldsymbol{p}_0$, so that the classical paths consist of a number of complete cycles of the classical orbit, and we separate the exponentials of the sine function:

$$\sum_c \exp\left\{\frac{\mathrm{i}S_{cE}(\boldsymbol{p}_0,\boldsymbol{p}_0)}{\hbar}\right\} = \sum_{c=0}^{\infty} \exp\left(\frac{\mathrm{i}c[S_E]}{\hbar}\right) \tag{23}$$

where $[S_E]$ is the increment in the action once around the orbit. This is a geometric progression, in which each term has the same magnitude, and so is not convergent except as a generalized function. As shown in II, destructive interference reduces the sum (when combined with its complex conjugate) to zero, unless $[S_E]$ is given by the Bohr–Sommerfeld condition, when constructive interference builds up the discrete spectrum.

Let us consider the same sum over the analytic classical paths of III for positive energies E. In this case the increment $[S_E] = \pm 2\pi \mathrm{i}\Pi$ given by III, equation (40), is purely imaginary, and if the positive sign is chosen we obtain

$$\begin{aligned}\sum_{c=0}^{\infty} \exp\left(\frac{ic[S_E]}{\hbar}\right) &= \sum_{c=0}^{\infty} \exp\left(-\frac{2\pi c\Pi}{\hbar}\right) \\ &= \sum_{c=0}^{\infty} \exp(-2\pi c\eta) \\ &= \frac{1}{1-\exp(-2\pi\eta)}.\end{aligned} \tag{24}$$

The series converges, and the sum is non-zero for all positive energies: the spectrum is thereby continuous. The factor (24) appears in the expression for the spectral operator (21).

If we consider the final momentum $\boldsymbol{p}$ to move around a fixed orbit continuously when $\boldsymbol{p}_0$ is fixed, then $\exp[\mathrm{i}\{S_{cE}(\boldsymbol{p}, \boldsymbol{p}_0)/\hbar\}]$ picks up a factor $\exp(-\pi\eta)$ every time the $\boldsymbol{p}$ passes through the 'barrier', which is the energy shell. The classical limit is given by $\eta \to \infty$, so that the barrier is then inpenetrable.

In symmetric representation, for positive energies E and for all regions I–IV, the operator J_E of equation (19) can be written as a sum over classical paths as

$$J_{E,k}(u_\lambda, u_\lambda^{(0)}) = \eta^2 \sum_{\text{attractive } c} \frac{\exp\{(i/\hbar)\overset{+}{S}_{cE}(u_\lambda, u_\lambda^{(0)})\} - \exp\{-(i/\hbar)\overset{-}{S}_{cE}(u_\lambda, u_\lambda^{(0)})\}}{2\mathrm{i}\sin(\text{analytic path length})}. \tag{25a}$$

The analytic path length and the appropriate analytic continuations for the classical action functions are given in table 1 of III. The sum is not over all paths, but only over those labelled attractive in the table. The suffix $k = Ze^2$ indicates that, for the quantal problem, the potential is attractive. The remaining paths contribute to the spectral operator of the repulsive potential, corresponding to scattering of positrons and labelled $-k$:

$$J_{E,-k}(u_\lambda, u_\lambda^{(0)}) = \eta^2 \sum_{\text{repulsive } c} \frac{\exp\{(i/\hbar)\overset{+}{S}_{cE}(u_\lambda, u_\lambda^{(0)})\} - \exp\{-(i/\hbar)\overset{-}{S}_{cE}(u_\lambda, u_\lambda^{(0)})\}}{2\mathrm{i}\sin(\text{analytic path length})}. \tag{25b}$$

To obtain a sum over all classical paths, these expressions have to be added together:

$$J_{E,k} + J_{E,-k} = \eta^2 \sum_{\text{all } c} \frac{\exp\{(i/\hbar)\overset{+}{S}_{cE}(u_\lambda, u_\lambda^{(0)})\} - \exp\{-(i/\hbar)\overset{-}{S}_{cE}(u_\lambda, u_\lambda^{(0)})\}}{2\mathrm{i}\sin(\text{analytic path length})}. \tag{25c}$$

The analytic path length is the analytic continuation of the path length for negative energies. When both $\boldsymbol{p}$ and $\boldsymbol{p}_0$ are in the classically accessible region, then for the shortest path the magnitude of the analytic path length is the hyperbolic angle between the two corresponding points on the Minkowski sphere. The analytic path length can be obtained directly from the classical action $S_{c,Z\,\mathrm{ryd}}$ when the energy of the incident particle, electron or positron, is Z ryd.

In momentum representation the spectral operator (21), the spectral operator for the repulsive potential and their sum are given by

$$\begin{aligned}I_{E,\pm k}(\boldsymbol{p}, \boldsymbol{p}_0) &= \frac{8\mu^3 p_{Ek}{}^2}{\pi^2\hbar^2} \frac{1}{(p^2-p_E{}^2)^2(p_0-p_E{}^2)^2} \\ &\times \sum_{\substack{\text{attractive } c \\ \text{or repulsive } c}} \frac{\exp\{(i/\hbar)\overset{+}{S}_{cE}(\boldsymbol{p}, \boldsymbol{p}_0)\} - \exp\{-(i/\hbar)\overset{-}{S}_{cE}(\boldsymbol{p}, \boldsymbol{p}_0)\}}{2\mathrm{i}\sin(\text{analytic path length})} \qquad (E > 0)\end{aligned} \tag{26a, b}$$

$$I_{E,k}+I_{E,-k} = \frac{8\mu^3 p_E k^2}{\pi^2\hbar^2}\frac{1}{(p^2-p_E{}^2)^2(p_0{}^2-p_E{}^2)}$$

$$\times \sum_{\text{all } c} \frac{\exp\{(i/\hbar)S_{cE}^{+}\}-\exp\{-(i/\hbar)S_{cE}^{-}\}}{2\mathrm{i}\sin(\text{analytic path length})} \qquad (E > 0). \qquad (26c)$$

These relations follow from equations (25) using the definition (14) of J_E and the fact that the action function for an analytic classical path between two momenta $\boldsymbol{p}, \boldsymbol{p}_0$ is the same as the action function for the corresponding path between the corresponding points $u_\lambda, u_\lambda{}^{(0)}$ on the Minkowski sphere (see III).

The form of equation (26*c*) is identical with that of equation (53) of II, because S_{cE}^{+} and S_{cE}^{-} are identical for negative energies, there being no cut in the action function there. Also the spectral operator $I_{E,-k}$ is zero for negative energies because the repulsive potential possesses no discrete spectrum. It should be noted that $p_E{}^2$ is defined with opposite signs in this paper and II. The correspondence identity (26*c*) is therefore valid for all real E, $\boldsymbol{p}$ and $\boldsymbol{p}_0$, except for a number of special singular points. It is a complete correspondence identity. The sum of the spectral operators integrated over the energy is twice the identity operator.

We may consider the correspondence identities (26*a*, *b*) for the separate spectral operators $I_{E,+k}$ and $I_{E,-k}$ to be complete correspondence identities only if we accept a definition of 'attractive' and 'repulsive' paths which is different for positive and negative energies E. These are defined for positive E in table 1 of III. It should be noted that they are *not* the classical paths for the attractive and repulsive potentials, but the paths that are required to make up the attractive and repulsive spectral operators. For negative E all paths are attractive in this sense. A full understanding of the reason for this choice of paths to make up the spectral operator would require a more detailed study of the analytic properties of the action functions and amplitudes than we have carried out.

The form of the equations (26) suggests that of equation (3). It is possible that the positive and negative exponentials arise from the Green functions $G_E{}^+$ and $G_E{}^-$, which tends to support the conjecture of Gutzwiller (1967) that the analytic continuation of his phase integral approximation to the bound-state momentum representation Green functions yields a well-defined discontinuity across the positive energy cut, even though part of momentum space is classically inaccessible. Moreover, the discontinuity would give the correct projection operators onto positive energy states.

The diagonal elements of the kernel of the spectral operator are proportional to the quantal microcanonical momentum distribution $\rho_E{}^{\mathrm{qm}}(\boldsymbol{p})$. The classical microcanonical momentum distribution $\rho_E{}^{\mathrm{cm}}(\boldsymbol{p})$, normalized to unit inward flux, can be obtained by integrating over position on the energy surface in phase space. For the attractive potential it is†

$$\rho_E{}^{\mathrm{cm}}(\boldsymbol{p}) = \frac{64\pi k^3\mu^4}{p_E{}^2(p^2-p_E{}^2)^4}\times\begin{Bmatrix}1 \text{ for } p > p_E\\ 0 \text{ for } p < p_E\end{Bmatrix}. \qquad (27a)$$

From (26*a*) the quantal distribution, having the same normalization in the classical limit, is

$$\rho_E{}^{\mathrm{qm}}(\boldsymbol{p}) = \frac{64\pi k^3\mu^4}{p_E{}^2(p^2-p_E{}^2)^4(1-\mathrm{e}^{-2\pi\eta})}\times\begin{Bmatrix}1 & \text{for } p > p_E\\ \mathrm{e}^{-2\pi\eta} & \text{for } p < p_E\end{Bmatrix}. \qquad (27b)$$

The Fock identity, whereby the classical and quantal momentum distributions are the same, therefore no longer holds for positive energies. This is the source of many of the difficulties which appear in subsequent sections.

4. Scattering and the spectral operator

We here obtain the kernel of the evolution operator in momentum representation for large times τ and hence the well-known Rutherford differential scattering cross section for

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† We should like to thank Mr. D. Banks for his derivation using classical theory.

an electron scattered by a fixed nucleus of charge Ze. Nowhere in the following analysis do we need to consider the distorting effects of the Coulomb potential at large distances on the incident electron wave. The effect is intrinsic in the kernel of the spectral operator itself.

In the classically accessible region of momentum space, the spectral operator kernel $I_E(\mathbf{p},\mathbf{p}_0)$ may be written as the sum $I_E^+(\mathbf{p},\mathbf{p}_0)+I_E^-(\mathbf{p},\mathbf{p}_0)$, where $I_E^-(\mathbf{p},\mathbf{p}_0)$ is just $[I_E^+(\mathbf{p},\mathbf{p}_0)]^*$, and

$$I_E^+(\mathbf{p},\mathbf{p}_0) = \frac{8\mu p_E^3\eta^2}{\pi^2(1-\mathrm{e}^{-2\pi\eta})(p^2-p_E^2)^2(p_0^2-p_E^2)^2}\frac{\mathrm{e}^{i\eta\beta}}{2i\sinh\beta}. \tag{28}$$

$I_E^\pm$ are obtained as classical path sums in the previous section. To a sufficiently good approximation, for large values of β, we may use the asymptotic form of sinh β, which is

$$\sinh\beta \sim \tfrac{1}{2}\mathrm{e}^{\beta} \sim \frac{E|\mathbf{p}-\mathbf{p}_0|^2}{\mu(T-E)(T_0-E)}. \tag{29}$$

Near the energy shell equation (28) becomes

$$I_E^+(\mathbf{p},\mathbf{p}_0) = \frac{8\mu p_E P_1^2(x_1x_2)^{i\eta-1}(x_3x_4)^{-i\eta-1}}{i\pi^2(1-\mathrm{e}^{-2\pi\eta})} \tag{30a}$$

where

$$\left.\begin{aligned} \eta &= \frac{P_1}{p_E} \\ x_1 &= 4p_E^2 \\ x_2 &= |\mathbf{p}-\mathbf{p}_0|^2 \\ x_3 &= p_0^2-p_E^2 \\ x_4 &= p^2-p_E^2 \end{aligned}\right\}. \tag{30b}$$

Here P_1 is the momentum of the electron in the first Bohr orbit. We see that the part of the spectral operator kernel which does not contain singularities, for fixed $\Theta \neq 0$, namely the term $(\mathbf{p}-\mathbf{p}_0)^{-2+2i\eta}$ reappears in the expression (1) for the cross section, apart from an irrelevant phase factor. The whole elaborate evaluation of this cross section which follows is only necessary to obtain the external constant. It does not alter the form, and it is for this reason that the identity arises.

The evolution operator $U(\tau)$ is related to the spectral operator by a Fourier transformation (see I):

$$U(\tau) = \int_{-\infty}^{\infty} \mathrm{d}E\,(I_E^+ + I_E^-)\exp\left(\frac{-iE\tau}{\hbar}\right). \tag{31}$$

In evaluating the scattering amplitude we are interested in the value of $U_\tau(\mathbf{p},\mathbf{p}_0)$ for large τ and β, and, by the Riemann–Lebesgue lemma, the only contributions to $U_\tau(\mathbf{p},\mathbf{p}_0)$ will arise from the singularities in $I_E^\pm(\mathbf{p},\mathbf{p}_0)$. These singularities occur when E takes on the values $T_0 = p_0^2/2\mu$, $T = p^2/2\mu$. Without loss of generality we assume that $T > T_0$ and investigate the singularities of $I_E^+(\mathbf{p},\mathbf{p}_0)$ as the energy E ranges from $-\infty$ to ∞ along the real energy axis. For negative energies there can be no contribution to the scattering as the wave functions are bounded.

If $\mathbf{p},\mathbf{p}_0$ lie in the accessible region, then, by taking the branch cuts of $\ln(T-E)$ in the complex E plane to run from T to $T-\mathrm{i}\infty$, we can define the phase of x_4, on the real axis, to be zero to the left and $-\pi$ to the right of the branch point. Similarly we can define the phases of x_3 on either side of the corresponding branch point to be 0 and $-\pi$, so that I_E^+ is uniquely defined for all regions of momentum space in accordance with equation (21). Because of the factor $\exp(-\mathrm{i}E\tau/\hbar)$ in equation (31), the contour must be closed in the lower half E plane to ensure convergence.

For $I_E^-(\mathbf{p},\mathbf{p}_0)$ the singularities again arise at the same points, but the branch cuts are now from T to $T+\mathrm{i}\infty$ and T_0 to $T_0+\mathrm{i}\infty$. Again the contour has to be closed in the lower half plane for convergence, and this means that the integral

$$\int_{-\infty}^{\infty} \mathrm{d}E\, I_E^{-}(\boldsymbol{p}, \boldsymbol{p}_0)\, \exp\left(\frac{-iE\tau}{\hbar}\right)$$

is zero for large positive τ. Thus

$$U_\tau(\boldsymbol{p}, \boldsymbol{p}_0) = \int_{\mathrm{C}} \frac{\mathrm{d}E\, 8\mu P_1{}^2 p_E (x_1x_2)^{i\eta-1}(x_3x_4)^{-i\eta-1}\exp(-\mathrm{i}E\tau/\hbar)}{i\pi^2(1-\mathrm{e}^{-2\pi\eta})} \tag{32}$$

where C is the contour shown in figure 2.

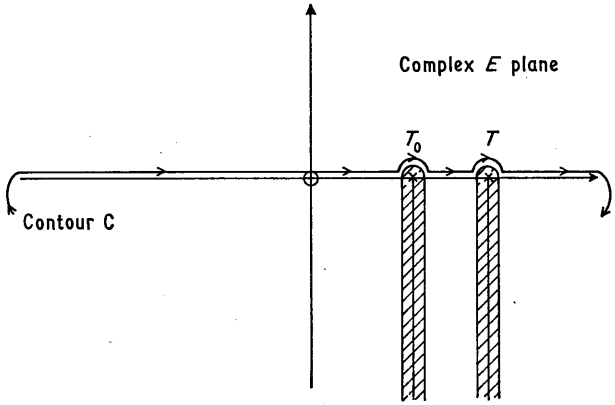

Figure 2. Contour C for integral of equation (32).

The terms in the integrand which are regular near the singular points may be considered constant and taken outside the integral to give

$$U_\tau(\boldsymbol{p}, \boldsymbol{p}_0) \sim \frac{8\mu p_m P_1{}^2 (x_1x_2)^{\mathrm{i}\eta_{\mathrm{m}}-1}\mathscr{I}}{i\pi^2\{1-\exp(-2\pi\eta_{\mathrm{m}})\}} \tag{33}$$

where the subscript m refers to the constant mean value near T and T_0, and

$$\mathscr{I} = \int_{\mathrm{C}} \mathrm{d}E \exp\left(\frac{-iE\tau}{\hbar}\right)(x_3x_4)^{-\mathrm{i}\eta_{\mathrm{m}}-1}. \tag{34}$$

The substitution $y = \{(p^2+p_0{}^2)-2p_E{}^2\}/(p^2-p_0{}^2)$ reduces this integral to the form

$$\mathscr{I} = \left(\frac{p^2-p_0{}^2}{2}\right)^{-2\mathrm{i}\eta_{\mathrm{m}}-1} \frac{1}{2\mu} \exp\left\{\frac{-\mathrm{i}(p^2+p_0{}^2)\tau}{4\mu\hbar}\right\}\mathscr{I}' \tag{35}$$

where $\mathscr{I}'$ is the integral

$$\mathscr{I}' = \int_{\mathrm{C}'} \mathrm{d}y\, \mathrm{e}^{i\alpha y}(y^2-1)^{\nu-\frac{1}{2}} \tag{36}$$

with

$$\alpha = \frac{(p^2-p_0{}^2)\tau}{4\mu\hbar} \tag{37}$$

$$\nu = -i\eta_{\mathrm{m}}-\tfrac{1}{2} \tag{38}$$

and C′ is the contour shown in figure 3. With this contour, $\mathscr{I}'$ is just Hankel's integral for

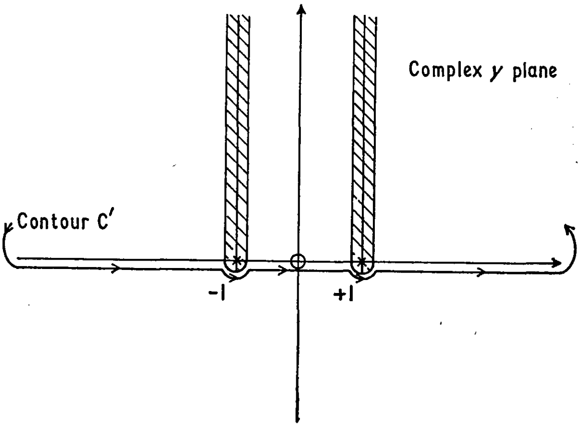

Figure 3. Contour C′ for integral of equation (36).

the Bessel function $J_{-\nu}(\alpha)$ given by Watson (1966, chap. VI)

$$J_{-\nu}(\alpha) = \frac{\Gamma(\frac{1}{2}-\nu)(\frac{1}{2}\alpha)^{\nu}\,e^{i\pi\nu}}{2\pi i\Gamma(\frac{1}{2})}\mathscr{I}'. \tag{39}$$

It now follows that the kernel of the evolution operator for large τ is

$$\begin{aligned} U_\tau(\mathbf{p},\mathbf{p}_0) = {} & \frac{i8p_m P_{.1}{}^2(x_1x_2)^{i\eta_m-1}}{\pi^{1/2}\{\exp(\pi\eta_m)-\exp(-\pi\eta_m)\}}\left(\frac{p^2-p_0{}^2}{2}\right)^{-2i\eta_m-1}\left\{\frac{(p^2-p_0{}^2)\tau}{8\mu\hbar}\right\}^{i\eta_m+\frac{1}{2}} \\ & \times \exp\left\{-\frac{i(p^2+p_0{}^2)\tau}{4\mu\hbar}\right\}\frac{J_{i\eta_m+\frac{1}{2}}\{(p^2-p_0)\tau/4\mu\hbar\}}{\Gamma(1+i\eta_m)} \end{aligned} \tag{40}$$

and

$$\begin{aligned} |U_\tau(\mathbf{p},\mathbf{p}_0)|^2 = {} & \frac{64p_m{}^2P_1^4x_1^{-2}x_2^{-2}}{\pi\{\exp(\pi\eta_m)-\exp(-\pi\eta_m)\}^2}\left(\frac{p^2-p_0{}^2}{2}\right)^{-2}\left(\frac{p^2-p_0{}^2}{8\mu\hbar}\right)\tau \\ & \times\frac{J_{i\eta_m+\frac{1}{2}}(\alpha)J_{-i\eta_m+\frac{1}{2}}(\alpha)}{\pi\eta_m\{\sinh(\pi\eta_m)\}^{-1}} \end{aligned} \tag{41}$$

$$= \frac{\eta_m{}^3\tau}{32\pi^2\sinh(\pi\eta_m)p_m{}^2\mu\hbar}\,\frac{1}{\sin^4\frac{1}{2}\Theta}\,\frac{1}{p^2-p_0{}^2}J_{i\eta_m+\frac{1}{2}}(\alpha)J_{-i\eta_m+\frac{1}{2}}(\alpha) \tag{42}$$

where Θ is the scattering angle.

For large times τ the value of $|U_\tau(\mathbf{p},\mathbf{p}_0)|^2$ as a function of p^2 is small except near $p_0{}^2$. The probability of scattering into unit solid angle is given by

$$\frac{dP}{d\Omega} = \int_0^\infty p^2\,dp|U_\tau(\mathbf{p},\mathbf{p}_0)|^2 \tag{43}$$

$$= \frac{\eta_m{}^3\tau\,\mathrm{cosec}^4\frac{1}{2}\Theta}{32\mu\hbar\pi^2\sinh(\pi\eta_m)p_m{}^2}\int_0^\infty\frac{p^2\,dp}{p^2-p_0{}^2}J_{i\eta_m+\frac{1}{2}}(\alpha)J_{-i\eta_m+\frac{1}{2}}(\alpha). \tag{44}$$

Noting that the only significant contribution to the integral arises near $p^2 = p_0{}^2$, we 'shift' the origin to $p_0{}^2$ and obtain

$$\frac{\partial P}{\partial\Omega} = \frac{\eta_m{}^3\tau\,\mathrm{cosec}^4\frac{1}{2}\Theta}{32\mu\hbar\pi^2\sinh(\pi\eta_m)p_m{}^2}p_m\int_0^\infty\frac{d(p^2-p_0{}^2)}{p^2-p_0{}^2}J_{i\eta_m+\frac{1}{2}}(\alpha)J_{-i\eta_m+\frac{1}{2}}(\alpha) \tag{45}$$

$$= \frac{\eta_m{}^3\tau\,\mathrm{cosec}^4\frac{1}{2}\Theta}{32\mu\hbar\pi^2\sinh(\pi\eta_m)p_m{}^2}\,p_m\frac{\sinh(\pi\eta_m)}{\pi\eta_m} \tag{46}$$

which on the energy shell becomes $\eta_{\mathrm{m}}{}^2\tau \operatorname{cosec}^4 \tfrac{1}{2}\Theta/32\mu\hbar\pi^3 p_E$. The angular differential cross section is given by

$$\sigma(\Theta) = \frac{1}{j\tau}\frac{\partial P}{\partial \Omega} \tag{47}$$

where $j = p_E/\mu(2\pi\hbar)^3$ is the flux of the incident wave. Therefore, if we substitute for the variables η_{m} and j, the differential cross section is

$$\sigma(\Theta) = \frac{Z^2e^4}{16E^2 \sin^4 \frac{1}{2}\Theta} \tag{48}$$

which is the well-known Rutherford formula.

5. Scattering and transition operators

In this section the scattering amplitude is derived from the spectral operator via the more conventional route of Green operators and transition operators.

The Green functions $G_E{}^{\pm}(\boldsymbol{p}, \boldsymbol{p}_0)$ and hence $I_E(\boldsymbol{p}, \boldsymbol{p}_0)$ are singular as one approaches the energy shell:

$$T = \frac{p^2}{2\mu} \to E, \qquad T_0 = \frac{p_0{}^2}{2\mu} \to E. \tag{49}$$

In fact, for short-range potentials we have identically

$$G_E{}^+(\boldsymbol{p}, \boldsymbol{p}_0) = \frac{\delta(\boldsymbol{p}-\boldsymbol{p}_0)}{E-T} - \frac{\mathbf{T}_E(\boldsymbol{p}, \boldsymbol{p}_0)}{(E-T)(E-T_0)} \tag{50}$$

and similarly for $G_E{}^-$ with $\mathbf{T}_E$ replaced by $\mathbf{T}_E{}^\dagger$. The $\mathbf{T}$ matrix $\mathbf{T}_E(\boldsymbol{p}, \boldsymbol{p}_0)$ is finite on the energy shell and for fixed values of $\boldsymbol{p}_0$ and $\boldsymbol{p}$:

$$\lim_{p^2,\, p_0{}^2 \to p_E{}^2} \mathbf{T}_E(\boldsymbol{p}, \boldsymbol{p}_0) = -\frac{1}{4\pi^2\hbar\mu} f(\boldsymbol{p}, \boldsymbol{p}_0). \tag{51}$$

We consider the limit for $\boldsymbol{p}, \boldsymbol{p}_0$ in the accessible region of momentum space. As $|\boldsymbol{p}|$ and $|\boldsymbol{p}_0|$ tend to p_E, then $\beta \to \infty$, and, using equation (35),

$$\frac{E|\boldsymbol{p}-\boldsymbol{p}_0|^2}{\mu(E-T)(E-T_0)} = \frac{8E^2 \sin^2 \frac{1}{2}\Theta}{(E-T)(E-T_0)} \tag{52}$$

where Θ is the scattering angle.

Hence, from equation (3) and Schwinger (1964), we find that

$$I_E(\boldsymbol{p}, \boldsymbol{p}_0) \sim -\frac{1}{4\pi^2\hbar\mu}\frac{Ze^2}{4E\sin^2 \frac{1}{2}\Theta}\frac{1}{2\pi \mathrm{i}}\{G_{0,T}^{-} \exp(\mathrm{i}\eta \ln \sin^2 \tfrac{1}{2}\Theta) G_{0,T_0}^{-} - \text{c.c.}\} \tag{53}$$

where

$$G_{0,T}^{-} = \frac{1}{E-T}\left(\frac{2\pi\eta}{1-\mathrm{e}^{-2\pi\eta}}\right)^{1/2} \exp\left\{-\mathrm{i}\eta \ln\left(\frac{4E}{T-E}\right)\right\}. \tag{54}$$

This agrees with the result obtained by Schwinger from his integral representation of the Coulomb Green functions. $G_{0,T}^{-}$ is the distorted free Green function, which in position representation represents asymptotically a distorted incoming spherical wave. Hence we identify the scattering amplitude

$$f(\Theta) = \frac{Ze^2}{4E\sin^2 \frac{1}{2}\Theta} \exp(\mathrm{i}\eta \ln \sin^2 \tfrac{1}{2}\Theta). \tag{55}$$

We note that $|f(\Theta)|$, which is the physically measurable quantity, arises from the density of paths $(\sinh \beta)^{-1}$, while the phase of $f(\Theta)$ comes from the sums of the real part of the actions $S_{cE}^{\pm}$ over the classical paths. The sums over the complex parts of $S_{cE}^{\pm}$ build up into the normalization factor $(1-e^{-2\pi\eta})^{-1}$ of the distorted free Green functions. This is in contrast with the discrete energy case, where the actions are all real and the phase terms interfere with one another, so that $I_E(\boldsymbol{p}, \boldsymbol{p}_0)$ vanishes except at the bound-state energies.

A similar result is obtained as one approaches the energy shell from the other three regions, the only difference being the presence of factors $e^{-\pi\eta}$ in equation (53), as one passes onto different sheets in the complex plane.

6. Conclusions

For the system of two charged particles we have obtained a complete correspondence identity, whereby the quantum dynamics of relative motion is completely determined for positive and negative energies E by rays in momentum space, which are the classical paths and their analytic continuations. Initially the kernel of the spectral operator $I_E = \delta(E-H)$ in momentum representation is obtained as a sum over classical paths involving classical action functions. From this relation energy levels, state vectors and the evolution of the system in time may all be obtained from the solution of the classical problem. The results of Gutzwiller (1967) and Norcliffe and Percival (1968 b) have thereby been extended to the continuous spectrum.

The study of correspondence identities, which are valid only for particular potentials, shows clearly that the relationship between quantal and classical dynamics depends crucially on the choice of representation. In the case of the Coulomb interaction the momentum representation and the related symmetric representations must be used both in the classical and quantal theory.

Also the choice of operator is important. The spectral operator I_E is given precisely by the classical path sum, whereas the Green operators $G_E^{\pm}$ are not. As shown in I, the Fourier transform of I_E for such a system is the two-sided evolution operator, which contains within itself all information about the quantum dynamics of the system. In particular, the scattering properties can be obtained directly from the spectral operator in momentum representation, as shown in § 4 of this paper. For the Coulomb potential the direct derivation of the angular differential cross section from the spectral operator has advantages over the more conventional approach using transition operators.

The three correspondence identities of II have all been derived from the complete correspondence identity. However, the lengthy derivation in § 4 of the constant external factor in the Rutherford scattering formula is not as satisfactory as the derivation of the Bohr–Sommerfeld and Fock identities for the bound states. The Fock identity is not valid for the continuum, and the quantum-mechanical phenomena which thereby intervene complicate matters considerably.

The scattering processes involving charges of opposite sign are intimately related. For positive energies, as seen in III, the classical orbit in momentum space for one is the analytic continuation of that for the other, and the rays or analytic classical paths which contribute to the spectral operator for, say, the attractive potential usually include many segments which represent classical motion of a charge of opposite sign. Furthermore, not all the rays contribute to the spectral operator, but only a set of them, although every ray contributes to one spectral operator or the other. Which ray belongs to which spectral operator is known, but not fully understood.

The O(4) (4-sphere) symmetry for the negative energies and the O(1, 3) (Minkowski sphere) symmetry for the positive energies were very helpful in the derivation of the correspondence identities, but we do not know if the presence of such dynamical symmetries is essential to the existence of correspondence identities.

Quantal barrier penetration in momentum space is obtained precisely, for the Coulomb potential, through the analytic continuation of classical action functions. Such analytic continuation is clearly of general importance for the study of the relation between classical and quantal mechanics.

We have provided a model of the H atom based on classical electron orbits which is an alternative to the Bohr–Sommerfeld model. The main difference between the two models for a given energy level is that ours includes a statistical distribution over all elliptic orbits consistent with this energy, whereas the Bohr–Sommerfeld model includes only those with particular eccentricities and restricted orientations, these being associated with quantum numbers l and m. Our model is better in that it leads to precisely the same physical results as modern non-relativistic quantum theory, and that it can be generalized to positive energies; but the problem of l and m quantization has not been solved in classical terms, so it is at a stage analogous to the original Bohr theory.

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