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ACTION ANGLE VARIABLES IN CLASSICAL AND QUANTUM MECHANICS

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Action angle variables in classical and quantum mechanics

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I. INTRODUCTION

The model theory of the strong interaction which has been widely studied in recent years is quantum chromodynamics (QCD). QCD is a theory in which many calculations are very difficult to carry out. As W. Marciano and H. Pagels (1) have said: "QCD is a Lagrangian field theory in search of a solution. Nothing comparable to the Feynman rules and the perturbation approximation series in QED exists for the bound state physics of QCD. There may even be difficulties in precisely defining the theory. According to QCD all the strongly interacting particles are bound states of permanently confined constituents called quarks. Yet no one has ever proven the existence of a single bound state ...." In view of the lack of a solution to the problem of bound states in QCD, perhaps a new approach is in order.

In classical mechanics one learns that many problems may be solved easily if an appropriate change of variables is employed. If one were to apply the change-of-variables approach to the bound-state problem in QCD, one would prefer to use some set of variables in which bound states are most naturally described. One method of deciding what specific type of new variables to choose for hadron problems is to study the resonances produced in two-body scattering.

Examination of scattering data, e.g., πN shows that if one plots the angular momentum (ℓ) versus the mass squared (m^2), the resonances tend to be located on straight lines, Regge trajectories. This grouping of the resonances into families tends to indicate that angular momentum

is an important quantity. In an attempt to calculate the masses and widths of these particles, it might prove useful to choose a set of variables in which angular momentum plays a prominent role.

In classical mechanics there is a system of variables which historically has been defined for bound-state two-body systems, and which uses angular momentum as one of the canonical momenta of the system. This set of coordinates and momenta is the action-angle variables. These classical quantities are Hamilton-Jacobi variables where the Hamiltonian of any system is a function only of the action variables, i.e., of the momenta (2). This property simplifies dynamical calculations. Furthermore, while these variables were developed for bound states of systems, their definition has been extended (3) to scattering states by analytic continuation. Thus, the action-angle variables may be applied to "quasi-bound" states (scattering states) as well as to the traditional bound states.

Since these variables can have angular momentum as a fundamental momentum (having a canonically conjugate variable associated with it), and since these variables have proven useful in the past for the study of the bound states of systems, they might prove useful for studying the hadronic resonances.

Before one can begin to calculate hadronic masses using action-angle variables it is necessary to understand them as quantum-mechanical objects. This thesis will treat the action-angle variables as operators in the context of nonrelativistic quantum mechanics. This is the first

step towards calculating hadronic processes using the concept of action-angle variables.

Quantum mechanical transformation theory has not been extensively investigated. Dirac (4,5) has considered using operators to effect transformations, and, in addition, has also considered using a quantum action-function, $S(q,q_0,t)$, to generate a transformation. His discussions of transformation theory are very general.

P. Jordan (6,7,8,9) has considered the problem of carrying out a general Hamilton-Jacobi transformation using generating functions ($S(\alpha,q)$ and $S(\beta,q)$, where α is the new momentum, β the new coordinate and q the old coordinate). Jordan does mention action-angle variables, J and w, but only defines the operator J in terms of a spectral decomposition ($J = h \Sigma |n'\rangle n'\langle n'|$). The definition of J given by Jordan is correct but not useful, since application of this definition requires knowledge of the wavefunctions, $\langle q'|n'\rangle$, i.e., of the solutions of Schrödinger's equation. Van Vleck (10) has applied Dirac's transformation theory (5) and shown that expectation values become averages in the classical limit. Van Vleck also briefly considered the problem of carrying out a quantum Hamilton-Jacobi transformation, but he does not consider action-angle variables.

Some authors have treated specific quantum systems using action-angle variables. The harmonic oscillator has been treated by Dirac (11). A calculation which was designed to find "proper angular-momentum" variables has been carried out by Biedenharn and Brussard (12). Their

proper angular variables are related to the action-angle variables J_θ and J_ϕ which will be discussed in Chapter III.

There has been a series of authors who have concerned themselves with the problem of defining angle variables for harmonic oscillators quantum mechanically. Jordan (9) and Susskind and Glowgower (13) have pointed out the difficulties of specifying the commutator of an angle variable with its canonically conjugate momentum. Carruthers and Nieto (14), Lévy-Leblond (15), and Newton (16) have considered this problem and recommended various solutions. The problem of defining angle variables is relevant because the action-angle variable, w, is an angle variable. A new treatment of this problem is found in Leacock (17) and at various points in this thesis.

As far as the author has been able to determine, while the above authors have treated various specific aspects of the problem of defining action-angle variables quantum mechanically, no author has developed a general definition of these variables. The purpose of this thesis is to define action-angle variables quantum mechanically. The quantum analogue of classical Hamilton-Jacobi action-angle-variable theory is constructed. The methods developed here are general and may be generalized to apply to quantum-relativistic problems.

The action-angle variables constitute a system of coordinates and momenta in which the Hamiltonian is a function only of the momentum. This is the case classically and is the case quantum-mechanically if the action-angle variables are properly defined. Classically, action-angle variables are useful if one wants certain specific information, e.g.,

the frequencies of a system. Quantum mechanically, we will see that these variables are useful if one wants certain specific information, e.g., energy levels. For example, the energy levels of the bound states of strongly interacting particles may be most easily found using action-angle variables.

The thesis is organized as follows. Chapter II is a brief review of the classical concepts and of the properties quantum action-angle operators should possess. We then apply these properties to the problem of using the classical transformation equations to deduce the corresponding quantum transformation equations, thus defining the action-angle operators for the system under consideration. After considering eigenvalue spectra and action-angle wavefunctions, we apply these concepts to a series of examples. This series includes the harmonic oscillator in Chapter II and in Chapter III includes the plane rotor, θ-motion or angular problem, and the radial part of a three-dimensional harmonic oscillator.

We return in Chapter IV to the general problem of defining action-angle variables quantum mechanically. The approach involves using a quantum-mechanical Hamilton-Jacobi eigenvalue equation to define a quantum generating function. The quantum generating function is used to govern the transformation to quantum action-angle variables. This method is applied in Chapter V to three examples, one of which is untreatable using the method of Chapters II and III.

II. CLASSICAL ANALOGUE THEORY

A. Classical Action-Angle Variables

In classical mechanics, Hamilton-Jacobi theory provides a mechanism by which problems may be solved using coordinate transformations (2). One transformation which has proven useful historically is the transformation from a set of coordinates and momenta p and q to the action angle variables, J and w. Under this change of coordinates all Hamiltonians in classical mechanics are functions of J only; they are independent of w. Since the transformation is canonical, Hamilton's equation of motion are preserved. We begin by defining the classical generating function, W(q,J).

A classical canonical transformation may be carried out using a generating function which is a function of the old coordinate, q, and the new momentum, J. This function, W(q,J), gives the old momenta, p, and new coordinate, w, as:

$$p = \partial W(q,J)/\partial q \quad , \tag{2.1}$$

$$w = \partial W(q,J)/\partial J \quad . \tag{2.2}$$

From Eqs. (2.1) and (2.2) it is possible to find one set of coordinates in terms of the other:

$$\begin{aligned} q &= \bar{f}(J,w) \quad , \\ p &= g(J,w) \quad , \\ J &= h(p,q) \quad , \\ w &= i(p,q) \quad . \end{aligned} \tag{2.3}$$

Equations (2.1), (2.2) or (2.3) are the equations of the canonical transformation. In order to carry out such a transformation it is necessary to find the generating function W(q,J).

The first step in finding W(q,J) is to find the associated function, $W_0(q,E)$, from which W(q,J) is found after defining J(E). The function $W_0(q,E)$ satisfies the time-independent Hamilton-Jacobi equation. Given a Hamiltonian of the form:

$$\frac{1}{2m} p^2 + V(q) = E \tag{2.4}$$

where m is the mass, p is the momentum, V(q) is the potential and E is the energy, from Eq. (2.1), a differential equation for $W_0(q,E)$ may be obtained under requirement:

$$W_0(q,E(J)) = W(q,J) \quad . \tag{2.5}$$

Using Eqs. (2.5) and (2.1) in Eq. (2.4), we obtain the time-independent Hamilton-Jacobi equation for the generating function:

$$\frac{1}{2m}\left(\frac{\partial W_0(q,E)}{\partial q} \right)^2 + V(q) = E \quad . \tag{2.6}$$

Equation (2.6) may be solved by quadrature, and we obtain:

$$W_0(q,E) = \int_{q_0}^{q} 2m[E - V(q')]^{1/2} dq' \quad . \tag{2.7}$$

Equations (2.6) and (2.7) define $W_0(q,E)$ up to a constant. It is now necessary to define J(E) so that W(q,J) may be obtained, and the transformation from p and q to J and w may be determined.

In order to define J(E) we use a method, advocated in Ref. 3, which uses a contour integral of the momentum, p. From Eq. (2.4), p may be regarded as a function of q and E:

$$p(q,E) = 2m[E - V(q)]^{1/2} \quad . \tag{2.8}$$

We assume for the moment that V(q) describes a potential well, and there are two values of q, q_+ and q_- such that:

$$p(q_+,E) = p(q_-,E) = 0 \quad . \tag{2.9}$$

The q_+ and q_- are the classical turning points.

Next, following Ref. 3, we allow q to be complex. On the complex q plane, Eq. (2.8) may be written:

$$p(q,E) = \sqrt{g(q,E)(q - q_+)(q - q_-)} \quad . \tag{2.10}$$

In the form (2.10), q_+ and q_- are seen to be square root branch points of the function p(q,E). We connect q_+ and q_- with a cut and choose that branch of p(q,E) which is positive along the bottom of the cut. This is illustrated in Figure 1.

Using this definition of p(q,E), J(E) is defined as a contour integral:

$$J(E) = \int_c p(q,E)\,dq \quad , \tag{2.11}$$

where the contour c is shown in Fig. 1. The contour c is chosen so that J(E) is the integral of p(q,E) around one cycle of the q-motion. The contour must be chosen so that it encloses only q_+, q_- and the cut connecting them; it does not enclose any other singularities of p(q,E).

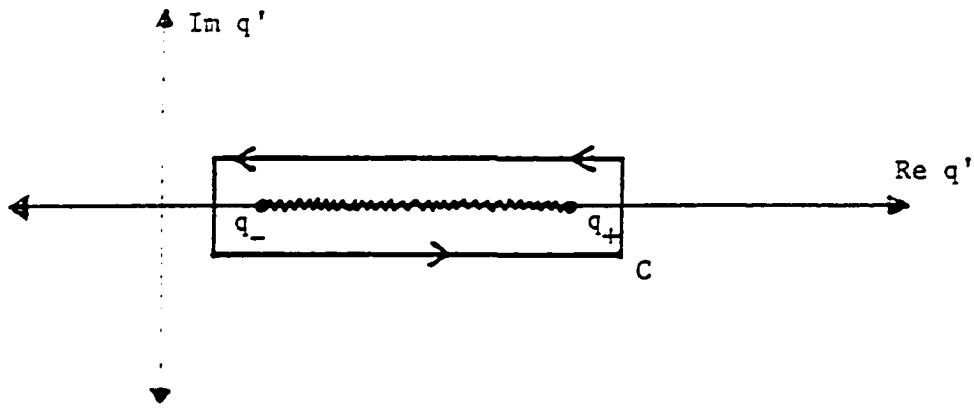

Figure 1. The q'-plane path, C, is used in defining J where q_+ and q_- are given by $p(q_+,E) = p(q_-,E) = 0$. The function $p(q,E)$ has a cut from q_+ to q_- with signs as shown. The contour, C, is chosen so that traversing once around the contour is equivalent to traversing one cycle of the q-motion

Combining the definition of J(E), Eq. (2.11), with the expression for $W_0(q,E)$, Eq. (2.7), we obtain W(q,J) from Eq. (2.5):

$$W(q,J) = W_0(q,E(J)) \quad . \tag{2.12}$$

Equation (2.12) along Eqs. (2.1) and (2.2) specify the canonical transformation from p and q to J and w.

Having defined J(E) and found W(q,J), we can use Eq. (2.2) to find w, the coordinate which is canonically conjugate to J:

$$w \equiv \frac{\partial W}{\partial J}(q,J) \quad . \tag{2.2}$$

w has the property that the change it undergoes over a cycle of the q motion is one. The change, Δw, in w around one cycle of the q-motion is defined as:

$$\Delta w = \int_c \frac{\partial w}{\partial q}\, dq \tag{2.13}$$

where c is the contour used to define J and is given in Fig. 1. The integral around c is interpreted as an integral over one cycle of the q-motion. Using Eqs. (2.2) and (2.11) with Eq. (2.13) it quickly follows that

$$\Delta w = 1 \tag{2.14}$$

around the cycle. The result (2.14) is a characteristic of action-angle variables. Had we defined J differently, Eq. (2.14) would be replaced by some other relation. This property that $\Delta w = 1$ will be important when we begin to consider the quantum theory.

We now have the basis of Hamilton-Jacobi theory using action-angle variables. A main importance of action-angle variables lies in the fact that the Hamiltonian, H'(J), depends on J only:

$$E = H(p,q) \rightarrow E = H'(J) \quad . \tag{2.15}$$

Thus, the transformation of p and q to J and w causes the coordinates, w, to be ignorable. Since transformations carried out using a generating function, W, are canonical, Hamilton's equations of motion hold and we have (2):

$$\begin{aligned} \frac{dw}{dt} &= \frac{\partial H'}{\partial J} = \nu(J) \quad , \\ \frac{dJ}{dt} &= -\frac{\partial H'}{\partial w} = 0 \quad , \end{aligned} \tag{2.16}$$

where ν is the classical frequency of oscillation of the system. This simple form of Hamilton's equations is another reason that a (p,q) to (J,w) transformation is desirable. We now proceed to see what features a quantum Hamilton-Jacobi theory should have.

B. Quantum Hamilton-Jacobi Theory, I

There is a close connection between classical and quantum mechanics with the salient features of one appearing in the other. In particular, if it is possible to solve problems in classical mechanics using transformation theory then one may be able to solve quantum mechanical problems using the same technique.

By analogy with classical mechanics, we have as our goal a quantum canonical transformation theory which would take us to a system of

coordinates in which the Hamiltonian is a function only of the new momenta. The wavefunction will be seen to take on a correspondingly simple form. In this section we will consider a one-dimensional system.

Before beginning, a few comments on notation are in order. First, all classical objects will have a "c" subscript (e.g., q_c, p_c, H_c, ...). All eigenvalues will have one prime " ' ". Operators will be unprimed. We will use a Dirac bra-ket notation (4). For example, suppose we have the operator q with a state $|q'\rangle$;

$$q|q'\rangle = q'|q'\rangle \quad . \tag{2.17}$$

Similarly, with E and the state $|E'\rangle$:

$$E|E'\rangle = E'|E'\rangle \quad . \tag{2.18}$$

Also, e.g.,

$$\langle q'|qE|E'\rangle = q'E'\langle q'|E'\rangle \quad . \tag{2.19}$$

Commutators will be designated by square brackets:

$$[p,q] = \hbar/i \quad . \tag{2.20}$$

The Hermitian conjugate will be denoted by a "+". Finally, the connection of a bra-ket to a wavefunction, ψ, is given by, for example:

$$\langle q'|E'\rangle = \psi(q',E') \quad . \tag{2.21}$$

Let us assume that we have a system whose classical transformation equations can be written in the form:

$$q_c = f_c(J_c,w_c) \quad , \tag{2.22}$$

$$p_c = g_c(J_c,w_c) \quad . \tag{2.23}$$

We would like to find analogous quantum equations:

$$q = f(J,w) \quad , \tag{2.24}$$

$$p = g(J,w) \quad . \tag{2.25}$$

We impose the following conditions, A through F, on the quantum equations (2.24) and (2.25). Condition A is that the quantum equations (2.24) and (2.25) must reduce to the corresponding classical equations in the limit of Planck's constant $\hbar$ going to zero. Condition B is that both sides of Eqs. (2.24) and (2.25) must be Hermitian. We assume that p, q and J, w are Hermitian and have:

$$q = q^+ = f(J,w) = (f(J,w))^+ \quad , \tag{2.26}$$

$$p = p^+ = g(J,w) = (g(J,w))^+ \quad . \tag{2.27}$$

Condition c requires that both sides of Eqs. (2.24) and (2.25) satisfy the same commutation relation:

$$[p,q] = [g(J,w),\ f(J,w)] \quad . \tag{2.28}$$

In order to calculate the commutator (2.28) directly we need information concerning the commutator of J and w. Since J and w are assumed to be a canonically conjugate set of coordinates and momentum, their commutator is:

$$[J,\ e^{\pm 2\pi i w}] = \pm 2\pi\hbar\ e^{\pm i 2\pi w} \quad . \tag{2.29}$$

Equation (2.29) is chosen so that it avoids problems in the definition of angle variables as discussed in Refs. 9, 15 and 17.

Condition D requires that if the quantum Hamiltonian in terms of p and q is H(p,g) then after the transformation (2.24) and (2.25) the Hamiltonian, H'(J), must be independent of the new coordinate w:

$$H(p,q) = H(g(J,w), f(J,w)) = H'(J) \quad . \tag{2.30}$$

Condition E states that given classical Hamiltonians $H_c(p_c,q_c)$ and $H'_c(J_c)$ such that, from Eqs. (2.22) and (2.23) we have:

$$H_c(p_c,q_c) = H_c(g_c(J_c,w_c), f_c(J_c,w_c)) = H'_c(J_c) \quad , \tag{2.31}$$

then we require that

$$H'(J) \xrightarrow{\hbar\to 0} H'_c(J_c) \quad . \tag{2.32}$$

Equation (2.32) also aids in interpreting J and w as the quantum analogues of the classical objects.

Classically, if the change in w_c, Δw_c, is calculated around one cycle of the motion, then this change is one. We interpret this to mean that the state of the system is invariant when w_c goes to $w_c + 1$. Quantum mechanically we require a similar invariance. We require that the wavefunction be invariant under the translation, $w' \to w' + 1$:

$$\langle w' + 1 | J' \rangle = \langle w' | J' \rangle \quad . \tag{2.33}$$

Equation (2.33) is the only boundary condition which we place on the wavefunctions $\langle w' | J' \rangle$.

As a result of this boundary condition on the wavefunction we are able to place a restriction on the form of Eqs. (2.24) and (2.25). p and q are the fundamental observables. We require that if the system

is unchanged by $w' \to w' + 1$, then the matrix elements of q and p should be unchanged:

$$\begin{aligned} \langle w' + 1|q|J'\rangle &= \langle w'|q|J'\rangle \quad , \\ \langle w' + 1|p|J'\rangle &= \langle w'|p|J'\rangle \quad . \end{aligned} \tag{2.34}$$

Equation (2.34) places a restriction on the form of f(J,w) and g(J,w). Specifically, let us suppose that both f(J,w) and g(J,w) can be written in the forms:

$$\begin{aligned} p &= f(J,w) = f_1(w)f_2(J) \quad , \\ q &= g(J,w) = g_1(w)g_2(J) \quad . \end{aligned} \tag{2.35}$$

Functions of operators of the form (2.35) are called well-ordered by Dirac (4) and their matrix elements are easily found.

For p, we substitute Eq. (2.35) into (2.34) and have from Eq. (2.17):

$$\langle w' + 1|f_1(w)f_2(J)|J'\rangle = f_1(w' + 1)f_2(J')\langle w' + 1|J'\rangle \quad , \tag{2.36}$$

$$\langle w'|f_1(w)f_2(J)|J'\rangle = f_1(w')f_2(J')\langle w'|J'\rangle \quad . \tag{2.37}$$

As a result of the boundary condition, Eq. (2.33), and the invariance of the matrix elements (2.34) we have:

$$f_1(w' + 1) = f_1(w') \quad . \tag{2.38}$$

Similarly for $q = g_1(w)g_2(J)$, we find

$$g_1(w' + 1) = g_1(w') \quad . \tag{2.39}$$

The final requirement, condition F, which we place on the transformation equations (2.24) and (2.25) is that they satisfy Eq. (2.34).

Inspection of expressions (2.35) shows that p and q are not necessarily Hermitian because J and w, being conjugate coordinates, do not commute. This inadequacy of the forms (2.35) is easily remedied as we now show.

For the examples which we will consider, both $f_1(w)$ and $g_1(w)$ have the form $e^{\pm i2\pi w}$. The exponential, $e^{\pm i2\pi w}$, clearly satisfies the cyclic property (2.38) and (2.39). Furthermore, as a result of Eq. (A.29), $f(J)e^{i2\pi w} = e^{i2\pi w}\, f(J + 2\pi\hbar)$, the reverse ordering of Eq. (2.35) is also allowed for this exponential:

$$\begin{aligned} p &= f_3(J)\, e^{\pm i2\pi w} = f_3(J)\, f_1(w) \quad , \\ q &= g_3(J)\, e^{\pm i2\pi w} = g_3(J)\, g_1(w) \quad . \end{aligned} \tag{2.40}$$

Combining Eqs. (2.35) and (2.40) we find that p and q can be written in the following forms which will prove useful when we work out examples:

$$\begin{aligned} p &= f^{+}(J)\, e^{+i2\pi w} + e^{-i2\pi w} f(J) \quad , \\ q &= g^{+}(J)\, e^{+i2\pi w} + e^{-i2\pi w} g(J) \quad . \end{aligned} \tag{2.41}$$

The forms of p and q given in Eq. (2.41) are useful because they satisfy the cyclic property (2.38) and (2.39) (which is condition F) and because they are manifestly Hermitian which is required of p and q by condition B.

The conditions A through F which we impose on the canonical transformation equations are designed to insure that p and q will remain Hermitian, will continue to satisfy the same classical limit and will have appropriate commutation relations. These conditions also require that the Hamiltonian in terms of J will be independent of w and have the correct classical limit. Also the transformation equations must be invariant when matrix elements between $\langle w'|$ and $|J'\rangle$ are calculated and w' is replaced by w' + 1. These requirements allow us to assert that the operators J and w which are defined by p = f(J,w) and q = g(J,w) are the quantum analogues of the classical coordinates and momentum.

Having imposed a boundary condition on the wavefunction $\langle w'|J'\rangle$ we are now able to calculate both the form of the wavefunction and the eigenvalues of J. This calculation completes our first specification of quantum mechanics in terms of J and w. A more general formulation will be given in Chapters IV and V.

Having Eqs. (2.29) and (2.33), we can find the wavefunction $\langle w'|J'\rangle$. The effect of J on a state $|J'\rangle$ as we have seen is:

$$J|J'\rangle = J'|J'\rangle \quad .$$

Therefore, we have:

$$\langle w'|J|J'\rangle = J'\langle w'|J'\rangle \quad . \tag{2.42}$$

Under the assumption that J and w form a canonically conjugate set we have consistent with Eqs. (2.29) and (2.33):

$$J = \frac{\hbar}{i} \frac{\partial}{\partial w} \tag{2.43}$$

where we are assuming a Schrödinger representation. Since $\langle w'|J'\rangle$ satisfies an appropriate periodic boundary condition (3) we have:

$$\langle w'|\frac{\hbar}{i} \frac{\partial}{\partial w}|J'\rangle = \frac{\hbar}{i} \frac{\partial}{\partial w'} \langle w'|J'\rangle \quad . \tag{2.44}$$

Combining Eqs. (2.42), (2.43) and (2.44) we find:

$$\frac{\hbar}{i} \frac{\partial}{\partial w'} \langle w'|J'\rangle = J'\langle w'|J'\rangle \quad . \tag{2.45}$$

The solution of Eq. (2.45) is:

$$\langle w'|J'\rangle = A\, e^{i/\hbar\, J'w'} \quad . \tag{2.46}$$

If we now impose the condition (2.33) on Eq. (2.46) we have

$$\langle w'|J'\rangle = \langle w' + 1|J'\rangle$$

or in terms of Eq. (2.46)

$$A\, e^{i/\hbar\, J'w'} = A\, e^{i/\hbar\, J'(w'+1)} \quad . \tag{2.47}$$

Equation (2.47) will hold only if

$$J' = 2\pi\hbar n \quad . \quad n = 0,\pm1,\pm2,\pm3, \ldots \tag{2.48}$$

Combining Eqs. (2.46) and (2.48) we have

$$\langle w'|J'\rangle = \langle w'|2\pi\hbar n\rangle = A\, e^{i2\pi n w'} \quad . \quad n = 0,\pm1,\pm2,\pm3, \ldots \tag{2.49}$$

Equations (2.48) and (2.49) are general and hold for systems described by action-angle variables, defined using the transformation equations

of the form (2.24) and (2.25). This completes our basic specification of J - w quantum mechanics.

The physics of J - w quantum mechanics lies in finding the transformation equations. Once they are found, the allowed energy levels of the system are easily found. Let us assume that we have found the system Hamiltonian in terms of J: H'(J). Using Eq. (2.42) we have:

$$\langle w'|H'(J)|J'\rangle = H'(J')\langle w'|J'\rangle$$

$$= H'(2\pi\hbar n)\langle w'|J'=2\pi\hbar n\rangle \qquad (2.50)$$

$$= E'_n\langle w'|J'=2\pi\hbar\rangle \qquad (2.51)$$

From Eqs. (2.48), (2.50) and (2.51) we have

$$E'_n = H'(2\pi\hbar n) \quad , \quad n = 0,\pm1,\pm2, \ldots \quad . \qquad (2.52)$$

Equation (2.52) is a general statement which holds for any system for which J is Hermitian. The allowed energy levels of the system are given by Eq. (2.52). Thus, the transformation from p and q to J and w not only provides the Hamiltonian H'(J), but also gives immediately the energy levels. This is one important reason for considering the action-angle variable Hamilton-Jacobi transformation.

C. The Harmonic Oscillator

In order to illustrate these ideas we will now apply them to the harmonic oscillator using a method similar to that of Dirac (11). The Hamiltonian for the harmonic oscillator is:

$$H = p^2 + \frac{1}{4}\omega^2 q^2 \quad , \tag{2.53}$$

$$[p,q] = \frac{\hbar}{i} \quad ,$$

where we have chosen a system of units in which twice the mass (2m) is one and where $\frac{\omega}{2\pi}$ is the frequency. The classical equations of transformation are (18):

$$\begin{aligned} q_c &= \sqrt{\frac{2J_c}{\pi\omega}}\ \sin(2\pi w_c) \quad , \\ p_c &= \sqrt{\frac{\omega J_c}{2\pi}}\ \cos(2\pi w_c) \quad , \end{aligned} \tag{2.54}$$

which give

$$H_c = \frac{\omega}{2\pi}\ J_c \quad .$$

We assert that the quantum transformation equations are:

$$\begin{aligned} q &= \frac{1}{2i}\sqrt{\frac{2}{\pi\omega}}\ (a^+ - a) \quad , \\ p &= \frac{1}{2}\sqrt{\frac{\omega}{2\pi}}\ (a^+ + a) \quad , \end{aligned} \tag{2.55}$$

where

$$\begin{aligned} a &= e^{-i2\pi w}\sqrt{J} \quad , \\ a^+ &= \sqrt{J}^+ e^{i2\pi w} \quad . \end{aligned} \tag{2.56}$$

We can check that Eq. (2.55) satisfies conditions A, B, C and F by inspection. First, in the limit of $\hbar \to 0$, $[\sqrt{J},\ e^{\pm i2\pi w}] = 0$, and

Eq. (2.55) reduces to Eq. (2.54) (condition A). Second, Eqs. (2.55) are Hermitian by inspection (condition B). Third, Eqs. (2.55) are of the form (2.41) and so the cyclic condition F is satisfied. Fourth, the commutator of q with p can be calculated using Eq. (2.29). We have from Eqs. (2.55)

$$[p,q] = \left[\frac{1}{2}\sqrt{\frac{\omega}{2\pi}}\ (a^+ + a), \frac{1}{2}\sqrt{\frac{2}{\pi\omega}}\ (a^+ - a)\right]$$

$$= \frac{i}{4\pi}\ 2[a^+,a] \quad . \tag{2.57}$$

Using Eq. (2.29), Eq. (2.57) becomes:

$$\frac{i}{2\pi}\ [a^+,a] = \frac{i}{2\pi}\ [\sqrt{J}^+\ e^{i2\pi w},\ e^{-i2\pi w}\ \sqrt{J}]$$

$$= \frac{i}{2\pi}\ \{\sqrt{J}\ \sqrt{J}^+ - e^{-i2\pi w}\ \sqrt{J}\ \sqrt{J}^+\ e^{i2\pi w}\} \quad . \tag{2.58}$$

In Ref. 17, it is shown that the Hilbert space: $|J'\rangle = |2\pi\hbar n\rangle$ must be restricted to those states having $J' \geq 0$. For this restriction of the Hilbert space it follows that

$$\sqrt{J} = \sqrt{J}^+ \quad . \tag{2.59}$$

Substituting Eq. (2.59) into Eq. (2.58) and using Eq. (2.29) we have:

$$\frac{i}{2\pi}\ [a^+,a] = \frac{\hbar}{i} \quad . \tag{2.60}$$

Substituting Eq. (2.60) into Eq. (2.57) we have:

$$[p,q] = \frac{\hbar}{i} \tag{2.61}$$

and condition C is satisfied. [Note that for $J' < 0$ a minus sign

occurs on the RHS of Eqs. (2.57), (2.58) and (2.61) resulting in $[p,q] = -\hbar/i$ which is clearly unphysical. See Ref. 17 for details.]

As a result of the restriction of the Hilbert space to states having $J' \geq 0$ and as a result of Eq. (2.59), Eq. (2.56) may be written as:

$$a = e^{-i2\pi w}\sqrt{J} \quad ,$$

$$a^+ = \sqrt{J}\, e^{i2\pi w} \quad . \tag{2.62}$$

The forms (2.62) will simplify many expressions.

We now verify that the Hamiltonian, H', depends on J only. We substitute Eq. (2.55) into Eq. (2.53) and obtain:

$$H = p^2 + \frac{1}{4}\omega^2 q^2 = \frac{1}{2}\sqrt{\frac{\omega}{2\pi}}\,(a + a^+)^2 + \frac{1}{4}\omega^2\,\frac{1}{2}\sqrt{\frac{2}{\pi\omega}}\,(a - a^+)^2$$

$$= \frac{\omega}{8\pi}\{aa + aa^+ + a^+a + a^+a^+ - aa + aa^+ + a^+a - a^+a^+\}$$

$$= \frac{\omega}{4\pi}\{aa^+ + a^+a\} \quad . \tag{2.63}$$

From Eq. (2.62) $a^+a = J$ and from Eq. (2.60) $aa^+ = a^+a + 2\pi\hbar$. Substituting these identities in Eq. (2.63) we obtain:

$$H = p^2 + \frac{1}{4}\omega^2 q^2 = \frac{\omega}{2\pi}\{J + \pi\hbar\} \quad . \tag{2.64}$$

Equation (2.64) shows that the Hamiltonian is independent of w. Also in the limit of $\hbar \to 0$, $J \to J_c$, and Eq. (2.64) becomes:

$$H' = \frac{\omega}{2\pi}\{J + \pi\hbar\} \xrightarrow{\hbar \to 0} \frac{\omega}{2\pi}\, J_c = H_c \quad . \tag{2.65}$$

so that the quantum Hamiltonian reduces to the classical Hamiltonian, H_c, as desired (condition E). Thus, Eqs. (2.64) and (2.65) verify conditions D and E by showing that H'(J) is independent of w and that H(J) has the right classical limit. We have now satisfied all of the conditions (A-F) which we imposed earlier, and conclude that Eqs. (2.55) and (2.56) constitute a valid (p,q) to (J,w) transformation where J, w are the quantum action-angle variables.

The energy levels of Eq. (2.64) are given by substituting Eq. (2.64) into Eq. (2.50) and obtain:

$$\langle w'|H'(J)|J'\rangle = \frac{\omega}{2\pi}\{2\pi\hbar n + \pi\hbar\}\langle w'|J'\rangle \qquad (2.66)$$

$$n = 0,+1,+2, \ldots$$

where we have restricted ourselves to the $n \geq 0$ part of the Hilbert space as discussed earlier. The reader will recognize these as the harmonic oscillator eigenvalues which can be obtained by other methods.

The procedure which we have followed entailed finding the classical transformation equations in the form

$$\begin{aligned} p_c &= f_1(J_c,w_c) \quad , \\ q_c &= g_1(J_c,w_c) \quad . \end{aligned} \qquad (2.67)$$

Once this was done, corresponding quantum equations were asserted:

$$\begin{aligned} p &= f_2(J,w) \quad , \\ q &= g_2(J,w) \quad . \end{aligned} \qquad (2.68)$$

We then verified that Eq. (2.68) had the six desired properties. One

of the most important properties is that the quantum Hamiltonian be independent of w:

$$H(p,q) \rightarrow H'(J) \quad . \tag{2.69}$$

Since we had already determined that the possible eigenvalues of J are $J' = 2\pi\hbar n$ ($n = 0,+1,+2, \ldots$), the harmonic oscillator energy levels were given by inspection:

$$E'_n = H'(J' = 2\pi\hbar n) \quad . \tag{2.70}$$

The method employed here works for the harmonic oscillator, and will now be applied to other problems. In each case the procedure is the same. We assert (or find) the transformation equations. We verify conditions A through F for the physical Hilbert space. Finally, the energy levels are given by inspection. This procedure works for systems having simple classical transformation equations.

III. SIMPLE QUANTUM SYSTEMS

A. Separation of Variables

In the previous chapter the idea of transforming from a set of coordinates and momenta (p,q) to a corresponding set of action-angle coordinates and momenta (J,w) was introduced. The six quantum conditions which such a transformation must satisfy were specified. In this chapter we will apply the same concept and set of conditions to the problem of motion in a central field. The Hamiltonian in spherical polar coordinates and momenta, which we will transform, is:

$$H(r,P_r,\theta,P_\theta,\phi,P_\phi) = (2mr^2)^{-1}\{P_r r^2 P_r + \sin^{-1}\theta\, P_\theta \sin\theta\, P_\theta + P_\phi^2/\sin^2\theta\} + V(r) \quad . \tag{3.1}$$

We will make our transformations in three steps:

$$\begin{aligned} &(1)\quad P_\phi,\phi \rightarrow J_\phi,w_\phi \quad , \\ &(2)\quad P_\theta,\theta \rightarrow J_\theta,w_\theta \quad , \\ &(3)\quad P_r,r \qquad J_r,w_r \quad . \end{aligned} \tag{3.2}$$

We are able to make the transformation to action-angle variables in this way because the full Hamiltonian (3.1) may be separated into three partial "Hamiltonia" each of which depends on only one coordinate and its canonically conjugate momentum:

$$L_z^2(P_\phi,\phi) \equiv P_\phi^2 \quad , \tag{3.3}$$

$$L^2(P_\theta,\theta) \equiv \sin^{-1}\theta\, P_\theta \sin\theta\, P_\theta + P_\phi^2/\sin^2\theta \quad , \tag{3.4}$$

$$H_r(P_r,r) \equiv (2mr^2)\{P_r r^2 P_r + L^{2'}\} + V(r) \quad . \tag{3.5}$$

In Eqs. (3.4) and (3.5) $P_\phi'^2$ and $L^{2'}$ are the constants of separation which connect Eq. (3.3) to Eq. (3.4) and Eq. (3.4) to Eq. (3.5), respectively. In quantum mechanics these separation constants take the values of the eigenvalues of L_z^2 and L^2 respectively, hence the primes on $P_\phi'^2$ and $L^{2'}$.

In carrying out the transformations listed in Eq. (3.2) we will use the procedure given in Chapter II. We will consider a transformation valid only if it satisfies all six conditions (A-F) which we established. These conditions will guide us through the examples of this chapter.

B. Rotor

In this section we will carry out step one of Eq. (3.2): $P_\phi,\phi \rightarrow J_\phi,\phi$. The "Hamiltonian" given by Eq. (3.3) may be interpreted as a particle rotating around the origin on a circle, as a "rotor". The procedure which we will follow for the rotor is to list the classical transformation equations, then the corresponding quantum equations, then verify the six conditions, and finally give the "energy levels" of L_z^2. While the rotor is trivial to transform in this way, it is instructive, and, more importantly, prepares the ground for more complicated transformations.

The classical transformation equations and "Hamiltonian", L_z^2, are:

$$P_{\phi c} = J_{\phi c}/2\pi \quad , \tag{3.6}$$

$$\dot{\phi}_c = 2\pi w_{\phi c} \quad , \tag{3.7}$$

so

$$L_z^2 = P_\phi^2 = (J_{\phi c}/2\pi)^2 \quad . \tag{3.8}$$

We assert that the quantum canonical transformation equations and Hamiltonian have the same form as the classical expressions:

$$P_\phi = J_\phi/2\pi \quad , \tag{3.9}$$

$$e^{i\phi} = e^{i2\pi w_\phi}{}^{1} \quad , \tag{3.10}$$

so

$$L_z^2 \equiv P_\phi^2 = (J_\phi/2\pi)^2 \quad . \tag{3.11}$$

We are assuming

$$[P_\phi, e^{i\phi}] = \hbar\, e^{i\phi} \quad .$$

The conditions which we have demanded that the transformation equations and Hamiltonian satisfy are quickly verified. In the limit $\hbar \to 0$, that is in the limit of

$$P_\phi \to P_{\phi c} \quad ,$$

$$\phi \to \phi_c \quad ,$$

---

[1] The forms $e^{i\vartheta}$ and $e^{i2\pi w_\phi}$ are used in order to avoid problems of defining angles as discussed in Jordan (9), Leacock (17), and Lévy-Leblond (15).

$$J_\phi \rightarrow J_{\phi c} \quad ,$$

$$w_\phi \rightarrow w_{\phi c} \quad ,$$

it is clear that the quantum expressions (3.9), (3.10) and (3.11) become the classical expressions (3.6), (3.7) and (3.8) (conditions A and E). The Hamiltonian is clearly independent of w_ϕ as required (condition D). The Eqs. (3.9) and (3.10) are of the form (2.41) (cyclic in w with period 1), hence condition F is satisfied. The commutator of the left hand sides of Eqs. (3.9) and (3.10) is:

$$[P_\phi, e^{i\phi}] = \hbar\, e^{i\phi} \quad . \tag{3.12}$$

After the substitution of Eqs. (3.9) and (3.10) into Eq. (3.12) we find:

$$[J_\phi/2\pi, e^{i2\pi w_\phi}] = 2\pi\hbar\, e^{i2\pi w_\phi} \quad . \tag{3.13}$$

Equation (3.13) is true because of the assumed canonical nature of J_ϕ and $e^{i2\pi w_\phi}$; so Eq. (3.12) is verifeid. Under the assumption (3.10), (3.12) and (3.13) are equal and condition C is verified. Finally, under the assumption that p_ϕ, J_ϕ, ϕ and w_ϕ are Hermitian we have:

$$P_\phi = p_\phi^+ = (J_\phi/2\pi) = (J_\phi/2\pi)^+ \quad , \tag{3.14}$$

$$(e^{i\phi})^+ = (e^{2\pi i w_\phi})^+ \quad . \tag{3.15}$$

Both sides of Eq. (3.14) are clearly Hermitian and thus condition B is satisfied. For Eq. (3.15) both sides are unitary with the Hermitian conjugate of the left side of Eq. (3.15) equal to the Hermitian

conjugate of the right side of Eq. (3.15). In the context of the rotor we will consider Eq. (3.15) as satisfying condition B. If one prefers, the real and imaginary parts of Eq. (3.10) may be considered separately:

$$\begin{aligned} \cos\phi &= (\cos\phi)^{+} = \cos(2\pi w_{\phi}) = (\cos(2\pi w_{\phi}))^{+} \\ \sin\phi &= (\sin\phi)^{+} = \sin(2\pi w_{\phi}) = (\sin(2\pi w_{\phi}))^{+} \end{aligned} \tag{3.16}$$

Whether one chooses Eqs. (3.15) or (3.16), the relationship between ϕ and w_{ϕ} remains the same and condition B is considered satisfied.

This completes the verification of conditions A-F. Hence, we consider Eqs. (3.9) and (3.10) as defining a valid transformation from ϕ and P_{ϕ} to the action-angle variables J_{ϕ} and w_{ϕ}. The only items left to consider for the rotor are the allowed states and eigenvalues of L_z^2.

As in other action-angle calculations the wavefunction is:

$$\langle w'_{\phi} | J'_{\phi} \rangle = \langle w'_{\phi} | 2\pi\hbar m \rangle = e^{i2\pi m w'_{\phi}} , \tag{2.49}$$

$$m = 0, \pm 1, \pm 2, \ldots .$$

Since the six conditions are valid for all states, all values of m are allowed. In contrast, for the harmonic oscillator the commutator (condition C) was valid only for states having $2\pi\hbar n \geq 0$. Here, we have no such restriction.

Having the states (2.49) and the allowed values of m, we can now calculate the eigenvalues of L_z^2. This is done using Eqs. (2.49) and (3.11):

$$\langle w'_\phi | L_z^2 | J'_\phi \rangle = \langle w'_\phi | (J_\phi/2\pi)^2 | J'_\phi \rangle \tag{3.17}$$

$$= (J'_\phi/2\pi)^2 \langle w'_\phi | J'_\phi \rangle \tag{3.18}$$

$$= (\hbar m)^2 \langle w'_\phi | J'_\phi = 2\pi\hbar m \rangle \quad . \tag{3.19}$$

Hence

$$L_z^2(J'_\phi) = (\hbar m)^2 \qquad m = 0, \pm 1, \pm 2, \ldots \quad . \tag{3.20}$$

This completes our treatment of the rotor. We have found the valid transformation equations from ϕ and P_ϕ to J_ϕ and w_ϕ. We have found the form of L_z^2 in terms of J_ϕ and have found the eigenvalues, $L_z'^2$. Having found the eigenvalues of L_z^2 we can proceed to step two, the transformation of P_θ and θ to J_θ and w_θ, since we now know the values of the separation constant connecting the ϕ problem and the θ problem.

C. The θ-Motion, L^2

Having solved the ϕ-motion and found the separation constant which connects the ϕ-motion to the θ-motion, we now proceed to the θ-problem. As in the harmonic oscillator and the ϕ-problem, the basic conditions required of a (p,q) to (J,w) transformation remain the same. In this problem, however, we will not be able to simply assert the form of the quantum transformation equations based on the classical equations. A derivation based on the commutation requirement and the w_θ-independence of $L^2(J_\theta)$ is needed, and is given in Appendix A in its entirety. After finding the form of $L^2(J_\theta)$ and the transformation equations, the verification of conditions A through F may be completed, and the

eigenvalues of $L^2(J_\theta)$ found. These eigenvalues provide the connection which we will later use between the θ and ϕ motions and the radial motion.

We begin by listing the classical total angular momentum and θ-transformation equations (18):

$$L_c^2 = P_\theta^2 + P_\phi^2/\sin^2\theta \quad , \tag{3.21}$$

$$= (J_\theta + J''_\phi)^2/4\pi^2 \quad , \tag{3.22}$$

$$\cos\theta_c = \sin i \sin(-2\pi w_\theta + 2\pi w_{\theta c}) \quad , \tag{3.23}$$

$$P_\theta \sin\theta_c = ((J_\theta + J''_\phi)/2\pi) \sin i \cos(-2\pi w_\theta + 2\pi w_{\theta c}) \quad , \tag{3.24}$$

$$\cos i = P_\phi/L_c = J_\phi/(J_\theta + J''_\phi) \quad , \tag{3.25}$$

$$\sin i = (1 - P_\phi^2/L_c^2)^{1/2} = (1 - J_\phi^2/(J_\theta + J''_\phi)^2)^{1/2} \quad . \tag{3.26}$$

$w_{\theta c}$ is a constant determined by initial conditions. We need to define J''_ϕ and begin by noting that $J_{\theta c}$ is defined by Born (18):

$$J_{\theta c} = 2\pi(L_c^2)^{1/2} - 2\pi(P_\phi^2)^{1/2} \quad . \tag{3.27}$$

The signs of the two square roots must be chosen. We choose the sign of $(L_c^2)^{1/2}$ to be positive so that this quantity, L_c, is interpreted as the length of the angular momentum vector. This sign of $(P_\phi^2)^{1/2}$ is also chosen to be positive so that $J_{\theta c}$ will be positive, will have a range of values from 0 to $2\pi L_c$, and will be interpreted as the "quantity of θ-motion." $J_{\theta c}$ equal to zero is the interpreted as the angular momentum

vector being oriented along the z-axis with $L_c^2 = P_\phi^2$. Finally, for the above choice of signs we define $2\pi[P_\phi^2]^{1/2} \equiv J_\phi''$, where J_ϕ'' is real and positive so that (3.20) follows.

The task at hand is to convert the above classical expressions into valid quantum operator equations with respect to the quantum "Hamiltonian":

$$L^2(P_\theta,\theta) \equiv \sin^{-1}\theta\, P_\theta \sin\theta\, P_\theta + P_\phi'^2/\sin^2\theta \quad . \tag{3.4}$$

Since the "ϕ" part of the problem has been solved (see the rotor calculation), we need only note that P_ϕ and J_ϕ enter only through their eigenvalues P_ϕ' and J_ϕ' (or $J_\phi'' \equiv |J_\phi'|$).

If one studies Eqs. (3.23) and (3.24) one observes that, by analogy to the harmonic oscillator, two operators b and b^+ may be defined as:

$$b = e^{-i2\pi w_\theta} f(J_\theta,J_\phi'') \quad , \tag{3.28}$$

$$b^+ = f^+(J_\theta,J_\phi'')\, e^{i2\pi w_\theta} \quad , \tag{3.29}$$

such that

$$\cos\theta = (b - b^+)/2i \tag{3.30}$$

$$P_\theta \sin\theta = [b(J_\theta + J_\phi'') + (J_\theta + J_\phi'')b^+]/4\pi \quad . \tag{3.31}$$

Before the canonical transformation (3.30) and (3.31) may be called complete, $f(J_\theta,J_\phi')$ must be specified.

In Appendix A the calculation for the form of $f(J_\theta, J''_\phi)$ and L^2 is given, using three requirements. First, the requirement that $L^2(J_\theta, J''_\phi)$ be independent of w_θ is used. Second, we require that the commutator of the right hand side of Eq. (3.30) with the right hand side of Eq. (3.31) be the same as the commutator of the left hand side of Eq. (3.30) with the left hand side of Eq. (3.31). This requirement involves substituting the transformation equations into:

$$[P_\theta \sin\theta, \cos\theta] = -\frac{\hbar}{i}(1 - \cos^2\theta) \quad , \tag{3.32}$$

and finding a restriction on the form of $f(J_\theta, J''_\phi)$. Finally, we require that the quantity $f(J_\theta, J''_\phi) f^{+}(J_\theta, J''_\phi)$ have positive eigenvalues since it is positive definite. This condition leads to the conclusion that $J'_\theta \geq 0$ for physically allowed states. Using these three requirements it is shown in Appendix A that:

$$f = \{[(J_\theta + J''_\phi)^2 - J''^2_\phi]/[(J_\theta + J''_\phi)^2 - \pi^2\hbar^2]\}^{1/2} \quad , \tag{3.33}$$

$$L^2(J_\theta, J''_\phi) = (J_\theta + J''_\phi + \pi\hbar)^2/4\pi^2 - 1/4\ \hbar^2 \quad , \tag{3.34}$$

where the physical Hilbert space is restricted to states $|J'_\theta, J'_\phi\rangle$ where $J'_\theta = 2\pi\hbar n_\theta$, $n_\theta = 0,1,2,3, \ldots$, $J'_\phi = 2\pi\hbar m$, $m = 0,\pm1,\pm2, \ldots$ and where $J''_\phi = |J'_\phi|$. As shown in the Appendix, if we use the notation:

$$J'_\theta + J''_\phi = 2\pi\hbar\ell \quad , \tag{3.35}$$

then the physical Hilbert space may be chosen to be:

$$\ell \geq |m| \quad , \quad \ell = 0, 1, 2, 3, \ldots$$
$$m = 0, \pm 1, \pm 2, \ldots \quad . \tag{3.36}$$

For this choice of the physical Hilbert space we have:

$$f(J_\theta, J''_\phi) = f^+(J_\theta, J''_\phi) \tag{3.37}$$

which simplifies Eqs. (3.28) and (3.29) to:

$$b = e^{-i2\pi w_\theta} f(J_\theta, J''_\phi) \quad ,$$
$$b^+ = f(J_\theta, J''_\phi)\, e^{i2\pi w_\theta} \quad . \tag{3.38}$$

Since we have now specified $f(J_\theta, J'_\phi)$ and $L^2(J_\theta)$, we can verify the six conditions which we imposed on a set of transformation equations. By expressing $\cos\theta$ and $P_\theta \sin\theta$ in terms of P_x, P_y, P_z, x, y and z, the reader may verify that

$$P_\theta \sin\theta = (P_\theta \sin\theta)^+ \quad ,$$
$$\cos\theta = (\cos\theta)^+ \quad . \tag{3.39}$$

Under the assumption that $J_\theta = J_\theta^+$ and $w_\theta = w_\theta^+$, it follows that both sides of the transformation equations (3.30) and (3.31) are Hermitian which is condition A. In the limit of $\hbar \to 0$ and J_θ, J''_ϕ, w_θ, P_θ, θ going to their corresponding classical variables, the quantum expressions (3.30), (3.31) and (3.34) reduce to the corresponding classical expressions (3.23), (3.24) and (3.22). Thus, conditions B and E are satisfied, as required. $L^2(J_\theta, J''_\theta)$ is independent of w_θ, which is condition D.

The commutator of $P_\theta \sin\theta$ with $\cos\theta$, Eq. (2.32), is satisfied when calculated in terms of J_θ and w_θ using the transformation equations, which is condition C. Finally, since the quantum transformation equations (3.30) and (3.31) are of the exponential form (2.41), their matrix elements are invariant under $w'_\theta \to w'_\theta + 1$, and thus condition F is satisfied. This completes the verification of conditions A-F and we conclude that the quantum action-angle variable transformation equations (3.30) and (3.31) are a valid set of canonical transformation equations with respect to the physical Hilbert space (Eq. (3.36)).

Having verified conditions A-F, we may now allow $L^2(J_\theta)$ to act on a state $|J'_\theta, J'_\phi\rangle$ and find its eigenvalues. Using Eq. (3.34) we find:

$$L^2|J'_\theta,J'_\phi\rangle = \frac{1}{4\pi^2}\left[(J'_\theta + J'_\phi + \pi\hbar)^2 - \pi^2\hbar^2\right]|J'_\theta,J'_\phi\rangle \quad . \tag{3.40}$$

Since $J'_\theta + J'_\phi = 2\pi\hbar\ell$ for the physical Hilbert space we have:

$$L^2|J'_\theta,J'_\phi\rangle = \hbar^2\ell(\ell+1)|J'_\theta,J'_\phi\rangle$$

or

$$L^{2'} = \hbar^2\ell(\ell+1) \quad \text{where} \quad \ell = 0,+1,2,\ldots \quad , \tag{3.41}$$
$$\ell \geq |m| \quad .$$

The finding of the eigenvalues of L^2 completes the θ-problem.

We now relist the relevant equations for future reference.

Angular momentum squared (old coordinates):

$$L^2(\theta,P_\theta,\phi,P_\phi) = \sin^{-1}\theta\, P_\theta \sin\theta\, P_\theta + P'^2_\phi/\sin^2\theta \quad ;$$

wavefunction (old coordinates):

$$\langle \theta',\phi' | \ell,m \rangle = Y_{\ell m}(\theta',\phi') \quad ; \quad \ell = 0, 1, 2, \ldots \geq |m| \quad , \quad m = 0,\pm1,\pm2, \ldots$$

angular momentum squared (new coordinates):

$$L^2(J_\theta,J''_\phi) = (J_\theta + J''_\phi + \pi\hbar)^2/4\pi^2 - 1/4\ \hbar^2 \quad ;$$

wavefunction (new coordinates):

$$\langle w'_\theta,w'_\phi | J'_\theta,J'_\phi \rangle = e^{i/\hbar(J'_\theta w'_\theta + J'_\phi w'_\phi)} \quad ,$$

$$J'_\theta = 2\pi\hbar n_\theta \quad , \quad n_\theta = 0, 1, 2, \ldots \quad ,$$

$$J'_\phi = 2\pi\hbar m \quad , \quad m = 0,\pm1,\pm2, \ldots \quad ,$$

$$J''_\phi = |J'_\phi| \quad .$$

Quantum canonical transformation (between old and new coordinates):

$$\cos\theta = (b - b^+)/2i \quad ,$$

$$P_\theta \sin\theta = [b(J_\theta + J''_\phi) + (J_\theta + J''_\phi)b^+]/4\pi \quad ,$$

$$b = e^{-i2\pi w_\theta} f(J_\theta,J''_\phi) \quad ,$$

$$b^+ = f(J_\theta,J''_\phi)\ e^{i2\pi w_\theta} \quad ,$$

$$f(J_\theta,J''_\phi) = \{[(J_\theta + J''_\phi)^2 - J''^2_\phi]/[(J_\theta + J''_\phi)^2 - \pi^2\hbar^2]\}^{1/2} \quad .$$

Eigenstates (old coordinates):

$$L^2|\ell m\rangle = \ell(\ell+1)\hbar^2|\ell m\rangle \quad ,$$

$$L_z|\ell m\rangle = m\hbar|\ell m\rangle \quad .$$

Eigenstates (new coordinates):

$$L^2|n_\theta m\rangle = (n_\theta + m'')(n_\theta + m'' + 1)\hbar^2|n_\theta m\rangle \quad ,$$

$$L_z|n_\theta m\rangle = m\hbar|n_\theta m\rangle \quad ,$$

$$J_\theta|n_\theta m\rangle = n_\theta 2\pi\hbar|n_\theta m\rangle \quad ,$$

$$J_\phi|n_\theta m\rangle = m2\pi\hbar|n_\theta m\rangle \quad ,$$

where $m'' \equiv |m|$. (See Eqs. (3.9)-(3.11) for the ϕ transformation equations.)

Reviewing what has been done so far in this chapter, we find that the angular part of the central force problem has been completed. We have transformed quantum mechanically from P_ϕ, ϕ, P_θ and θ to J_ϕ, w_ϕ, J_θ and w_θ, which was our original aim. In the process of this canonical transformation we have found $L_z(J_\phi)$ and $L^2(J_\theta, J_\phi'')$ and have found their eigenvalues and eigenfunctions. We thus have systematically replaced the old operators and eigenfunctions with new operators and eigenfunctions. In both cases, however, the eigenvalue spectrum of the observables, L_z^2 and L^2, remains the same as it must.

Since we now have the eigenvalues of L^2, we have the values of the separation constant connecting the angular coordinates and the r-motion in Eq. (3.5). We will now proceed to the r-problem using the information gathered thus far.

D. The Radial Problem

At the beginning of this chapter it was stated that we would treat in succession the three separate parts of a full three-dimensional spherical potential, Hamiltonian. Having completed the angular problems we now treat the "radial" Hamiltonian.

The Hamiltonian given by Eq. (3.3) is for $2m = 1$:

$$H_r(r,P_r) = r^{-2} P_r r^2 P_r + L^{2'}/2mr^2 + V(r) \quad . \quad (3.5)$$

$L^{2'}$ is the eigenvalue of L^2, the total angular momentum, and has values $\hbar^2 \ell(\ell + 1)$ for $\ell = 0,1,2,3, \ldots$. The kinetic part of Eq. (3.5) may be rewritten in terms of $P_r r + \hbar/2i$. This quantity is chosen at this point since it is Hermitian as can be shown by writing it in terms of x, y, z, P_x, P_y, P_z and verifying that:

$$(P_r r + \frac{\hbar}{2i}) = (P_r r + \frac{\hbar}{2i})^{+} \quad (3.42)$$

where

$$[P_r,r] = \frac{\hbar}{i} \quad . \quad (3.43)$$

By rewriting Eq. (3.5), using $P_r r + \hbar/2i$, we obtain:

$$H(r,P_r) = r^{-1}\left(Pr_r + \frac{\hbar}{2i}\right)^2 r^{-1} + (L^{2'} + \frac{1}{4}\hbar^2)/r^2 + V(r) \quad .(3.45)$$

Substituting $\hbar^2\ell(\ell + 1)$ for $L^{2'}$ we have:

$$H(r,P_r) = r^{-1}\left(P_r r + \frac{\hbar}{2i}\right)^2 r^{-1} + \hbar^2(\ell + 1/2)^2/r^2 + V(r) \quad . (3.46)$$

An advantage to the form (3.46) of $H(r,P_r)$ is that $(P_r r + \hbar/2i)$ is a combination which proves to be convenient. The convenience lies in the fact that for the first example which we will consider, the three-dimensional harmonic oscillator, one of the transformation equations involves $(P_r r + \hbar/2i)$ explicitly because the classical transformation equations involve "$P_r r$" and $(P_r r + \hbar/2i)$ is the quantum analogue of this classical quantity.

We will now consider the three-dimensional harmonic oscillator. The process which we will follow is essentially the same as was used for the one-dimensional harmonic oscillator, the rotor, and the θ-motion for L^2. Our aim as always is to find valid quantum transformation equations and the eigenvalue spectrum of the relevant "Hamiltonian".

Equation (3.68) is the form of the "Hamiltonian" which we will use for the example of the three-dimensional harmonic oscillator with $V(r) = 1/4\ \omega^2 r^2$:

$$H(r,P_r) = r^{-1}\left(P_r r + \frac{\hbar}{2i}\right)^2 r^{-1} + \hbar^2(\ell + 1/2)^2/r^2 + 1/4\ \omega^2 r^2 \quad . \tag{3.47}$$

As in the other problems which we have considered, we begin by listing

the classical transformation equations and Hamiltonian:

$$H_c = P_{rc}^2 + L_c^2/r_c^2 + \frac{1}{4}\omega^2 r^2$$

$$= \frac{\omega}{2\pi}\{2J_{rc} + J_{\theta c} + J''_{\phi c}\} \quad , \tag{3.48}$$

$$P_r r = f_c \cos 2\pi(w_r - w_{r0}) \quad , \tag{3.49}$$

$$\frac{1}{2}\omega r^2 - H_c/\omega = f_c \sin 2\pi(w_r - w_{r0}) \quad , \tag{3.50}$$

$$f_c \equiv \frac{1}{2\pi}\left((2J_{rc} + J_{\theta c} + J''_{\phi c})^2 - (J_{\theta c} + J''_{\phi c})^2 \right)^{1/2} \quad . \tag{3.51}$$

This form of the transformation equations relies on J_{rc} defined as:

$$J_{rc} = \frac{1}{2}\left(\frac{2\pi}{\omega} H_c - [\, L_c^2 \,]^{1/2} \right) \quad , \tag{3.52}$$

where J_{rc} is found using the integral of P_r around one cycle of the motion. The branch of P_r which is chosen is pictured in Figure 1 (with positive signs on the bottom of the cut. Using this branch of P_r with a counterclockwise direction of integration, J_{rc} is defined to be a positive quantity. In Eq. (3.52), the positive square root is chosen for $[L_c^2]^{1/2}$ which is cousistent with the branch of P_r which we have chosen, and which is consistent with the choice of sign made for the classical angular problem (Chapter III, Section C).

We begin the quantum process by defining an operator d such that:

$$d^+ \equiv f(J_r, J'_\theta + J'_\phi)\, e^{i2\pi w_r} \quad , \tag{3.53}$$

$$d \equiv e^{-i2\pi w_r} f(J_r, J''_\theta + J'_\phi) \quad , \tag{3.54}$$

$$f(J_r, J'_\theta + J'_\phi) \equiv \frac{1}{2\pi} \{[2J_r + J'_\theta + J''_\phi + \pi\hbar]^2 - [J'_\theta + J''_\phi + \pi\hbar]^2\}^{1/2} \tag{3.55}$$

where $J'_\theta + J''_\phi$ is discussed in Chapter III, Section C on the angular momentum problem.

Using the d operator we assert that the quantum transformation equations are:

$$P_r r + \frac{\hbar}{2i} = \frac{1}{2}(d^+ + d) \quad , \tag{3.56}$$

$$\frac{1}{2}\omega r^2 - H/\omega = +\frac{1}{2i}(d^+ - d) \quad . \tag{3.57}$$

We assert that Eqs. (3.56) and (3.57) are the quantum analogues of the classical transformation equations (3.52) and (3.53), and we now demonstrate the validity of the assertion. Since $P_r r + \hbar/2i$ is Hermitian, we have:

$$(P_r r + \hbar/2i) = (P_r r + \hbar/2i)^+ = \frac{1}{2}(d^+ + d) = [\frac{1}{2}(d^+ + d)]^+ \quad ,$$

$$(\frac{1}{2}\omega r^2 - H/\omega) = (\frac{1}{2}\omega r^2 - H/\omega)^+ = +\frac{1}{2i}(d^+ - d) = [+\frac{1}{2i}(d^+ - d)]^+ .$$

Thus, the quantum transformation equations have both sides Hermitian and condition B is satisfied. Condition C is that both sides of the transformation equations satisfy the same commutator.

The commutator of $P_r r + \hbar/2i$ and $\frac{1}{2}\omega r^2 - H/\omega$ is:

$$\left[P_r r + \frac{\hbar}{2i} , \frac{1}{2}\omega r^2 - \frac{H}{\omega} \right] = \frac{2\hbar}{i\omega} H \quad . \tag{3.58}$$

Substituting the quantum forms (3.56) and (3.57) into the LHS of Eq. (3.58), one obtains after simplifying:

$$\frac{1}{2i} [d,d^+] = \frac{2\hbar}{i\omega} H \quad . \tag{3.59}$$

Substituting the expressions for d^+,d, Eqs. (3.53) and (3.54) into Eq. (3.59) we have

$$e^{-i2\pi w_r} f f^+ e^{i2\pi w_r} - f^+ f = \frac{4\hbar}{\omega} H \quad . \tag{3.60}$$

Using Eq. (A.29), $f(J_r)f^+(J_r)e^{i2\pi w_r} = f(J_r + 2\pi\hbar)f^+(J_r + 2\pi\hbar)$, Eq. (3.60) becomes:

$$f(J_r + 2\pi\hbar)\, f^+(J_r + 2\pi\hbar) - f^+(J_r)\, f(J_r) = \frac{4\hbar}{\omega} H \quad . \tag{3.61}$$

The quantum Hamiltonian, H, as given by Eq. (3.47) is a positive definite quantity and, hence, has positive eigenvalues. Referring to the form of $f(J_r)$ as given by Eq. (3.55), the left hand side of Eq. (3.61) will have positive eigenvalues only for those states having $J_r' \geq 0$. We will call this the restricted or physical Hilbert space. It is important to note that for the physical Hilbert space, $f(J_r) = f^+(J_r)$. This will simplify some expressions. Substituting the form of f, Eq. (3.55) into Eq. (3.61) and using the commutator $[J_r, e^{i2\pi w_r}] = 2\pi\hbar\, e^{i2\pi w_r}$, we have:

$$\frac{1}{2\pi}\{[2(J_r + 2\pi\hbar) + J'_\theta + J''_\phi + \pi\hbar]^2 - [2J_r + J'_\theta + J''_\phi + \pi\hbar]^2\} = \frac{4\hbar}{\omega} H$$

or

$$H = \frac{\omega}{2\pi}[2J_r + J'_\theta + J''_\phi + 3\pi\hbar] \quad . \tag{3.62}$$

Thus, the commutator of $(P_r r + \hbar/2i)$ with $(1/2\ \omega r^2 - H/\omega)$ is verified providing the Hamiltonian has the form given in Eq. (3.62). The form of the Hamiltonian (3.62) is correct as may be seen by directly substituting the quantum transformation equations (3.56) and (3.57) into the quantum Hamiltonian, $H(r,P_r)$, as given in Eq. (3.62). Thus, condition C is satisfied. Condition D is that the quantum Hamiltonian $H(J_r, J'_\theta + J''_\phi)$ be independent of w_r, w_θ and w_ϕ. The form of the quantum Hamiltonian (3.62) clearly satisfies this condition. Condition E requires that the quantum Hamiltonian, $H(J_r, J'_\theta + J''_\phi)$, Eq. (3.62), reduce to the classical Hamiltonian, $H(J_{rc}, J_{\theta c} + J''_{\phi c})$, as given in Eq. (3.48). In the limit of $\hbar \to 0$ where $J'_r \to J_{rc}$, $J''_\theta + J''_\phi \to J_{\theta c} + J''_{\phi c}$, this is the case. Condition A (that the quantum equations have the correct classical limit) is easily verified for the physical Hilbert space. In the $\hbar \to 0$ limit where $J'_r \to J_{rc}$, $J'_\theta \to J_{\theta c}$ and $J''_\phi \to J''_{\phi c}$, $f(J'_r, J'_\theta + J''_\phi)$ becomes $f_c(J_{rc}, J_{\theta c} + J''_{\phi c})$ and in the limit of $w'_r \to w_{rc}$, the quantum equations (3.78) and (3.79) become the corresponding classical expressions (3.71) and (3.72). Finally, condition F which requires that the matrix elements of $(P_r r + \hbar/2i)$ and $(1/2\ \omega r^2 - H/\omega)$ be invariant under the translation in w'_r, $w'_r \to w'_r + 1$, is satisfied since the quantum transformation equations depend only on exponentials of w_r and hence are of the form (2.37).

This completes the verification of conditions A through F for the restricted Hilbert space. We therefore conclude that the quantum transformation equations which we have given are a valid set, and define J_r and w_r as being the quantum analogues of the classical variables.

Since we have found the form of the Hamiltonian, $H(J_r, J'_\theta + J''_\phi)$, we may now find its eigenvalues for the restricted Hilbert space, $(J'_r \geq 0)$. Allowing the Hamiltonian to act on a state $|J'_r, J'_\theta, J'_\phi\rangle$ we have:

$$H(J_r, J'_\theta + J''_\phi)|J'_r,J'_\theta,J'_\phi\rangle = \frac{\omega}{2\pi}(2J_r + J'_\theta + J''_\phi + 3\pi\hbar)|J'_r,J'_\theta,J'_\phi\rangle$$

$$= \frac{\omega}{2\pi}(2J'_r + J'_\theta + J''_\phi + 3\pi\hbar)|J'_r,J'_\theta,J'_\phi\rangle \qquad (3.63)$$

where $J'_r = 2\pi\hbar n_r$, $n_r = 0, 1, 2, \ldots$ and where $J'_\theta + J''_\phi = 2\pi\hbar\ell$, $\ell = 0, 1, 2, \ldots$ (as given by the angular problem in Chapter III, Section C). Using these values of the eigenvalues the energy levels $E_{n_r,\ell}$ are:

$$E_{n_r,\ell} = \hbar\omega(2n_r + \ell + 3/2) \quad . \qquad (3.64)$$

This completes our treatment of the three-dimensional harmonic oscillator since we have asserted and verified the transformation equations and have found the energy levels of the quantum Hamiltonian, $H(J_r, J'_\theta + J''_\phi)$.

In addition to completing the radial part of the three-dimensional harmonic oscillator, we have now completed an entire three-dimensional problem. We have transformed from P_ϕ, ϕ, P_θ, θ, P_r and r to J_ϕ, w_ϕ, J_θ,

w_θ, J_r and w_r using the following transformation equations and "Hamiltonia":

$$
\begin{aligned}
P_\phi &= J_\phi/2\pi \quad , \\
e^{i\phi} &= e^{i2\pi w_\phi} \quad , \\
L_z^2 &= P_\phi^2 = (J_\phi/2\pi)^2 \quad ;
\end{aligned}
\tag{3.65}
$$

$$
\begin{aligned}
&P_\theta \sin\theta = (b - b^+)/2i \quad , \\
&\cos\theta = [b(J_\theta + J_\phi) + (J_\theta + J_\phi)b^+]/4\pi \quad , \\
&b = e^{-i2\pi w_\theta} \{[(J_\theta + |J_\phi|)^2 - J_\phi^2]/[(J_\theta + |J_\phi|)^2 - \pi^2\hbar^2]\}^{1/2} \quad , \\
&L^2 = \sin^{-1}\theta\, P_\theta \sin\theta\, P_\theta + P_\phi^2/\sin^2\theta = (J_\theta + |J_\phi| + \pi\hbar)^2/4\pi^2 - \tfrac{1}{4}\hbar^2 \quad ;
\end{aligned}
\tag{3.66}
$$

for $V(r) = \frac{1}{4}\omega^2 r^2$:

$$
\begin{aligned}
&P_r r + \hbar/2i = \tfrac{1}{2}(d^+ + d) \quad , \\
&\tfrac{1}{2}\omega r^2 - H/\omega = \frac{1}{2i}(d^+ - d) \quad , \\
&d = e^{-i2\pi w_r} \frac{1}{2\pi} \{[2J_r + J_\theta + J_\phi + \pi\hbar]^2 - [J_\theta + J_\phi + \pi\hbar]^2\}^{1/2} \quad , \\
&H(P_r, r) = r^{-1}(P_r r + \hbar/2i)^2\, r^{-1} + (L^{2'} + \tfrac{1}{4}\hbar^2)/r^2 + \tfrac{1}{4}\omega^2 r^2 \\
&\qquad = \frac{\omega}{2\pi}(2J_r + J_\theta + |J_\phi| + 3\pi\hbar) \quad .
\end{aligned}
\tag{3.67}
$$

These are valid transformation equations and satisfy conditions A-F for the following eigenfunctions:

$$|J_r', J_\theta', J_\phi'\rangle = |2\pi\hbar n_r,\ 2\pi\hbar(\ell - m),\ 2\pi\hbar m\rangle \quad ,$$

$$n_r = 0,\ 1,\ 2,\ 3,\ \ldots \quad , \tag{3.68}$$

$$\ell = 0,\ 1,\ 2,\ 3,\ \ldots \geq |m| \quad ,$$

$$= 0, \pm 1, \pm 2, \pm 3,\ \ldots \quad .$$

With respect to the states (3.68), (3.65)-(3.67) are equivalent to the equations given earlier in this chapter. The eigenvalues of L_z^2, L^2 and H_r are found by allowing these operators to act on a state (3.68):

$$L_z^2|J_r', J_\theta', J_\phi'\rangle = \hbar^2 m^2 |J_r', J_\theta', J_\phi'\rangle \tag{3.69}$$

$$L^2|J_r', J_\theta', J_\phi'\rangle = \hbar^2(\ell + 1)\ell |J_r', J_\theta', J_\phi'\rangle \tag{3.70}$$

$$H_r|J_r', J_\theta', J_\phi'\rangle = \frac{\omega}{2\pi}(2n_r + \ell + 3/2)|J_r', J_\theta', J_\phi'\rangle \quad . \tag{3.71}$$

From Eqs. (3.65)-(3.67) it is clear that we have systematically replaced each operator in the old system with an operator in the new system. Thus, action-angle variables are a valid set of variables (operators) with which to do quantum mechanical calculations. It is important to note that for potentials which depend only on r, the entire angular calculation remains valid. Thus, Eqs. (3.65), (3.66), (3.69) and (3.70) remain the same for all potentials V(r). These angular equations may be viewed as a different way of treating angular motion.

The radial equations listed are valid only for the three-dimensional harmonic oscillator. For other potentials, other transformation equations will result. It is not clear whether all potentials may be

treated using the techniques we have employed so far. There is one potential which seems intractable using these methods, the Coulomb potential.

E. Comments on the Coulomb Problem

In all the problems which have been done so far, it has been possible to write the classical transformation equations in the form:

$$\begin{aligned} g_c(q,p) &= s_c(J,w) \quad , \\ h_c(q,p) &= t_c(J,w) \quad . \end{aligned} \tag{3.72}$$

Having the classical forms (3.72) we were then able to assert or derive the corresponding operator relations. Turning now to the Coulomb potential, the classical Coulomb Hamiltonian and transformation equations are (18): $(2m = 1)$

$$H_c = p_r^2 + \frac{L^2}{r^2} - \frac{g}{r} = \frac{-\pi^2 g^2}{(J_r + J_\theta + J_\phi)^2} \tag{3.73}$$

$$r = a(1 - \varepsilon \cos u) \tag{3.74}$$

$$u - t \sin u = 2\pi w_r \tag{3.75}$$

$$a = \frac{(J_r + J_\theta + J_\phi)^2}{2\pi^2 g} \tag{3.76}$$

$$\varepsilon^2 = 1 - \frac{(J_\theta + J_\phi)^2}{(J_r + J_\theta + J_\phi)^2} \quad . \tag{3.77}$$

Since Eqs. (3.74) and (3.75) constitute a transcendental transformation equation, it has proven impossible to put it conveniently into the form (3.72). This inability to find a suitable expression means that we are unable to use the method which we have employed so far on the Coulomb problem. Although in principle one can find the transformation equations, this author has been unable to do so and asserts the need for an alternate technique. This technique will begin to unfold in the following chapter.

IV. A QUANTUM TRANSFORMATION THEORY

A. The Hamilton-Jacobi Eigenvalue Equation and $W_0(q',E')$

The method that we have been using thus far to make the (p,q) to (J,w) transformation has several drawbacks which make a more general method desirable. First, it applies only to systems having classical analogues since we are "updating" the classical transformation equations to find the corresponding quantum expressions. Second, the method works only when the classical equations are algebraically simple. In the case of the Coulomb problem, the difficulty of manipulating the classical equations means that the method of Chapters II and III is useless. Finally, it would be convenient to have a method which is sufficiently general that a computer could carry out the transformation. The method of Chapters II and III is difficult to program. Thus, at least at present, it appears that a more general method is desirable.

In order to develop another method of performing (p,q) to (J,w) transformations we will rely on two ingredients. First, classical mechanics will be used to guide the development and notation. Second, Dirac (4,5) and Jordan (6,7,8,9) have considered various forms of transformation theories. In the initial development we will follow the general transformation methods discussed in Dirac's Section 32 (4). We, of course, modify his methods to suit our particular problem. It will be seen that these two ingredients combine to form a theory which is more general and less dependent on algebraic manipulations than the earlier method. We begin this development by reviewing the classical mechanics that was introduced in Chapter II.

In classical mechanics a generating function (2) governs the transformation from one set of canonical coordinates to another. As was discussed in Chapter II, Section A, for action-angle variables, the transformation takes the form:

$$p_c = \frac{\partial W_c(q_c,J_c)}{\partial q} = \frac{\partial W_{0c}(q_c,E_c)}{\partial q} \tag{2.1}$$

$$c = \frac{\partial W_c(q,J)}{J} \tag{2.2}$$

where $W_{0c}(q_c,E_c) = W_c(q_c,J_c(E_c))$ and where $W_c(q_c,J_c)$ is Hamilton's characteristic function which satisfies the Hamilton-Jacobi equation:

$$H_c = p_c^2 + V(q_c)$$

$$\left(\frac{\partial W_c}{\partial q_c}\right)^2 + V(q_c) = E_c \tag{2.6}$$

in units where the mass m obeys 2m = 1. The above equations are converted to the corresponding quantum expressions by properly defining quantum w and J.

In order to generalize the classical theory, we begin by writing the wavefunction, $\langle q'|E'\rangle$, in a manner similar to that used by Dirac and Jordan (see Refs. 4-9):

$$\langle q'|E'\rangle \equiv e^{iW_0(q',E')/\hbar} \tag{4.1}$$

where all primes denote eigenvalues. Equation (4.1) defines the function $W_0(q',E')$. We use Eq. (4.1) with a time-independent

Schrödinger's equation so that a differential equation for W_0 results. Using a Hamiltonian of the form:

$$H = p^2 + V(q) \quad . \tag{4.2}$$

Schrodinger's equation is:

$$\langle q'|H|E'\rangle = E'\langle q'|E'\rangle$$

$$\langle q'|p^2 + V(q)|E'\rangle = E'\langle q'|E'\rangle \quad . \tag{4.3}$$

Using $\langle q'|p|E'\rangle = \frac{\hbar}{i}\frac{\partial}{\partial q'}\langle q'|E'\rangle$ (see Ref. 4) with Eq. (4.3) and the wavefunction, Eq. (4.1), we have:

$$\left\{\frac{\hbar}{i}\frac{\partial^2 W_0(q',E')}{\partial q'^2} + \left(\frac{\partial W_0(q',E')}{\partial q'}\right)^2 + V(q')\right\}\langle q'|E'\rangle = E'\langle q'|E'\rangle \quad . \tag{4.4}$$

Canceling the wavefunctions, $\langle q'|E'\rangle$, from both sides of Eq. (4.4) and using the notation:

$$W_{0qq} \equiv \frac{\partial^2}{\partial q'^2} W_0(q',E') \quad , \quad W_{0q} \equiv \frac{\partial}{\partial q'} W_0(q',E')$$

we obtain:

$$\frac{\hbar}{i} W_{0qq} + W_{0q}^2 + V(q') = E' \quad . \tag{4.5}$$

Equation (4.5) has the property that, for $\hbar = 0$, it becomes the classical Hamilton-Jacobi equation, Eq. (2.2), for the function $W_{0c}(q_c,E_c)$.

$W_0(q',E')$ and Eq. (4.5) reduce to Hamilton's characteristic function and the classical Hamilton-Jacobi equation, respectively.

This classical limit suggests designating Eq. (4.5) as a quantum mechanical Hamilton-Jacobi eigenvalue equation. This is an "eigenvalue equation" because its solution, W_0, is a function of the eigenvalues, q' and E', and not a function of the corresponding operators.

Let us suppose that Eq. (4.5) has been solved and its general solution, W_0, has been found. The wavefunction $\langle q'|E'\rangle$ has boundary conditions imposed on it (for physical reasons), and therefore W_0 has corresponding boundary conditions imposed on it. The two sets of boundary conditions are related by Eq. (4.1). For example, we often require the wavefunction to be zero at some point, q_0 (e.g., the origin or infinity). As q' approaches q_0 we have:

$$\lim_{q' \to q_0} \langle q'|E'\rangle = e^{iW_0(q',E')/\hbar} = 0 \quad . \tag{4.6}$$

Therefore,

$$\lim_{q' \to q_0} W_0(q',E') \to +i\infty \quad . \tag{4.7}$$

Thus the requirement that the wavefunction vanishes at a certain point leads to the conclusion that $W_0(q',E')$ must have a positive infinite imaginary part at that point. Other boundary conditions on W_0 are handled similarly.

Having solved the differential equation (4.5) and satisfied the physical boundary conditions imposed on W_0, we now need to find the operator associated with $W_0(q',E')$.

Let us assume that the Hamilton-Jacobi eigenvalue equation has been solved for $W_0(q',E')$. If we were working with classical mechanics we would then find $E_c(J_c)$, substitute it into $W_{0c}(q_c,E_c)$, and hence find the full generating function $W_c(q_c,J_c)$. Having the generating function, the coordinate, w_c, and the momentum, p_c, are then given by derivatives of the generating function with respect to J_c and q_c, respectively. Quantum mechanically we would like to carry out a similar procedure. This procedure could be carried out providing a definition of J' existed which was analogous to the classical contour integral definition, (Eq. (2.11)). Such a contour integral definition requires knowing the quantum analogue of the classical momentum function, $p_c(q_c,E_c)$, as in Eq. (2.1). Classically, this quantum momentum function may be found using the form of the Hamiltonian or from:

$$p_c(q_c,E_c) = \partial W_{0c}(q_c,E_c)/\partial q_c \qquad (2.1)$$

where

$$W_{0c}(q_c,E_c) = W_c(q_c,J_c(E_c)) \quad .$$

In order to find the quantum analogue of the classical momentum function, $p_c(q_c,E_c)$, we will use the following procedure. First, we will find the function of operators, $W_0(q,E)$, which is associated with $W_0(q',E')$. Then we will define an operator, p, as a derivative of $W_0(q,E)$ such that $[p,q] = h/i$. Finally, we will find the function of eigenvalues, $p^*(q',E')$, which is associated with p. Since p has commutator $\hbar/i$ with q and is found using $W_0(q',E')$ and $W_0(q,E)$, we will assert that $p^*(q'E')$ is the quantum analogue (in eigenvalue form) of

the classical momentum. This $p^*(q',E')$ will be used to define J' as a contour integral from which the quantum analogues of the classical quantities, $W_c(q_c,J_c)$, p_c and w_c, will follow.

We begin this process by finding the function of operators $W_0(q,E)$ which is associated with $W_0(q',E')$. To do this we use the notion of a well-ordered function of operators (4). An operator, M(q,E), is a well-ordered function of two operators q and E if all occurrences of q appear to the left of all occurrences of E. In general M(q,E) takes the form:

$$M(q,E) = \sum_{ij} d_i(q)\, f_j(E) + \int a(q,\lambda)\, b(E,\lambda)\, d\lambda \quad . \tag{4.8}$$

The important feature is that q appear to the left of E. For the sake of illustration we assume that a well-ordered operator, M(q,E), may be written in the form:

$$M(q,E) = d(q)\, f(E) \quad , \tag{4.9}$$

while keeping in mind that the more general form (4.8) is allowed and implied.

The utility of well-ordering a function of operators, M(q,E), lies in the fact that it can be related to a corresponding function of eigenvalues, M(q',E'), by the relation:

$$\langle q'|M(q,E)|E'\rangle = \langle q'|d(q)f(E)|E'\rangle \tag{4.10}$$

$$= d(q')f(E')\langle q'|E'\rangle$$

$$= M(q',E')\langle q'|E'\rangle \quad . \tag{4.11}$$

We now apply the concept of a well-ordered function of operators to define the function $W_0(q,E)$ which corresponde to $W_0(\sigma',E')$, the solution of the Hamilton-Jacobi eigenvalue equation.

Let us assume that $W_0(q',E')$ can be written in a well-ordered form:

$$W_0(q',E') = g(q')\, h(E') \quad . \tag{4.12}$$

The function of eigenvalues, $W_0(q',E')$, is connected to the well-ordered function of operators, $W_0(q,E)$, by:

$$\langle q'|W_0(q,E)|E'\rangle = \langle q'|g(q)h(E)|E'\rangle \tag{4.13}$$

$$= g(q')h(E')\langle q'|E'\rangle$$

$$\equiv W_0(q',E')\langle q'|E'\rangle \quad . \tag{4.14}$$

Equations (4.13) and (4.14) establish the desired relationship and define the function of operators, $W_0(q,E)$:

$$W_0(q,E) \equiv g(q)\, h(E) \tag{4.15}$$

from the corresponding function of eigenvalues. This function of operators will now be used to define an operator p which we will eventually call the quantum momentum.

Having defined the operator function, W_0, we can define the operator, p, as in classical mechanics:

$$p = \frac{\partial W_0(q,E)}{\partial q} \equiv \frac{\partial g(q)}{\partial q}\, h(E) \quad . \tag{4.13}$$

p is interpreted as a well-ordered function of the operators q and E, which we will eventually designate as the momentum. We may also

relate p to a function of eigenvalues, p^*, in the same way that we related $W_0(q,E)$ and $W_0(q',E')$:

$$\langle q'|p|E'\rangle = \langle q'\left|\frac{\partial g(q)}{\partial q}\,h(E)\right|E'\rangle$$

$$= \frac{\partial g(q')}{\partial q'}\,h(E')\langle q'|E'\rangle \qquad (4.14)$$

$$\equiv p^*(q',E')\langle q'|E'\rangle \quad ,$$

where

$$p^*(q',E') \equiv \frac{\partial g(q')}{\partial q'}\,h(E') \quad . \qquad (4.15)$$

We now calculate the commutator of p and q by relating p to $\frac{\hbar}{i}\frac{\partial}{\partial q}$. For states satisfying appropriate boundary conditions (4) we have

$$\langle q'\left|\frac{\hbar}{i}\frac{\partial}{\partial q}\right|E'\rangle = \frac{h}{i}\frac{\partial}{\partial q'}\langle q'|E'\rangle \quad . \qquad (4.16)$$

Since we have wavefunctions in an exponential form, Eq. (4.1), we can relate p to $\frac{\hbar}{i}\frac{\partial}{\partial q}$ easily. Using Eqs. (4.16) and (4.1) we have:

$$\langle q'\left|\frac{h}{i}\frac{\partial}{\partial q}\right|E'\rangle = \frac{h}{i}\frac{\partial}{\partial q'}\,e^{i/\hbar\,W_0(q',E')} \quad , \qquad (4.17)$$

$$= \frac{\partial g(q')}{\partial q'}\,h(E')\langle q'|E'\rangle \quad . \qquad (4.18)$$

Comparing Eq. (4.18) to the matrix element, $\langle q'|p|E'\rangle$, Eq. (4.14), we see that p and $\frac{\hbar}{i}\frac{\partial}{\partial q}$ have the same matrix elements with respect to $\langle q'|$ and $|E'\rangle$. We thus conclude that:

$$p = \frac{\hbar}{i} \frac{\partial}{\partial q} \quad . \tag{4.19}$$

Using Eq. (4.19) it follows that:

$$[p,q] = pq - qp = \frac{\hbar}{i} \tag{4.20}$$

when p is defined by Eq. (4.13).

The importance of relating p to $\frac{\hbar}{i} \frac{\partial}{\partial q}$ is easily seen. First, as we have seen the commutator of p and q is $\frac{\hbar}{i}$. Second, Dirac (4) has shown that for states satisfying suitable boundary conditions $\frac{\hbar}{i} \frac{\partial}{\partial q}$ is Hermitian, hence p defined by Eq. (4.13) is Hermitian. With a correct commutator and hermiticity we assert that p is the momentum canonically conjugate to q. From this assertion, it follows that $p^*(q',E')$ is the "eigenvalue" analogue of the classical momentum function $p_c(q_c,E_c)$. $p^*(q',E')$ is the object which will be used to define the eigenvalue, J'. Before defining J', we will study the quantum Hamilton-Jacobi eigenvalue equation, $p^*(q',E')$ and related equations in more detail, since they differ from their classical counterparts and since this treatment is different from the "normal" treatment in quantum mechanics.

B. $p^*(q',E')$ and the Ricatti Equation

We have introduced $p^*(q',E')$ and have asserted that it is the quantum analogue of the classical momentum, $p_c(q_c,E_c)$. Before using $p^*(q',E')$ to define quantum action-angle variables we examine briefly the mathematics of $p^*(q',E')$. An understanding of this function is necessary if one is to understand why and how it is used to define the quantum action variable.

From the definition of $p^*(q',E')$, Eq. (4.15), it follows that:

$$p^*(q',E') = \frac{\partial W_0(q',E')}{\partial q'} \quad . \tag{4.21}$$

In the Hamilton-Jacobi eigenvalue equation, Eq. (4.5), only the first and second derivatives of $W_0(q',E')$ are used. Substituting $p^*(q',E')$ as given by Eq. (4.21) and its first derivative (with respect to q') into the Hamilton-Jacobi eigenvalue equation, Eq. (4.5), we obtain a differential equation for $p^*(q',E')$:

$$\frac{\hbar}{i} p_q^* + p^{*2} + V(q') = E' \quad , \tag{4.22}$$

where

$$p_q^* \equiv \frac{\partial p^*(q',E')}{\partial q'} \quad .$$

Equation (4.22) is a generalized Ricatti equation and is sufficient to define $p^*(q',E')$ uniquely everywhere in the complex q'-plane, provided that a boundary condition is specified at a regular point, q_0, of $p^*(q',E')$:

$$p^*(q'=q_0, E') = p_0^* \quad . \tag{4.23}$$

The Ricatti equation, Eq. (4.22), has a simple classical limit. In the classical limit with $h \to 0$, the Ricatti equation becomes:

$$p_c^2 + V(q_c) = E_c \quad , \quad (h \to 0) \quad . \tag{4.24}$$

Equation (4.24) is identical to the classical Hamiltonian, Eq. (2.4), (with $2m = 1$) and, hence, Eq. (4.24) defines the classical momentum

function $p_c(q_c,E_c)$. Thus, $p^*(q',E')$ does become $p_c(q_c,E_c)$ in the classical limit. This also aids in the interpretation of $p^*(q',E')$ as the quantum analogue of the classical momentum function.

The Ricatti equation, Eq. (4.22), can be generalized to encompass different types of coordinates. This is done using the quantum Hamiltonian in the form:

$$\frac{1}{f(q)}\ p\ f(q)p + V(q) = E \quad . \tag{4.25}$$

This form of the Hamiltonian applies to one-dimensional Cartesian coordinates (x,p_x) where $f = 1$. It applies to angular coordinates where $f = 1$ for (ϕ,p_ϕ) and where $f = \sin\vartheta$, when the coordinate is ϑ and the momentum is p_ϑ. For the radial part of spherical polar coordinates f is equal to r^2. The reader may verify these specifications of f(q) by referring to the Hamiltonia which were treated in Chapters II and III, Eqs. (2.53), (3.3), (3.4), and (3.5).

Using the commutator of p with f(q) as given by Dirac (4):

$$[p,f(q)] = \frac{\hbar}{i}\frac{\partial f}{\partial q} \quad ,$$

the Hamiltonian, Eq. (4.25), becomes:

$$p^2 + \left(\frac{\hbar}{i}\frac{1}{f(q)}\frac{\partial f}{\partial q}\right)p + V(q) = E \quad . \tag{4.26}$$

Using the wavefunction in the form (4.1) we obtain the generalized Hamilton-Jacobi eigenvalue equation:

$$\frac{\hbar}{i}W_{0qq} + W_{0q}^2 + \frac{\hbar}{i}\frac{1}{f}f_q\,W_{0q} + V(q') = E' \tag{4.27}$$

where the subscript "q" denotes differentiation with respect to q, i.e.,

$$W_{0q} \equiv \frac{\partial W_0(q',E')}{\partial q'} \quad , \quad W_{0qq} \equiv \frac{\partial^2 W_0(q',E')}{\partial q'^2} \quad .$$

Substituting $p^*(q',E')$ as defined in Eq. (4.21) into Eq. (4.27) we obtain a generalized Ricatti equation of the form:

$$\frac{\hbar}{i} p^*_q + p^{*2} + \frac{\hbar}{i} \frac{1}{f} f_q p^* = E' - V(q') \quad , \tag{4.28}$$

where

$$p^*_q \quad \frac{\partial p^*(q',E')}{\partial q'} \quad .$$

Before proceeding to use $p^*(q',E')$ to define quantum action-angle variables, we will present some of the basic mathematics associated with Ricatti equations and their solutions. The reader is referred to Refs. 19, 20 and 21 for more complete treatments.

Since Eq. (4.28) is a generalized Ricatti equation if any particular solution y can be found, the general solution has the form:

$$p^*(q) = y(q) + \frac{1}{u(q)} \quad . \tag{4.29}$$

Substituting Eq. (4.29) into the generalized Ricatti equation, Eq. (4.28), we obtain the differential equation for u(q).

$$\frac{\hbar}{i} \frac{\partial u}{\partial q} - (2y + \frac{\hbar}{i} \frac{1}{f} f_q)u = 1 \quad . \tag{4.30}$$

Equation (4.30) may be solved by quadratures (19):

$$u(q) = u = C\, e^{-iB(q)/\hbar} + e^{-iB(q)/\hbar} \int_{a(q')} \frac{i}{\hbar} e^{iB(q')/\hbar}\, dq' \tag{4.31}$$

where

$$B(q) \equiv \int_{a(q')} (-2y - \frac{\hbar}{i}\frac{1}{f} f_q)dq'' \quad , \tag{4.32}$$

where a(q) is a contour in the q' plane from a point q_0 to the point q, and where C is a constant of integration with respect to q' (but may in general depend on E'). Using the definition of u(q), Eq. (4.30) and $p^*(q)$ as given in Eq. (4.29) we have

$$p^*(q) = y(q) + \frac{e^{iB(q)/\hbar}}{C + \int_{a(q)} \frac{i}{h} e^{iB(q')/\hbar}\, dq'} \quad . \tag{4.33}$$

Equation (4.33) reduces the solving of the generalized Ricatti equation (4.28) to the finding of any particular solution of Eq. (4.28). All other solutions are obtained by adjusting the parameter C in Eq. (4.33).

A particular solution of Eq. (4.28) may be found by inspection if f(q) and V(q) are sufficiently simple. If V(q) and $\frac{1}{f} f_q$ can be expanded as power series (e.g.,

$$V(q) = \sum_{\ell=0}^{\infty} d_\ell\, q^\ell \quad) \quad ,$$

then there exists a power series of form:

$$y(q) = \sum_{\ell=1}^{\infty} g_\ell \, q^\ell \tag{4.34}$$

which satisfies the generalized Ricatti equation (4.28), and hence Eq. (4.34) is a valid particular solution. More general equations must be studied on a case by case basis.

A full discussion of the singularities of solutions first-order nonlinear differential equations is beyond the scope of this paper. A good discussion may be found in Ince, Chapter 12 (19). For our purposes it is sufficient to point out that solutions of Ricatti equations may have both poles and branch points. Such solutions may have fixed poles and fixed branch points whose location and type can be determined by inspection of the differential equation. (Their location may depend on values of parameters of the differential equation (e.g., E' in Eq. (4.28).) Solutions of Ricatti equations may also have movable poles (but no movable branch points) whose locations depend on the boundary conditions imposed and on parameters in the differential equation.

For the purposes of the discussions which follow it is sufficient to notice that since the branch points are fixed a simply connected region, S, in the complex q-plane can be found in which the solution of a Ricatti equations, $p^*(q)$, is regular, single valued, analytic and has only poles as singularities. Thus, it will be reasonable to define integrals of $p^*(q)$ within the region S. We will always assume (or prove) that we are operating within such a region.

With these general considerations we will now proceed to apply, $p^*(q',E')$, the quantum momentum eigenvalue function, to the problem of defining w and J, the action-angle variables. We will follow closely the classical theory. There will, however, be differences since $p^*(q',E')$ is very different from $p_c(q_c,E_c)$ except when $\hbar \to 0$.

C. J' - the Action Variable

In classical mechanics the momentum function, $p_c(q_c,E_c)$, is used to define J_c, the classical action variable. We will now use $p^*(q',E')$ to do exactly the same thing quantum mechanically. After defining J(E), the quantum action-variable operator, we will continue to follow classical mechanics and define W(q,J), the generating function, and w which is the operator canonically conjugate to J.

Let us suppose that from a Hamiltonian, the corresponding Hamilton-Jacobi "eigenvalue" equation and the corresponding Ricatti equation have been found and solved yielding $p^*(q',E')$. Let us further suppose that a boundary condition, $p^*(q'=q_0, E') = p_0^*$, has been imposed on $p^*(q',E')$. (This boundary condition is imposed on physical grounds and is normally obtained from the boundary condition imposed on $W_0(q',E')$.) Having imposed the boundary condition, $p^*(q',E')$ is now uniquely specified. We will not define J', the eigenvalue of the operator J, as the integral around the closed contour D:

$$J' \equiv \int_D p^*(q',E')dq' \quad . \tag{4.35}$$

Equation (4.35) defines J' once the contour D is specified and the direction (around D) in which the integral is to be evaluated is specified.

The two choices which we need to make are largely conventional. In classical mechanics, one chooses a particular branch of the function $p_c(q_c,E_c)$ (in Fig. 1, this corresponded to choosing "+" signs along the bottom of the cut). Next one chooses the contour, which normally encloses the classical turning points and the cut between them, but which encloses no other singularities of $p_c(q_c,E_c)$. Finally, one chooses the direction (around the contour) in which the integral is to be evaluated. In order to maintain the correct classical limit for J', one must make a corresponding set of choices quantum mechanically.

We have argued that $p^*(q',E')$ becomes $p_c(q_c,E_c)$ in the classical limit. Instead of using the wavefunction to impose a boundary condition on $p^*(q',E')$, one may use the classical limit. This is done by choosing a point q_0 at which both $p^*(q',E')$ and $p_c(q_c,E_c)$ are defined (or their limits are defined in the limit of $q' \to q_0$ and $q_c \to q_0$). Assuming that one has specified $p_c(q_c,E_c)$, one now chooses the boundary condition for $p^*(q',E')$ such that in the classical limit one has:

$$p^*(q_0,E') \to p_c(q_0,E_c) \quad . \tag{4.36}$$

Again, once such a boundary condition has been imposed $p^*(q',E')$ is uniquely determined. If one imposes a boundary condition on $p^*(q',E')$ by some other method, Eq. (4.36) should be verified or should be used to choose the branch of $p_c(q_0,E_c)$ with which the classical J_c is defined. The reason that one uses such limits is to guarantee that in the classical limit J' will become J_c.

We emphasize here that $p^*(q',E')$ is the physical quantum momentum eigenvalue function. For example, when using $p^*(q',E')$ to define $J'(E')$, it must satisfy all physical boundary conditions imposed on it which may be possible, in some cases, only at discrete values of E'.

Assuming that $p^*(q',E')$ and $p_c(q_c,E_c)$ have been specified such that $p_c(q_c,E_c)$ is the classical limit of $p^*(q',E')$, we now choose the contour D and the direction of integration. First, we choose the quantum direction of integration to be the same as the corresponding classical direction. For example, if we were calculating the quantum analogue of Fig. 1, we would choose the counterclockwise direction.

In order to choose the contour, two considerations are important. First, in the classical momentum function $p_c(q_c,E_c)$ is normally defined as having a cut between the two classical turning points on the real axis (as was discussed briefly in Chapter II). The contour is chosen to enclose this cut. The quantum contour must enclose at least that segment of the real axis which terminates on the classical turning points. (We will call this segment the classical region.)

The other consideration which is important is the singularity structure of $p^*(q',E')$. As discussed in Appendix C, at an eigenstate of the system, for some simple potentials (The harmonic oscillator and Coulomb potentials are discussed in Appendix C, in detail.), $p^*(q',E')$ has poles only on the real axis with a set of poles between the classical turning points, with at most one pole to the right of the classical region, and with at most one pole to the left of the classical region. While such a simple singularity structure will probably occur

only for simple potentials, the methods of Appendix C will aid in the choice of the contour and evaluation of the integral defining J'.

With the understanding that the singularity structure of $p^*(q',E')$ must be studied on a case by case basis, and with a desire to maintain the classical limit, we choose the quantum contour to be identical to the classical contour. This contour will enclose the segment of the real axis between and including the classical turning points.

We have decided that for systems having a classical analogue, we will normally choose the contour and direction of integration to be the same as the corresponding classical contour and direction of integration. We have decided also that the boundary condition imposed on $p^*(q',E')$ should be chosen so that $p_c(q_c,E_c)$ is given in the classical limit. These considerations are sufficient to specify the elements of the integral, Eq. (4.35), which we are using to define J'. As a result of this definition we obtain from Eq. (4.35) $J' \equiv J'(E')$.

We interpret the E' in J'(E') as the eigenvalue of the Hamiltonian (i.e., the energy eigenvalue) obtained by allowing the Hamiltonian to act on a physically allowed state. Recall that J' is the eigenvalue of the operator J.

Having now discussed the definition of J'(E'), we will now assume that we have found $J' = J'(E')$ for some system using the above definition. Having J', we will now use this object to define the operator J, the canonically conjugate operator w, and the eigenstates $\langle w'|J'\rangle$. This will complete the quantum discussion of our formal action-angle variable theory.

We conclude this section with an addendum on the properties of $p^*(q',E')$ at an eigenstate of the system. This will be useful when we evaluate the contour integral, Eq. (4.35), which defines $J'(E')$.

The normal requirement that a wavefunction must satisfy in order to consider it a physically allowed state is normalizability. This requirement in general will demand that the wavefunction $\langle q'|E'\rangle$ have a certain asymptotic behavior. This asymptotic form of the wavefunction can be interpreted as applying to $p^*(q',E')$. Since $p^*(q',E')$ is the derivative of $W_0(q',E')$ and since the wavefunction, $\langle q'|E'\rangle$, is the exponential of $(i/\hbar)W_o(q',E')$ we have:

$$p^*(q',E') = -i\hbar \frac{1}{\langle q'|E'\rangle} \frac{\partial}{\partial q'} (\langle q'|E'\rangle) \quad . \tag{4.37}$$

For bound state problems (for which one has $V(q')>E'$, for q' real and $|q'|$ large) one can make general statements about the sign of the product $\langle q'|E'\rangle^{-1}\partial(\langle q'|E'\rangle)/\partial q'$ (for q' real and $|q'|$ large) at an eigenstate of the system. These statements will apply when $\langle q'|E'\rangle$ is a real function of q' and E' for real q' and real E' and when the boundary condition on $\langle q'|E'\rangle$ is $\langle q'|E'\rangle \to 0$ when $|q'| \to \pm\infty$.

These statements will refer to a simple potential for which at two points on the real q'-axis, q_+ and q_-, $(q_+ > q_-)$ $V(q_+) = V(q_-) = E'$. Between q_+ and q_- we assume that on the real axis, $V(q') < E'$. For $q- < q_-$ we demand $V(q')<E'$ and for $q' < q_+$ we demand $V(q') > E'$, on the real q'-axis. By specifying the potential in this way on the real axis, the relative size of $V(q')$ and E' in an interval determines the behavior of the wavefunction, $\langle q'|E'\rangle$, in that interval.

At an eigenstate of the system the product $\langle q'|E'\rangle\partial(\langle q'|E'\rangle)/\partial q'$ and hence the product $\langle q'|E'\rangle^{-1}\partial(\langle q'|E'\rangle)/\partial q'$ has the following signs (19,22). For q' real and $q' > q_+$, this product is negative and for q' real and $q' < q_-$ this product is positive providing one is in the region where $V(q') > E'$ (inside the potential hill). When $\langle q'|E'\rangle$ is <u>not</u> a physically allowed wavefunction of the system, for large q' (i.e., $|q'| \to \infty$), the product is positive for q' real and $q' > q_+$, and/or the product is negative for q' real and $q' < q_-$. Thus, we conclude that at an eigenstate of the system and only at an eigenstate of the system, inside the "potential hill" ($V(q') > E'$) on the real q'-axis $p^*(q',E')$ is positive imaginary for q' real and $q' > q_+$, and is negative imaginary when q' is real and $q' < q_-$. Both of these conditions must be satisfied at an eigenstate. If the boundary condition on the wavefunction is changed, these conditions change. For example, in central potential it is normally demanded that the wavefunction vanish at the origin. If q_- is positive, then at an eigenstate $p^*(q',E')$ must be negative imaginary in the interval $(0,q_-)$ on the real q'-axis. Such changes in these conditions must be studied on a case by case basis.

The importance of these conditions is that they allow one to quickly decide whether a certain energy E' corresponds to an eigenenergy of a system. This will prove very useful in a practical sense when we calculate J'(E') for the Coulomb problem in Chapter V.

D. The Operators

Let us assume that we have found $J'(E')$ for some Hamiltonian where E' are the eigenvalues of energy for that system. Using classical mechanics as a guide we will now define the operators which correspond to the classical objects, J_c, w_c, $W(q_c,J_c)$. We will define these objects with respect to wavefunctions of the system $\langle q'|E'\rangle$ (or $\langle q'|J'\rangle$).

Let us assume that $J' = J'(E')$ has been found and let us further assume that $J' = J'(E')$ may be inverted to yield

$$E' = E'(J') \quad . \tag{4.38}$$

Using the substitution (4.38) at the eigenvalues of energy, the function $W_0(q',E')$, Eq. (4.4), may be transformed to $W(q',J')$ by:

$$W_0(q',E'(J')) = W(q',J') \quad . \tag{4.39}$$

Using the wavefunction, Eq. (4.1), and Eqs. (4.38) and (4.39), we can redesignate the physical states of the system as:

$$\langle q'|E'\rangle = e^{iW_0(q',E')/\hbar} = e^{iW(q',J')/\hbar} = \langle q'|J'\rangle . \tag{4.40}$$

$\langle q'|J'\rangle$ is interpreted as the wavefunction of the system described using the states $|J'\rangle$ where $E' = E'(J')$ from Eq. (4.42). Recall $J|J'\rangle = J'|J'\rangle$.

Using the wavefunctions, $\langle q'|E'\rangle$ and $\langle q'|J'\rangle$, we define the operators, $J(E)$ and $H(J)$, as:

$$\langle q'|J(E)|E'\rangle \equiv J'(E')\langle q'|E'\rangle \tag{4.41}$$

$$\langle q'|H(J)|J'\rangle \equiv E'(J')\langle q'|J'\rangle \quad . \tag{4.42}$$

J(E) or simply J is the action-angle operator and H(J) is the Hamiltonian operator written in terms of the operator J. Since H(J) is independent of w, the coordinate conjugate to J, a Hamilton-Jacobi transformation has been effected, using the operator J.

Using the well-ordered operator function $W_0(q,E)$ the well-ordered operator W(q,J) is defined using Eq. (4.42) as (see Eq. (4.15)):

$$W_0(q,\ E=H(J)) = g(q)h(H(J)) \tag{4.43}$$

$$= W(q,J) \tag{4.44}$$

Since each occurrence of E is to the right of q in W_0, each J will be to the right of every q, causing W(q,J) to be a well-ordered operator function. For the sake of this discussion, using Eq. (4.43), we rewrite W as:

$$W(q,J) = g(q)\ k(J) \tag{4.45}$$

where a more general well-ordered form as in Eq. (4.8) is allowed (and implied).

We can now find the operator w. By analogy to the classical theory and the definition of p, we define the canonically conjugate operator to J as:

$$w \equiv \frac{\partial W(q,J)}{\partial J} \tag{4.46}$$

or using Eq. (4.45):

$$w = g(q)\ \frac{\partial k(J)}{\partial J} \quad . \tag{4.47}$$

With wavefunctions of the form $\langle q'|J'\rangle$ the eigenvalue function $w^*(q',J')$ is defined as:

$$\langle q'|w|J'\rangle \equiv w^*(q',J')\langle q'|J'\rangle \quad , \tag{4.48}$$

$$= g(q')\frac{\partial k(J')}{\partial J'}\langle q'|J'\rangle \quad , \tag{4.49}$$

so

$$w^*(q',J') \equiv g(q')\frac{\partial k(J')}{\partial J'} \quad . \tag{4.50}$$

Earlier we defined p as $p \equiv \partial W_0(q,E)/\partial q$. Since $W_0(q,E) = W(q,J)$, we can update our definition with

$$p \equiv \frac{\partial W_0(q,E)}{\partial q} = \frac{\partial W(q,J)}{\partial q} = \frac{\partial g(q)}{\partial q}k(J) \quad . \tag{4.51}$$

Using wavefunctions of the type $\langle q'|J'\rangle$ we can also find $p_j^*(q',J')$ using W(q,J) from Eq. (4.45):

$$\langle q'|p|J'\rangle = \left\langle q' \left| \frac{\partial g(q)}{\partial q}k(J) \right| J'\right\rangle \quad ,$$

$$= \frac{\partial g(q')}{\partial q'}k(J')\langle q'|J'\rangle \quad ,$$

$$\equiv p_j^*(q',J')\langle q'|J'\rangle \quad . \tag{4.52}$$

where

$$p_j^*(q',J') \equiv \frac{\partial g(q')}{\partial q'}k(J') \quad .$$

The earlier $p^*(q',E')$ is equal to $p_j^*(q',J')$ using $E' = E'(J')$ or $J' = J'(E')$. Thus both p and w are defined using W(q,J) in the same

way as p_c and w_c are defined using $W_c(q_c,J_c)$. This parallel construction gives us confidence that the quantities, p and w, have been defined in a reasonable way.

One way to increase our confidence in J and w is to verify that they have the proper commutation relation. If J and w are a canonically conjugate coordinate and momentum, they have commutator $\hbar/i$. This can be shown using the same method that we used for p and q. The commutator of w and J is calculated using the $\langle q'|J'\rangle$ wavefunction (4.40), provided that it satisfies suitable boundary conditions (as given in Dirac (4)). For acceptable states we have:

$$\left\langle q' \left| -\frac{\hbar}{i}\frac{\partial}{\partial J} \right| J' \right\rangle = \frac{\hbar}{i}\frac{\partial}{\partial J'}\langle q'|J'\rangle \quad . \tag{4.53}$$

Using the exponential form of the wavefunction, $\exp[(i/\hbar)W(q',J)]$, Eq. (4.53) becomes

$$\left\langle q' \left| -\frac{\hbar}{i}\frac{\partial}{\partial J} \right| J' \right\rangle = \frac{\partial W(q',J')}{\partial J'}\langle q'|J'\rangle \quad . \tag{4.54}$$

Using $W(q',J') = g(q')k(J')$, Eq. (4.54) is:

$$\left\langle q' \left| -\frac{\hbar}{i}\frac{\partial}{\partial J} \right| J' \right\rangle = g(q')\frac{\partial k(J')}{\partial J'}\langle q'|J'\rangle \quad . \tag{4.55}$$

Since right hand sides of Eqs. (4.49) and (4.55) (which gives $\langle q'|w|J'\rangle$) are equal, we equate the operators:

$$w = -\frac{\hbar}{i}\frac{\partial}{\partial J} \quad . \tag{4.56}$$

Using Eq. (4.55) we quickly verify that:

$$[J,w] = Jw - wJ = \frac{\hbar}{i} \quad . \tag{4.57}$$

Thus, J and w have the proper commutation relation and we conclude they are canonically conjugate.

We also note that (23)

$$[J,\ e^{-2\pi i(\hbar/i\ \partial/\partial J)}] = [J,\ e^{2\pi i w}]$$

$$= J \sum_{n=0}^{\infty} \frac{1}{n!} (-2\pi\hbar \frac{\partial}{\partial J})^n - \sum_{n=0}^{\infty} \frac{1}{n!} (-2\pi\hbar \frac{\partial}{\partial J})^n J$$

$$= - \sum_{n=1}^{\infty} \frac{1}{(n-1)!} (-2\pi\hbar \frac{\partial}{\partial J})^{n-1}$$

$$= 2\pi\hbar\ e^{-2\pi i(\hbar/i\ \partial/\partial J)}$$

$$= 2\pi\hbar\ e^{2\pi i w} \quad .$$

This commutator will be more useful than Eq. (4.57) because of the difficulties defining angle variables mentioned earlier (9).

In addition, for states satisfying suitable boundary conditions, $(-\hbar/i)\partial/\partial J$ is Hermitian and since w is equal to this operator w is Hermitian.

We have argued earlier that $p^*(q',E')$, $W_0(q',E')$ and $J'(E')$ all have correct classical limits. From these limits we conclude that $W(q',J'(E')) = W_0(q',E')$ has the correct classical limit. In addition, we conclude that $E'(J')$ and $w' = w^*(q',J')$ have correct limits since they are derived from objects having correct classical limits in the same way as the classical derivation is done.

In order to aid in the interpretation of w as the quantum analogue of the classical angle variable, we calculate the change in $w^*(q',J')$

around the contour D which is used to define J'(E'). We interpret this as the quantum analogue of the classical calculation which shows that the change in w_c around one cycle of the classical motion is one. Specifically, we calculate:

$$\Delta w^* = \int_D dq' \frac{\partial w^*}{\partial q'} \quad ,$$

and using Eqs. (4.48)-(4.50)

$$= \int_D dq' \frac{\partial}{\partial q'} \frac{\partial W(q',J')}{\partial J'} \quad . \tag{4.58}$$

Now, using $W(q',J') = g(q')k(J')$, Eq. (4.58) becomes:

$$\Delta w^* = \int_D dq' \frac{\partial g(q')}{\partial q'} \frac{\partial k(J')}{\partial J'} \tag{4.59}$$

$$= \frac{\partial}{\partial J'} \int_D dq' \frac{\partial g(q')}{\partial q'} k(J') \quad . \tag{4.60}$$

Using the definition of $p^*(q',J')$ and the fact that $p_j^*(q',J') = p^*(q',E')$ we have:

$$\Delta w^* = \frac{\partial}{\partial J'} \int_D dq' \, p^*(q',E') \quad . \tag{4.61}$$

From the definition of J' we have:

$$\Delta w^* = \frac{\partial}{\partial J'} J' \tag{4.62}$$

or

$$\Delta w^* = 1 \quad . \tag{4.63}$$

Equation (4.63) is interpreted as the total change in $w^*(q',J')$ around the contour D. Classically, the change in w_c around the classical contour is one, leading to the conclusion that the system is unchanged when w_c is increased by one. Quantum mechanically, we interpret $\Delta w^* = 1$, Eq. (4.63), as motivating an interpretation of $w^*(q',J')$ in which the wavefunction which describes the system is unchanged when $w^*(q',J')$ increases by one. Let us define $w' \equiv w^*(q',J')$ and introduce the bra $\langle w'|$. For an allowed state of the system we interpret $\Delta w^* = 1$ as motivating the following boundary condition.

$$\langle w'|J'\rangle = \langle w' + 1|J'\rangle \quad . \tag{4.65}$$

Equation (4.65) is the statement of the boundary condition which we impose on the wavefunctions $\langle w'|J'\rangle$. It states that these wavefunctions are periodic in w' with period one. This relation is basic to quantum action-angle variables.

For periodic wavefunctions we have (4):

$$\langle w' \left| \frac{\hbar}{i} \frac{\partial}{\partial w} \right| J'\rangle = \frac{\hbar}{i} \frac{\partial}{\partial w'} \langle w'|J'\rangle \quad . \tag{4.66}$$

The operator $(\hbar/i)\partial/\partial w$ is Hermitian (4) and may be related to the operator, J, providing J is Hermitian. (J will be Hermitian if J'(E') is real.) Thus, when J is Hermitian, for a proper choice of the phase for $\langle w'|$ (4), we have:

$$J = \frac{\hbar}{i} \frac{\partial}{\partial w} \quad . \tag{4.67}$$

Expression (4.67) is the Schrödinger representation for J clearly this J is canonically conjugate to w. Having the boundary condition on the

wavefunction and J in this form, we may now calculate the wavefunctions $\langle w'|J'\rangle$, and find the possible eigenvalues J'.

The eigenvalues and eigenfunctions of J are found by calculating $\langle w'|J|J'\rangle$:

$$\langle w'|J|J'\rangle = J'\langle w'|J'\rangle \quad . \tag{4.68}$$

Combining Eqs. (4.66), (4.67) and (4.68) we find:

$$\frac{h}{i}\frac{\partial}{\partial w'}\langle w'|J'\rangle = J'\langle w'|J'\rangle \quad . \tag{4.69}$$

The solution of Eq. (4.69) is:

$$\langle w'|J'\rangle = A\, e^{i/\hbar\, J'w'} \quad . \tag{4.70}$$

Equation (4.70) will satisfy the boundary condition (4.65) if and only if:

$$J' = 2\pi\hbar n \quad , \quad n \in \{0,\pm 1,\pm 2, \ldots\} \quad . \tag{4.71}$$

These results, Eqs. (4.70) and (4.71), are general and apply to all systems having J Hermitian. Equation (4.71) gives the possible values of J'. Some of these values of J' may not be consistent with the definition of J', Eq. (4.39), and hence must be excluded for a given system under consideration. Such decisions limiting the allowed values of J' must be made on a case by case basis.

An advantage in using action-angle variables is that if the integral defining J' = J'(E') (where E' is an eigenvalue of energy) can be evaluated, and if J' = J'(E') can be inverted to give E' = E'(J'), then the quantum energy levels of the system are given by:

$$E' = E'(J')$$

$$= E'(2\pi\hbar n) \quad , \quad n \in \{0,\pm1,\pm2, \ldots\} \quad . \tag{4.72}$$

Thus, the energy levels of the system are given by inspection once J'(E') and E'(J') have been found. Equation (4.72) gives the energy levels of the system. If any of the values of n are inconsistent with the definition of J'(E'), Eq. (4.39), they must be excluded for the system under consideration. (This limitation will occur, e.g., in the Coulomb problem which we will treat in Chapter V. In the Coulomb case the allowed values are $n_r = 0,1,2, \ldots$.)

Having found the eigenfunctions and eigenvalues of J, we now conclude our formal presentation of quantum action-angle variables. In Chapter V we will apply these concepts to the rotor, harmonic oscillator and Coulomb problems. We now list the relevant equations:

Wavefunction: $\langle q'|E'\rangle = e^{iW_0(q',E')/\hbar}$

Hamiltonian: $p^2 + V(q) = H$

Hamilton-Jacobi eigenvalue equation:

$$\frac{\hbar}{i}\frac{\partial^2 W_0(q',E')}{\partial q'} + \left(\frac{\partial W_0(q',E')}{\partial q'}\right)^2 + V(q') = E'$$

Definitions of $p^*(q',E')$ and p: $p^*(q',E') = \dfrac{\partial W_0(q',E')}{\partial q'}$

$$p = \frac{\partial W_0(q,E)}{\partial q}$$

Ricatti equation for $p^*(q',E')$:

$$\frac{\hbar}{i}\frac{\partial p^*(q',E')}{\partial q'} + p^*(q',E')^2 + V(q') = E'$$

Definition of J': $J' = J'(E') = \int_D p^*(q',E')dq'$

Hamiltonian in J: $J' = J'(E') \rightarrow E' = E'(J')$

$$\langle q'|H|E'\rangle = E'\langle q'|E'\rangle$$

$$\langle q'|H(J)|J'\rangle = E'(J')\langle q'|J'\rangle$$

Definition of W(q,J) and W(q',J'): $W(q',J') = W_0(q',E'(J'))$

$$W(q,J) = W_0(q,H(J))$$

Definition of w, p, $w^*(q',J')$, and $p^*(q',J')$

$$w = \frac{\partial W(q,J)}{\partial J}$$

$$w^*(q',J') = \frac{\partial W(q',J')}{\partial J'} \qquad (\text{where } w^*(q',J') \equiv w')$$

$$p = \frac{\partial W(q,J)}{\partial q} = \frac{\partial W_0(q',E')}{\partial q}$$

$$p^*(q',J') = \frac{\partial W(q',J')}{\partial q'} = \frac{\partial W(q',E')}{\partial q'}$$

Wavefunction and boundary condition: $\langle w'|J'\rangle = e^{iJ'w'/\hbar}$

$$\langle w'+1|J'\rangle = \langle w'|J'\rangle$$

Possible eigenvalues of J': $J' = 2\pi\hbar n \quad , \quad n \in \{\ldots, -1,0,1,2, \ldots\}$

Possible energy levels of H(J):

$$E'_n = E(J') \qquad \text{where } J' = 2\pi\hbar n \text{ as above}$$

Commutation relations: $[p,q] = \hbar/i$

$$[J, e^{i2\pi w}] = 2\pi\hbar\, e^{i2\pi w}$$

Hermitian operators: p, q, J, w

where q and J are Hermitian by assumption

Classical limits: $W_0(q',E') \to W_0(q_c,E_c)$

$$p^*(q',E') \to p_c(q_c,E_c)$$

$$J' \to J_c$$

$$q' \to q_c \quad \text{by assumption}$$

$$W(q',J') \to W_c(q_c,J_c)$$

$$w' \to w_c$$

$$E'(J') \to E_c(J_c) = H_c$$

If one glances through the above set of expressions, one sees that the objects which we have defined have correct classical limits, and commutation relations. The basic variables are Hermitian. The wavefunction, $\langle w'|J'\rangle$, has the correct boundary condition and the Hamiltonian, H(J), is independent of w. We have in the context of this theory satisfied conditions A through E and have satisfied the essence of condition F (invariance of matrix elements under $w' \to w' + 1$). Thus,

the theory satisfies the basic requirements that we earlier imposed on a set of quantum transformation equations. We conclude that this canonical transformation theory is reasonable.

In the next chapter, we will apply these theoretical constructs to three problems. The rotor will provide an exercise in the formalism, and the harmonic oscillator and Coulomb problems will demonstrate the power of action-angle variables to find energy levels. These examples will reaffirm our assertion that the quantum action-angle variables have been defined in a reasonable way.

V. THREE APPLICATIONS OF THE GENERAL THEORY

In the last chapter a quantum transformation theory was developed, and action-angle variables were defined quantum mechanically. In this chapter we will apply our transformation theory to three systems, the rotor, the harmonic oscillator, and the Coulomb problem. The rotor is a simple example which will provide an exercise in using these transformation techniques, and the harmonic oscillator and Coulomb problems will demonstrate the power of these variables in finding energy levels. We will follow the general procedure of the last chapter.

A. Rotor Revisited

The method of defining quantum mechanical action-angle variables, J and w, developed in the last chapter can be applied to the rotor which we discussed earlier in Chapter III. For the rotor it will be possible to find simple expressions for all relevant quantities: J, w, p^*, p, W_0, W and H(J).

We begin by remembering that Schrödinger's equation for the rotor is (see Eq. (3.3) or Eq. (3.8)):

$$\left(\frac{\hbar}{i}\frac{\partial}{\partial\phi'}\right)^2 \langle\phi'|E'\rangle = E'\langle\phi'|E'\rangle \quad . \tag{5.1}$$

Relating W_0 to the wavefunction in the usual way:

$$\langle\phi'|E'\rangle = e^{iW_0(\phi',E')/\hbar} \quad , \tag{5.2}$$

we obtain the quantum Hamilton-Jacobi eigenvalue equation:

$$\frac{\hbar}{i}\frac{\partial^2 W_0}{\partial \phi'^2} + \left(\frac{\partial W_0}{\partial \phi'}\right)^2 = E' \quad . \tag{5.3}$$

Defining $p^*(\phi',E')$ as:

$$p^*(\phi',E') = \frac{\partial W_0(\phi',E')}{\partial \phi'} \quad . \tag{5.4}$$

Equation (5.3) becomes the appropriate Ricatti equation:

$$\frac{\hbar}{i}\frac{\partial p^*(\phi',E')}{\partial \phi'} + p^*(\phi',E')^2 = E' \quad . \tag{5.5}$$

Comparing Eq. (5.5) to the Ricatti equation (4.26), we see that f_q and $V(\phi')$ are both zero. Equation (5.5) is easily solved since a particular solution is:

$$p^* = \sqrt{E'} \equiv k \tag{5.6}$$

where we choose the positive square root for "$\sqrt{E'}$". In Chapter IV, we stated that once a particular solution to a Ricatti equation has been found the general solution follows (see Eqs. (4.31), (4.32) and (4.33)). Using the above particular solution, the general solution of the rotor is:

$$p^*(\phi',E') = k + \frac{2k\, e^{-2\frac{i}{\hbar}k\phi'}}{2kC - e^{-2\frac{i}{\hbar}k\phi'}} \tag{5.7}$$

where C is a constant (or more generally may be a function of E') which is chosen so that $p^*(\phi',E')$ satisfies a given boundary condition.

Note that $p^*(\phi',E')$ has poles where $C = (1/2\ k)\exp(-2ik\phi'/\hbar)$. This pole structure is illustrated in Figure 2.

The physical boundary condition which is imposed on the wavefunction, $\langle\phi'|E'\rangle$, is that it be periodic with a period of 2π. This boundary condition may be applied to $p^*(\phi',E')$ by noting (see Appendix C) that

$$p^*(\phi',E') = \frac{\hbar}{i}\frac{1}{\langle\phi'\ E'\rangle}\frac{\partial\langle\phi'|E'\rangle}{\partial\phi'} \quad . \tag{C.3}$$

From this form of $p^*(\phi',E')$ it follows that if the wavefunction is periodic, then $p^*(\phi',E')$ must also be periodic with a period of 2π. Applying this restriction to $p^*(\phi',E')$, Eq. (5.7), it follows that k must have the values $(\hbar m)/2$ where $m = 0,\pm1,\pm2, \ldots$, or a subset of these values.

After choosing values of C and E' (or k), the location of the poles of $p^*(\phi',E')$ are fixed. A path in the ϕ'-plane may be chosen on which to integrate $p^*(\phi',E')$ to yield $W_0(\phi',E')$. Integrating $p^*(\phi',E')$ from ϕ_0 to ϕ' one finds (24):

$$W_0(\phi',k,C) = k\phi' + \frac{\hbar}{i}\ln\left(2kC - e^{-2\frac{i}{\hbar}k\phi'}\right) + C_0 \quad . \tag{5.8}$$

Using Eq. (5.8) with the exponential form of the wavefunction, Eq. (5.2), $\langle\phi'|E'\rangle$ have been found, with:

$$\langle\phi'|E'\rangle = e^{\frac{i}{\hbar}C_0}\left(2kC\ e^{\frac{i}{\hbar}k\phi'} - e^{-\frac{i}{\hbar}k\phi'}\right) \quad . \tag{5.9}$$

The reader may verify that these wavefunctions satisfy Schrödinger's equation (5.1) and that $W_0(\phi',k,C)$ satisfies the Hamilton-Jacobi eigenvalue equation (5.3).

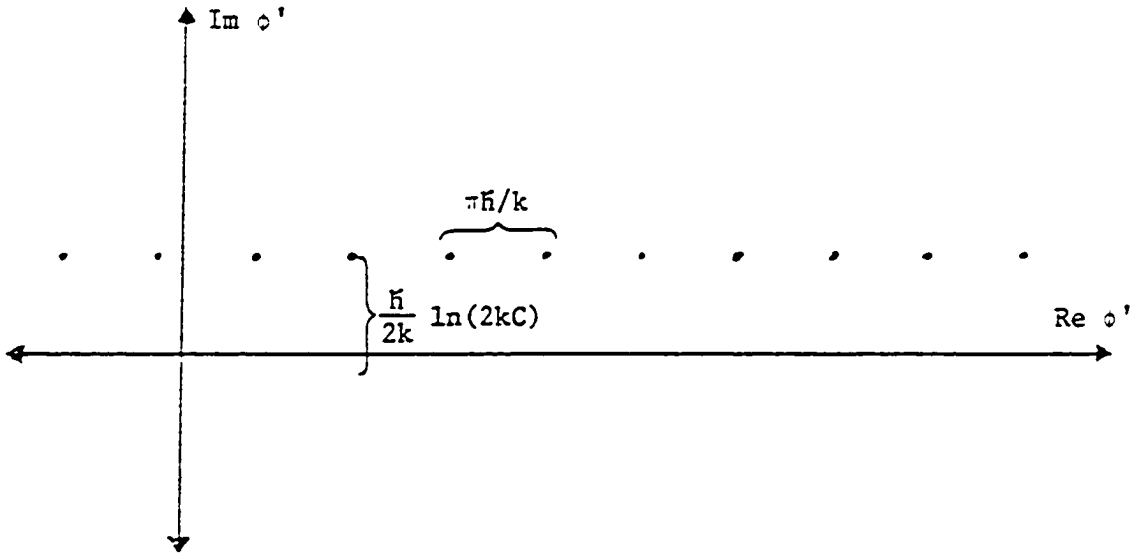

Figure 2. φ'-plane poles of $p^{*}(\varphi',E')$, Eq. (5.7), for k real and C real

Since the rotor is a simple problem, we could now impose a boundary condition on the wavefunction and find the energy eigenvalues. However, since our purpose is to use our action-angle formalism, we instead define J'_ϕ (or $J'_\phi(E')$) which will be used to find the energy eigenvalues. Before defining J'_ϕ, we review the definition of the classical J_c for this problem.

Classically, J_c is defined as the integral of $p_c(\phi_c,E_c)$ from 0 to 2π:

$$J_c \equiv \int_0^{2\pi} p_c(\phi_c,E_c)d\phi_c \quad . \tag{5.10}$$

The integral from 0 to 2π is interpreted as an integral over one cycle of the ϕ_c-motion, since the configuration of the physical system is considered to be the same when ϕ_c is 0 or ϕ_c is 2π. Quantum mechanically we define J'_ϕ in an analogous manner.

We define J'_ϕ as the integral of $p^*(\phi',E')$ from 0 to 2π:

$$J'_\phi \equiv \int_0^{2\pi} p^*(\phi',E')d\phi' \quad . \tag{5.11}$$

This integral is again considered to be an integral over one cycle of the physical motion as in the classical case. Using $p^*(\phi',E')$ as given in Eq. (5.7), J'_ϕ is:

$$J'_\phi = \int_0^{2\pi} \left\{ k + \frac{2k\, e^{-2\frac{i}{\hbar}k\phi'}}{2kC - e^{-2\frac{i}{\hbar}k\phi'}} \right\} d\phi'$$

$$= [W_o(\phi',k,C)]_0^{2\pi} \quad ,$$

where $W_0(\phi',k,C)$ is given by Eq. (5.8). As noted earlier, k has the values $m\hbar/2$, $m = 0,\pm1,\pm2, \ldots$, or a subset of these values. Using these values of k in Eq. (5.8) for W_0 yields

$$J'_\phi = [W_0(\phi',k,C)]_0^{2\pi} = 2\pi k = 2\pi\sqrt{E'} \quad . \tag{5.12}$$

Thus,

$$E' = \left(\frac{J'_\phi}{2\pi}\right)^2 \quad . \tag{5.13}$$

Note that Eqs. (5.12) and (5.13) are independent of the constant C which determines the initial conditions of the motion.

In Chapter IV, the general theory for action-angle variables states that the possible values of J' at an eigenstate of the system are:

$$J' = 2\pi\hbar m \quad , \quad m = 0,\pm1,\pm2, \ldots \quad . \tag{5.14}$$

Equating these values of J' with J'_ϕ as given in Eq. (5.12) we find:

$$2\pi\hbar m = 2\pi\sqrt{E'} = 2\pi k \tag{5.15}$$

where we restrict m to nonnegative values because "$\sqrt{E'}$" has been chosen to be positive. Thus, the eigenvalues of E' are:

$$E'_m = (\hbar m)^2 \quad , \quad m = 0, 1, 2, \ldots \quad . \tag{5.16}$$

We may check that the energy eigenstates (5.16) are reasonable by noticing that for k as given in Eq. (5.15), the wavefunction $\langle\phi'|E'\rangle$,

Eq. (5.9), satisfies the boundary condition:

$$\langle\phi'|E'\rangle = \langle\phi' + 2\pi|E'\rangle \quad . \tag{5.17}$$

Thus, our eigenstates do not lead to an inconsistency with regard to the wavefunction $\langle\phi'|E'\rangle$.

Having found the eigenvalues of energy, J'_ϕ at the eigenstates and $W_0(\phi',k,C)$, we will now find $W(\phi',J'_\phi,C)$, the function $\langle\phi'|J'_\phi\rangle$ and the Hamiltonian $H(J_\phi)$. We will follow the procedure of Chapter IV. Using $W_0(\phi',k,C)$, Eq. (5.8), and $E'(J'_\phi)$, $W(\phi',J'_\phi)$ is given by:

$$W(\phi',J',C) = \frac{J'_\phi}{2\pi}\,\phi' + \frac{\hbar}{i}\ln\left(\frac{J'_\phi}{\pi}C - e^{-2\frac{i}{\hbar}\frac{J'_\phi}{2}\phi'}\right) + C_0 \quad . \tag{5.18}$$

$E'(J'_\phi)$ and Eq. (5.18) furnish the connection between states of the form $\langle\phi'|E'\rangle$ and $\langle\phi'|J'_\phi\rangle$:

$$\langle\phi'|E' = \left(\frac{J'_\phi}{2\pi}\right)^2\rangle = e^{\frac{i}{\hbar}W_0(\phi',\, E' = (\frac{J'_\phi}{2\pi})^2,\, C)} \quad ,$$

$$= e^{\frac{i}{\hbar}W(\phi',J'_\phi,C)} \quad ,$$

$$= \langle\phi'|J'_\phi\rangle \quad . \tag{5.19}$$

Using states of the form $\langle\phi'|J'_\phi\rangle$ the Hamiltonian, $H(J_\phi)$, is defined from $E'(J'_\phi)$:

$$\langle\phi'|H(J_\phi)|J'_\phi\rangle = E'(J'_\phi)\langle\phi'|J'_\phi\rangle \quad ,$$

$$= \left(\frac{J'_\phi}{2\pi}\right)^2\langle\phi'|J'_\phi\rangle \quad . \tag{5.20}$$

From Eq. (5.20) it follows that:

$$H(J_\phi) = \left(\frac{J_\phi}{2\pi} \right)^2 \quad . \tag{5.21}$$

The energy levels of Eq. (5.21) are, of course, given by $E'(J'_\phi)$ in Eq. (5.15), using the values of J' given in Eq. (5.14).

In order to find the operator, w, the well-ordered operator function $W(\phi,J_\phi)$ must be found. This is done by expanding $W(\phi',J'_\phi,C)$, Eq. (5.18), about a regular point $\phi' = \phi_0$:

$$W(\phi',J'_\phi,C) = \phi' \frac{J'_\phi}{2\pi} + \frac{\hbar}{i} \sum_{\ell=0}^{\infty} \frac{(\phi'-\phi_0)^\ell}{\ell!} \frac{d^\ell}{d\phi'^\ell} \ln\left(\frac{J'_\phi}{\pi} C - e^{-2 \frac{i}{\hbar} \frac{J'_\phi}{2\pi} \phi'} \right)\Bigg|_{\phi'=\phi_0} + C_0 \quad . \tag{5.22}$$

If in Eq. (5.22) we demand that in any term all ϕ' appear to the left of all J'_ϕ, then the operator function is found by replacing each ϕ' by ϕ and J'_φ by J_ϕ since for each term we have:

$$\langle \phi' | f(\phi) g(J_\phi) | J' \rangle = f(\phi') g(J') \langle \phi' | J' \rangle \quad . \tag{5.23}$$

Using this device, Eq. (5.22) produces the operator function:

$$W(\phi,J_\phi,C) = \frac{J_\phi}{2\pi} + \frac{\hbar}{i} \sum_{\ell=0}^{\infty} \frac{(\phi-\phi_0)^\ell}{\ell!} \frac{d^\ell}{d\phi'^\ell} \ln\left(\frac{J_\phi}{\pi} C - e^{-2 \frac{i}{\hbar} \frac{J_\phi}{2} \phi'} \right)\Bigg|_{\phi'=\phi_0} + C_0 \quad . \tag{5.24}$$

From Eq. (5.24) and the definitions of p_ϕ and w given in Chapter IV we have:

$$w = \frac{\partial W(\phi, J_\phi, C)}{\partial J_\phi} \quad , \tag{5.25}$$

$$p_\phi = \frac{\partial W(\phi, J_\phi, C)}{\partial \phi} \quad . \tag{5.26}$$

As a more concrete example, let us choose $C = -1/2k = -\pi/J'_\phi$. For this choice, $W(\phi', J'_\phi, C)$ becomes after simplification:

$$W(\phi', J'_\phi, C) = \frac{\hbar}{i} \ln[\cos\left(\frac{\phi}{2\pi\hbar} J'_\phi \phi'\right)] + C_1 \quad . \tag{5.27}$$

where $C_1 = C_0 + \ln(-2)$. In the sense of the well-ordered series (5.24), the operator functions may be written as:

$$W(\phi, J_\phi, C) = \frac{\hbar}{i} \overset{\cdot\cdot}{\ln}[\cos\left(\frac{\phi}{2\pi\hbar} J_\phi\right)]^{\cdot\cdot} + C_1 \quad . \tag{5.28}$$

From the definitions of p_ϕ and w we have:

$$p_\phi = -\frac{\hbar}{i} \overset{\cdot\cdot}{\tan}\left(\frac{\phi}{2\pi\hbar} J_\phi\right) \frac{J_\phi}{2\pi\hbar} \quad , \tag{5.29}$$

$$w = -\frac{\hbar}{i} \frac{\phi}{2\pi\hbar} \overset{\cdot\cdot}{\tan}\left(\frac{\phi}{2\pi\hbar} J_\phi\right) \quad . \tag{5.30}$$

Using the exponential forms of the wavefunction in terms of $W_0(\phi', J'_\phi, C)$ and $W(\phi', J'_\phi, C)$, we have for the above choice of C the following wavefunctions:

$$\langle \phi' | J' \rangle = e^{C_1} \cos\left\{\frac{\phi' J'_\phi}{2\pi\hbar}\right\} \quad , \tag{5.31}$$

$$\langle \phi' | E' \rangle = e^{C_1} \cos\left\{\frac{\phi'}{\hbar} \sqrt{E'}\right\} \quad . \tag{5.32}$$

These wavefunctions and the operators, $W(\phi,J_\phi,C)$, p_ϕ and w depend on the above choice of C.

As a second example, if one evaluates the integrals defining $W(\phi',J'_\phi,C)$ and J'_ϕ as functions of C and then takes the limit of C going to zero, the operator functions and wavefunctions take on familiar forms:

$$W(\phi',J'_\phi,C) = \frac{1}{2\pi}\,\phi'\,J'_\phi + C_1 \quad , \tag{5.33}$$

$$W(\phi,J_\phi,C) = \frac{\phi J_\phi}{2\pi} \quad , \tag{5.34}$$

$$p_\phi = \frac{J_\phi}{2\pi} \quad , \tag{5.35}$$

$$w = \frac{\phi}{2\pi} \quad , \tag{5.36}$$

$$\langle\phi'|J'\rangle = e^{C_1}\, e^{\frac{i}{2\pi\hbar}\,\phi'\,J'_\phi} \quad , \tag{5.37}$$

$$\langle\phi'|E'\rangle = e^{C_1}\, e^{\frac{i}{\hbar}\,\phi'\sqrt{E'}} \quad . \tag{5.38}$$

Comparing the operators $W(\phi,J_\phi,C)$, p_ϕ and w for these two choices of the constant C, one sees that the operator functions depend on the choice of C (the boundary condition) with which they were obtained. Since the procedure involves finding $W(\phi',J'_\phi)$ and then using it to find $W(\phi,J_\phi)$, p_ϕ and w, this will be a general feature of all problems treated using these techniques.

While the rotor may be treated by traditional methods, it also provides a simple application of the full action-angle variable formalism. Its simplicity does however obscure the power of action-angle variables. The power of action-angle variables to find energy levels of systems is demonstrated for the harmonic oscillator and Coulomb problems in the next sections.

B. Harmonic Oscillator Revisited

The rotor has provided a fairly complete illustration of the application of the methods of Chapter IV. An example which shows how action-angle variables can be used to find quickly and easily the energy levels of a system is the harmonic oscillator. We now apply the methods of Chapter IV to find $J'(E')$ for the harmonic oscillator at eigenstates of the system. Having found $J'(E')$, the energy levels $E_n'(J')$ of the system follow immediately.

We begin our discussion of the harmonic oscillator by giving the appropriate Ricatti equation. From Eq. (4.22) with $V(q') = \frac{1}{4}\omega^2 x'^2$, the Ricatti equation which defines $p^*(x',E')$ is:

$$\frac{\hbar}{i} p_x^* + p^{*2} + \frac{1}{4}\omega^2 x'^2 = E' \tag{5.39}$$

where

$$p_x^* = \frac{\partial}{\partial x'}(p^*(x',E')) \quad .$$

Equation (5.39) defines $p^*(x',E')$ which will be used to define $J'(E')$.

Before defining $J'(E')$, some properties of $p^*(x',E')$ are worth discussing. First, in the finite x'-plane the solution $p^*(x',E')$ of

Eq. (5.39) has no branch points. $p^*(x',E')$ may have poles in the finite x'-plane whose locations depend on ω, E' and the initial conditions imposed on $p^*(x',E')$. By studying the truncated equation $(\hbar/i)p_x^* + p^{*2} = 0$, one observes that the residue of each pole of $p^*(x',E')$ in the finite x'-plane is $\hbar/i$. At an eigenstate of the system (see Appendix C), $p^*(x',E')$ has poles on the real axis between the classical turning points ($x' = \pm(4E'/\omega^2)^{1/2}$). $p^*(x',E')$ also has a pole at infinity. There are no other singularities of $p^*(x',E')$ at an eigenstate of the system. Finally, as discussed in Chapter IV, Section C, at an eigenstate of the system, $p^*(x',E')$ is positive imaginary for $x' \to +\infty$ (x' real) and $p^*(x',E')$ is negative imaginary for $x' \to -\infty$ (x' real). These general features of $p^*(x',E')$ will be used when we evaluate the contour integral which defines J'(E') at an eigenstate of the system.

Consistent with Chapter IV, Section C, we define J'(E') as a contour integral:

$$J'(E') \equiv \int_C p^*(x',E')dx' \quad , \tag{5.40}$$

where the direction of integration is taken to be counterclockwise, and where the contour C is identical to the classical contour. Specifically, C encloses the classical turning points ($x' = \pm(4E/\omega^2)^{1/2}$) and the real axis between them. $p^*(x',E')$ is the solution of the Ricatti equation (5.39). We now evaluate the integral, Eq. (5.40).

As discussed earlier and in Appendix C, at an eigenstate of the harmonic oscillator, the only singularities of $p^*(x',E')$ are on the real axis between the classical turning points and at $x' = \pm\infty$. In our

evaluation of the integral, Eq. (5.40), we distort the contour and enclose the singularity of $p^*(x',E')$ at $x' = \pm\infty$.

In order to carry out this calculation we make the transformation, $x' = S^{-1}$. Under this transformation, the integral defining $J'(E')$ becomes:

$$J'(E') = \int_{C_S} - p^*(S,E') \frac{dS}{S^2} \tag{5.41}$$

where the integral around C_S is taken in the clockwise direction and where C_S encloses only the point $S = 0$ (which corresponds to $x' = \pm\infty$). Applying the Residue theorem to Eq. (5.41), $J'(E')$ becomes:

$$J'(E') = 2\pi i \, \text{Res}(p^*(S,E')/S^2)\Big|_{S=0} \quad . \tag{5.42}$$

In order to evaluate Eq. (5.42), we now need only find $p^*(S,E')$ at $S = 0$.

In order to find $p^*(S,E')$, we apply the transformation, $x' = S^{-1}$, to the Ricatti equation which defines $p^*(x',E')$. Under this transformation, the Ricatti equation (5.39) becomes:

$$\frac{\hbar}{i} p_S^* - \frac{p^{*2}}{S^2} = - \frac{E'}{S^2} + \frac{1}{4}\omega^2 \frac{1}{S^4} \tag{5.43}$$

where

$$p_S^* \equiv \frac{\partial}{\partial S} (p^*(S,E')) \quad .$$

A solution of Eq. (5.43) is:

$$p^*(S,E') = \frac{A}{S} + \sum_{n=0}^{\infty} b_n S^n \tag{5.44}$$

where

$$A = \frac{i\omega}{2}$$

$$b_0 = 0$$

$$b_1 = \left(- \frac{iE}{\omega} - \frac{\hbar}{2i} \right)$$

$$b_2 = 0$$

$$b_3 = - \frac{1}{2A} \left(b_1^2 - \frac{\hbar}{i} b_1 \right)$$

$$b_j = - \frac{1}{2A} \left[- \frac{\hbar}{i} (j-2) b_{j-2} + \sum_{\ell=0}^{j-1} b_\ell \, b_{(j-\ell-1)} \right] \quad , \quad j \geq 3 \quad .$$

Earlier it was stated that at an eigenstate of the system $p^*(x',E')$ is positive imaginary for $x' \to +\infty$ (x' real) and $p^*(x',E')$ is negative imaginary for $x' \to -\infty$ (x' real). As applied to $p^*(S,E')$, this means that for $|S| \to 0$ (S real), $p^*(S,E')$ must be positive imaginary for S positive and negative imaginary for S negative. By Eq. (5.44), in the neighborhood of $S = 0$, $p^*(S,E') \approx i\omega/S$. For ω real and positive, this boundary condition is clearly satisfied and $p^*(S,E')$ is the solution of the Ricatti equation near $S = 0$ at an eigenstate of the system. [Note that other solutions of Eq. (5.43) exist. For example, one could have $A = -i\omega/S$, but such a solution fails to satisfy the physical boundary condition imposed on $p^*(S,E')$ at an eigenstate of the system.]

Having found the appropriate form of $p^*(S,E')$ near $S = 0$, we can return to the problem of evaluating the integral defining $J'(E')$, Eq. (5.40). The residue of $p^*(S,E')/S^2$ at $S = 0$ is:

$$\text{Res}(p^*(S,E')/S^2)\Big|_{S=0} = -\frac{iE}{\omega} - \frac{\hbar}{2i} \quad . \tag{5.45}$$

Using this residue with $J'(E')$ as given by Eq. (5.42) we have:

$$J'(E') = 2\pi i \, \text{Res}(p^*(S,E')/S^2)\Big|_{S=0}$$

$$= + 2\pi \left\{ \frac{E'}{\omega} - \frac{\hbar}{2} \right\} \quad . \tag{5.46}$$

At an eigenstate of the system we have evaluated the integral defining $J'(E')$. From the general theory of Chapter IV we have:

$$J' = 2\pi\hbar n \quad , \quad n = 0,\pm1,\pm2, \ldots \quad . \tag{5.47}$$

Equating $2\pi\hbar n$ with $J'(E')$ as given in Eq. (5.46), we have:

$$2\pi\hbar n = 2\pi \left\{ \frac{E'}{\omega} - \frac{\hbar}{2} \right\} \quad , \tag{5.48}$$

Thus,

$$E'_n = \frac{2\pi\hbar}{\omega} (n + 1/2) \quad , \quad n = 0, 1, 2, \ldots \tag{5.49}$$

where n is restricted to non-negative values so that E'_n will be positive (see below Eqs. (5.52), (5.53), and Ref. 17). From Eqs. (5.46)-(5.49), we have:

$$E' = \frac{1}{\omega} (J' + 1/2\ h) \quad . \tag{5.50}$$

Note that the energy levels, Eq. (5.40), are the same as those found in Chapter II, Eq. (2.66). Also, the classical limit of J'(E') is the same as that found in Chapter II, Eq. (2.65).

By evaluating the integral which defines J'(E'), we have found the energy levels of the system, Eq. (5.49). We must note that the contour distortion technique only is possible at an eigenstate of the system. When $p^*(x',E')$ does not satisfy the boundary conditions for an eigenstate, there are in general other poles in the x'-plane which will contribute to J'(E'). Only at an eigenstate is the pole structure simple, as discussed in Appendix C.

Before leaving the discussion of the evaluation of the integral, Eq. (5.40), which defines J'(E'), we note that this integral may be evaluated in another way which helps to illustrate why J'(E') is $2\pi\hbar n$. As discussed in Appendix C, $p^*(x',E')$ may be related to the wavefunction $\langle x'|E'\rangle$ by:

$$p^*(x',E') = \frac{\hbar}{i}\frac{1}{\langle x'|E'\rangle}\frac{d}{dx'}\langle x'|E'\rangle \quad . \tag{5.51}$$

From Eq. (5.51) it follows that a simple zero of the wavefunction corresponds to a simple pole of $p^*(x',E')$ with residue $\hbar/i$. As discussed in Appendix C, the wavefunction may have zeros on the real x'-axis between the classical turning points at an eigenstate. Associated with each of these zeros there is a pole of $p^*(x',E')$. Let us assume that there are n such poles of $p^*(x',E')$ located between the classical turning points. The contour C used to define J'(E') in Eq. (5.40) encloses these n poles and we can apply the Residue theorem

to evaluate the integral (5.40). We have:

$$J'(E') = \int_C p^*(x',E')dx'$$

$$= 2\pi i \sum_{\ell=1}^{n} \text{Res } p^*(x'=x'_\ell, E') \qquad (5.52)$$

$$= 2\pi\hbar n \quad , \quad n = 0, 1, 2, \ldots \qquad (5.53)$$

where the n poles are assumed to be at $x' = x'_1, x'_2, x'_3, \ldots, x'_n$.

Thus, the statement that $J'(E')$ is $2\pi\hbar n$ where $n = 0, 1, 2, \ldots$ is a statement that at an eigenstate of the harmonic oscillator the wavefunction has n zeros. $J'(E')$ is then an object which counts the zeros of the wavefunction (for the harmonic oscillator) and relates the number of zeros to the energy eigenvalue, E'.

At this point in the calculation, we could continue the process and find $W_0(q',E')$, $W_0(q,E)$, $W(q',J')$, $W(q,J)$, p, $p_j^*(q',J')$, w and $w^*(q',J')$. Such a calculation might be instructive and would duplicate other solutions of the harmonic oscillator (23). We, therefore, forego this process in order to point out that we have found the energy levels of the system without carrying out the full transformation to action-angle variables. For practical calculations, the advantage in using action-angle variables lies in the fact that certain information (energy levels) can be found without a full solution of the problem. The formalism guarantees that the quantities listed above may be found if desired. These quantities do not need to be found if one wishes to find the energy levels. We remark that the quantum process of finding the energy levels without solving the full problem is the exact

analogue of the process followed in classical action-angle variables where the system frequencies are found without solving the full motion.

We emphasize that if the singularity structure had been complicated, if the boundary conditions at the relevant singularities had been difficult to apply, or if the relevant residues had been energy (E') independent, the procedure which we employed might not have given the energy levels so easily. While the energy levels of a general potential might be difficult to find using action-angle variables, the procedure worked well for the harmonic oscillator. As we will see in the next section, this procedure also works well for finding the energy levels of the Coulomb problem.

C. Coulomb Potential

The harmonic oscillator and rotor have provided examples of problems in which the energy levels of systems can be found using action-angle variables (without necessarily finding the wavefunction $\langle q'|E'\rangle$). We now treat the radial Coulomb problem using the same techniques as were employed for the harmonic oscillator. We find the energy levels of the attractive Coulomb potential without solving Schrödinger's equation for the wavefunction $\langle q'|E'\rangle$.

We begin our treatment of the Coulomb problem by giving the appropriate Hamiltonian. We assume that the angular part of the Coulomb problem has been completed yielding the eigenvalues of L^2: $L^{2'} = \hbar^2 \ell(\ell+1)$ for $\ell = 0, 1, 2, \ldots$. With these values of $L^{2'}$, the radial attractive Coulomb Hamiltonian is: $(2m = 1)$

$$H(r,P_r) = \frac{1}{r^2} P_r r^2 P_r + \frac{\hbar^2 \ell(\ell+1)}{r^2} - \frac{g}{r} \quad . \tag{5.54}$$

Using the wavefunction in the exponential form:

$$\langle r'|E'\rangle = e^{\frac{i}{\hbar} W_0(r',E')} \quad . \tag{5.55}$$

A substitution is made into the Schrödinger's equation based on Eq. (5.54) in order to obtain the Hamilton-Jacobi eigenvalue equation:

$$\frac{\hbar}{i} W_{0rr} + \frac{2\hbar}{i} \frac{1}{r'} W_{0r} + W_{0r}^2 = E' - \frac{\hbar^2 \ell(\ell+1)}{r'^2} + \frac{g}{r'} \quad , \tag{5.56}$$

where $W_{0rr} \equiv \partial^2 W_0(r',E')/\partial r'^2$, and where $W_{0r} = \partial W_0(r',E')/\partial r'$. This equation for $W_0(r',E')$ will now be used to find the Ricatti equation for the quantum momentum eigenvalue function $p^*(r',E')$. Defining $p^*(r',E')$ as:

$$p^*(r',E') \equiv \frac{\partial W_0(r',E')}{\partial r'}$$

we have the Coulomb Ricatti equation:

$$\frac{\hbar}{i} \frac{\partial p^*(r',E')}{\partial r'} + \frac{2\hbar}{i} \frac{1}{r'} p^*(r',E') + p^*(r',E')^2 = E' - \frac{\hbar^2 \ell(\ell+1)}{r'^2} + \frac{g}{r'} \tag{5.57}$$

which has been obtained by substituting $p^*(r',E')$, into the Hamilton-Jacobi eigenvalue equation.

Before defining $J'(E')$ in terms of $p^*(r',E')$ two points need to be made about $p^*(r',E')$ which solves Eq. (5.57). First, (for E' real and negative) as discussed in Appendix C, at an eigenstate of the

system $p^*(r',E')$ has a pole at the origin, and may have poles on the real axis between the classical turning points (the points r_+ and r_- for which the right hand side of Eq. (5.57) is zero). Second, the poles in the classical region (between r_+ and r_-) each have residue $\hbar/i$. This is shown by studying Eq. (5.57) in the neighborhood of a pole where the right hand side of Eq. (5.57) can be neglected.

These considerations are important because at an eigenstate the quantum singularity structure is very similar to the classical structure. Classically, in the finite plane the momentum, $p_c(r_c,E_c)$, has a cut between the classical turning points and a pole at the origin. The action variable J is defined as the integral around a contour which encloses only the cut and is taken in a counterclockwise direction. The branch of $p_c(r_c,E_c)$ is chosen which is positive along the bottom of the cut (as in Figure 1). For this definition J_{rc} is positive. Normally, the integral is evaluated by distorting the contour so that it encloses only the point at infinity and the origin (3). The residue theorem is then applied to these two points. This is the method which we will use quantum mechanically.

Quantum mechanically we define J_r' for the Coulomb problem as the integral of $p^*(r',E')$ around a contour, D, (in a counterclockwise direction) which encloses the real line from one classical turning point to the other and which also encloses the turning points r_+ and r_- themselves. In order to evaluate this integral, we first assume that we are at an eigenstate of energy, E', (where E' is real and negative). Next, as in the harmonic oscillator, we assert that at

this eigenstate there are n poles on the real axis in the classical region. Each of these poles has residue $\hbar/i$ and by the residue theorem:

$$J_r' = \int_D p^*(r',E')dr' = 2\pi i \sum_{k=1}^{n} \text{Res}(p^*(r',E')) = 2\pi\hbar n \quad , \tag{5.58}$$

where n = 0, 1, 2, ... This is the same result as was obtained for the harmonic oscillator and may be interpreted as stating that there are n simple zeros of $\langle r'|E'\rangle$ between the classical turning points at a given eigenstate. Next we connect J_r' as given by Eq. (5.58) to the corresponding energy eigenvalue, E'. This is done by distorting the contour, D, in the same way as the contour is distorted in the classical problem (3).

As shown in Appendix C, the singularities at an eigenstate are in the classical region on the real axis, at the origin and possibly at infinity (which we investigate below). Thus, the distorted contour will enclose the singularity at the origin and the point at infinity. This distorted contour is equivalent to two individual contours which enclose the origin and the point at infinity providing that the integral is now taken in a clockwise direction.

The integrals which define J_r' in this way may be evaluated using the residue theorem once $p^*(r',E')$ has been found at r' = 0 and at r' = ∞. Calling the distorted contours D_0 and D_∞ the integrals which now define J_r' are:

$$J_r' = \int_D p^*(r',E')dr' = \int_{D_0} p^*(r',E')dr' + \int_{D_\infty} p^*(r',E')dr' \tag{5.59}$$

where the integrals around D_0 and D_∞ are now to be taken in a clockwise direction.

The integrals around D_0 and D_∞ can be evaluated using the residue theorem. The change of $r' = S^{-1}$ ($dr' = - S^{-2}\, dS$) is performed on the integral around D_∞ changing it to an integral around $S = 0$ on a contour D'_∞. With this change of variables J'_r in Eq. (5.59) becomes:

$$J'_r = \int_{D_0} p^*(r',E')dr' + \int_{D'_\infty} - p^*(S,E')S^{-2}\, dS \quad . \tag{5.60}$$

Using the residue theorem we have:

$$J'_r = - 2\pi i \, \mathrm{Res}[p^*(r',E')]_{r'=0} + 2\pi i \, \mathrm{Res}[p^*(S,E')S^{-2}]_{S=0} \quad . \tag{5.61}$$

Evaluating the integral J'_r has now been reduced to finding the residues of $p^*(r',E')$ and $p^*(S,E')S^{-2}$ at $r' = 0$ and $S = 0$, respectively. These residues may be found easily once the Coulomb Ricatti equation is solved.

In order to evaluate the residues which now define J'_r, we need to solve the Coulomb Ricatti in ways which yield solutions which are valid near $r' = 0$ and $S = 0$ ($r' = \infty$), such that these solutions satisfy the physical boundary conditions which we will impose on them. A solution of the Coulomb Ricatti equation (5.57), valid near $r' = 0$ is:

$$p^*(r',E') = - \frac{i\hbar\ell}{r'} + \sum_{n=0}^{\infty} E_n \, r'^n \quad , \tag{5.62}$$

where

$$C_0 = - \frac{g}{2i\hbar(1 + \ell)} \quad ,$$

$$C_1 = -\frac{E - C_0^2}{i\hbar(3 + 2\ell)} \quad ,$$

$$C_k = \frac{1}{i\hbar(k + 3 + 2\ell)} \sum_{\ell=0}^{k-1} C_\ell \, C_{(k-1-\ell)} \quad , \qquad k \geq 2 \quad .$$

For the sake of the discussions which follow we will call this solution p_0^* since it is valid near $r' = 0$.

Using the change of variables $r' = S^{-1}$, we can study the behavior of $p^*(r',E')$ near $S = 0$ or $r' = \infty$. Using this transformation of variables the Coulomb Ricatti equation becomes:

$$\frac{\hbar}{i}\frac{\partial p^*(S,E')}{\partial S} - \frac{2\hbar}{i}\frac{1}{S}p^*(S,E') - \frac{1}{S^2}p^*(S,E')^2 = -\frac{E'}{S^2} + \hbar^2\ell(\ell+1) - \frac{g}{S} \quad . \tag{5.63}$$

Equation (5.63) has as a particular solution:

$$p^{\pm}(S,E') = \sum_{n=0}^{\infty} b_n S^n \tag{5.64}$$

where

$$b_0 = +i\hbar \quad , \quad \kappa = \sqrt{-E'} > 0 \quad , \quad \text{for } E' > 0 \quad ,$$

$$b_1 = \frac{g}{2i\kappa} - \frac{\hbar}{i} \quad ,$$

$$b_2 = \frac{-\hbar^2\ell(\ell+1) + b_1^2 - i\hbar\, b_1}{2i} \quad ,$$

$$b_j = -\frac{1}{2i\hbar}\left\{-\frac{\hbar}{i}(j-3)b_{j-1} + \sum_{\ell=1}^{\infty} b_\ell\, b_{(j-1-\ell)}\right\} .$$

We will call this solution p_S^* for the discussion which follows.

As discussed in Chapter IV, solutions like p_S^* and p_0^* are not the most general solutions, but are correct in the neighborhood of $r' = 0$ and in the neighborhood of $S = 0$ providing they satisfy appropriate boundary conditions. As was discussed in Chapter IV (or see Appendix C), for an eigenstate of a system, if one has $E' < V(r')$, then between the origin and the left classical turning point, r_- (where $E' = V_{eff}(r_-)$), $p^*(r',E')$ must be negative imaginary. We can check that p_0^* satisfies this condition by noting that in the limit of $r' \to 0$ (r' real, positive), p_0^* or $p^*(r',E')$ as given by Eq. (5.62) is negative imaginary. Thus, p_0^* is the valid physical solution near $r' = 0$. In Chapter IV, the condition imposed on $p^*(r',E')$ in the region between the right classical turning point, r_+ (where $E' = V_{eff}(r_+)$), and positive infinity, is that $p^*(r',E')$ must be positive imaginary. We may check that p_S^* is valid near $S = 0$, because in the limit of $S \to 0$ (S real, positive) p_S^* or $p^*(S,E')$ as given by Eq. (5.64) becomes $i\kappa$ which is positive imaginary.

Thus, p_S^* is physically valid near $S = 0$ (or $r = \infty$). The two solutions, p_0^* and p_S^*, which we have found are valid near $r' = 0$ and $S = 0$, respectively, at an eigenstate of the Coulomb potential. [We note that other p^* solutions exist at $r = 0$ and $S = 0$ besides $p_0^*(r',E')$ and $p_S^*(S,E')$, but these solutions do not satisfy physical boundary conditions.]

Since we have found solutions which are valid at $r' = 0$ and $S = 0$ ($r' = \infty$), we can now return to the definition of J_r' which is given in Eq. (5.61) as the sum of two residues. The two residues of interest are:

$$\text{Res}[p^*(r',E')]_{r'=0} = \text{Res}[p^*]_{r'=0} = -i\hbar\ell \quad , \tag{5.65}$$

$$\text{Res}[p^*(S,E')S^{-2}]_{S=0} = \text{Res}[p_S^* S^{-2}]_{S=0} = \frac{g}{2i\kappa} - \frac{\hbar}{i} \quad . \tag{5.66}$$

Putting these residues into J_r' as given in Eq. (5.61) we find:

$$J_r' = -2\pi\hbar\ell + \frac{\pi g}{\kappa} - 2\pi\hbar \quad , \tag{5.67}$$

$$= -2\pi\hbar\ell + \frac{\pi g}{\sqrt{-E'}} - 2\pi\hbar \quad . \tag{5.68}$$

Equations (5.67) and (5.68) give $J_r' = J_r'(E')$. They can be inverted to give $E' = E'(J_r')$:

$$E' = -\frac{\pi^2 g^2}{(J_r' + 2\pi\hbar\ell + 2\pi\hbar)^2} \quad . \tag{5.69}$$

Expression (5.69) is the desired relation between the physical eigenvalues E' and J_r'. Note that it is an exact quantum mechanical result.

Using Eq. (5.22) we can find the energy levels. We have evaluated the integral defining J_r' two mathematically equivalent ways. One way produced J_r' as in Eq. (5.68) and the other way produced $J_r' = 2\pi\hbar n_r$, $n_r = 0, 1, 2, \ldots$ (which is also given by the general theory of Chapter IV). Since these ways are equivalent, the energy levels are found by

substituting $J'_r = 2\pi\hbar n_r$ into $E'(J'_r)$:

$$E'_n = \frac{-\pi^2 g^2}{(2\pi\hbar n_r + 2\pi\hbar\ell + 2\pi\hbar)^2} \quad \text{where} \quad \ell, n_r = 0, 1, 2, \ldots \quad . \quad (5.70)$$

The reader will notice that these are the exact Coulomb bound state energy levels in agreement with other calculations. E'_n, Eq. (5.70), also has the correct classical limit (3):

$$E_c = \frac{-\pi^2 g^2}{(J_{rc} + J_{\theta c} + J''_{\phi c})^2} \quad .$$

The fact that we have found the correct quantum energy levels and have maintained the correct classical limit gives us confidence that J'_r was defined in a reasonable way.

From Eq. (5.70) we see that the exact quantum energy levels of the system have been found without solving for the wavefunction $\langle q'|E'\rangle$. For this problem, finding the energy levels involved using the definition of $J'(E')$ in terms of $p^*(r',E')$, and then finding the two relevant residues of $p^*(r',E')$. Thus, the energy levels have been found without solving Schrödinger's equation, and without finding the quantum momentum function $p^*(r',E')$ for all r'.

At this point in the calculation we could go on to find $W_0(r',E')$, $W(r',J'_r)$, $W_0(r,E)$, $W(r,J)$, w, $H(J_r)$, p and the various wavefunctions. However, we have accomplished what we set out to do. We have found the Coulomb energy levels without carrying out the full canonical transformation. This is analogous to the classical use of action-angle variables which gives $E_c(J_c)$ without reference to w_c. For problems

which have a simple singularity structure (like the Coulomb problem), the use of action-angle variables to find energy-levels is a quick way to find the energy eigenvalues without any approximations.

D. Concluding Remarks

In this dissertation we have defined action-angle variables quantum mechanically using two methods. First, we used the classical transformation equations as a guide in the choice of a set of quantum transformation equations. We accepted this set of equations as valid if it satisfied certain conditions, not the least of which was producing a Hamiltonian independent of the coordinates w. This method worked well for systems having simple classical transformation equations, and did produce correct energy levels for all systems considered. However, the method failed when applied to the Coulomb problem.

The second and more general method involved starting with Schrödinger's equation and an exponential form of the wavefunction. From these a quantum Hamilton-Jacobi eigenvalue equation was found. From this eigenvalue equation a Ricatti equation was found whose solution $p^*(q',E')$ is the quantum analogue of the classical momentum $p_c(q_c,E_c)$. J' was defined as a contour integral of $p^*(q',E')$.

The definition of J' and a consideration of the boundary conditions appropriate for $p^*(q',E')$ led us to the definitions of the quantum generating functions $W_0(q,E)$ and $W(q,J)$. These generating functions allowed us to define p and w, the operators canonically conjugate to q and J, respectively. We verified the desired properties of p and w. We found the appropriate boundary condition for the wavefunction $\langle w'|J'\rangle$.

We found the eigenvalues of J and the operator H(J) with its eigenvalues, the energy levels of the system. This method is more powerful than the earlier "classical-update" method. In particular, this second method gave us the energy levels of the Coulomb problem which the earlier method was not able to do. We emphasize that the second method (Chapter IV) is completely general, i.e., it is applicable to any quantum system.

The central expression of the quantum action-angle variable theory proposed here is the definition of the action-variable eigenvalue J' in terms of the energy eigenvalue E', i.e., the definition J'(E'). Although we must solve the Hamilton-Jacobi eigenvalue equation for $p^*(q',E')$ in order to find J'(E'), it is not necessary to know $p^*(q',E')$ at all points q' (e.g., $p^*(q',E')$ must be known only at the origin and infinity for the Coulomb problem) in order to find J'(E') and the energy levels of the system. In contrast, finding energy levels using Schrödinger's equation requires a knowledge of the wavefunction $\langle r'|E'\rangle$, throughout the region of interest (e.g., from r' = 0 to r' = ∞ for the Coulomb problem). Thus, in principle, one can find the energy levels of a quantum system without finding a complete solution of the equation of motion, i.e., without finding a complete solution of Schrödinger's equation.

While quantum action-angle variables are equivalent to normal "p-q" quantum mechanics, the strength of these new variables lies in their ability to calculate energy levels without carrying out a full canonical transformation. The analogous use is made of them in

classical mechanics. These variables are ideally suited to calculate bound state energy levels, and may be generalizable to systems which have no classical analogue. It is in the context of carrying out bound state energy level calculations for systems for which traditional methods have failed, that action-angle variables may find their greatest utility.

VI. APPENDIX A: ANGULAR PROBLEM

As given in Chapter III, the hypothesized quantum transformation equations are:

$$\cos\theta = (b - b^{+})/2i \quad , \tag{3.30}$$

$$P_\theta \sin\theta = \frac{1}{4\pi}\left[b(J_\theta + J'_\phi) + (J_\theta + J''_\phi)b^{+}\right] \quad , \tag{3.31}$$

$$b = e^{-i2\pi w_\theta} f(J_\theta, J''_\phi) \quad , \tag{3.28}$$

$$b^{+} = f^{+}(J_\theta, J''_\phi)\, e^{i2\pi w_\theta} \quad , \tag{3.29}$$

where $J''_\phi = |J'_\phi| = 2\pi\hbar m''$, $m'' = 0, 1, 2, \ldots$.

It is desired to find $L^2(J_\theta, J''_\phi)$ and the function f so that conditions A-F are satisfied. This is done by first rewriting the "Hamiltonian" L^2 (3.4) so that is is a function of $\cos\theta$ and $P_\theta \sin\theta$ only so that we can use the transformation equations (3.30) and (3.31) directly. L^2 is defined by

$$L^2 \equiv \frac{1}{\sin\theta} P_\theta \sin\theta P_\theta + \frac{P'^2_\phi}{\sin^2\theta} \quad . \tag{3.4}$$

In the rewriting process we use the following commutators:

$$[P_\theta, \cos\theta] = -\frac{\hbar}{i}\sin\theta \quad , \tag{A.1}$$

$$[P_\theta, \sin\theta] = \frac{\hbar}{i}\cos\theta \quad , \tag{A.2}$$

$$[P_\theta, P'_\phi] = [P'_\phi, \cos\theta] = [P'_\phi, \sin\theta] = 0 \quad , \tag{A.3}$$

$$[L^2, \sin\theta] = \frac{\hbar}{i}\left(P_\theta \cos\theta + \cos\theta\, P_\theta + \frac{\hbar}{i}\frac{\cos^2\theta}{\sin\theta}\right) \quad . \tag{A.4}$$

We begin to rewrite L^2 in terms of P_θ $\sin\theta$ and $\cos\theta$ by multiplying both sides of L^2 by $\sin\theta$:

$$\sin\theta\, L^2 \sin\theta = P_\theta \sin\theta\, P_\theta \sin\theta + P'^2_\phi \tag{A.5}$$

$$= (P_\theta \sin\theta)^2 + P'^2_\phi \quad . \tag{A.6}$$

The left side of Eq. (A.6) may be rewritten using Eq. (A.4) to yield:

$$\sin\theta\, L^2 \sin\theta = \frac{1}{2}\left(\sin^2\theta\, L^2 + L^2 \sin^2\theta + \sin\theta[L^2, \sin\theta] - [L^2, \sin\theta]\sin\theta\right)$$

$$= \frac{1}{2}\left(2L^2 - \cos^2\theta\, L^2 - L^2 \cos^2\theta + 2\hbar^2\cos^2\theta\right) \quad . \tag{A.7}$$

Using Eq. (A.7) on the LHS of Eq. (A.6) we now have an expression which depends only on L^2, P'^2_ϕ, P_θ $\sin\theta$ and $\cos\theta$:

$$L^2 - P'^2_\phi = \frac{1}{2}\left[\cos^2\theta\left(L^2 + \frac{1}{4}\hbar^2\right) + \left(L^2 + \frac{1}{4}\hbar^2\right)\cos^2\theta\right] - \frac{5}{4}\hbar^2\cos^2\theta$$

$$+ P_\theta \sin\theta\, P_\theta \sin\theta \quad . \tag{A.8}$$

Equation (A.8) is now in a form into which both Eqs. (3.30) and (3.31) may be substituted. Also to save writing we introduce the notation

$$J \equiv J_\theta + J''_\phi \quad . \tag{A.9}$$

Expression (A.8) contains only P_θ $\sin\theta$ and $\cos\theta$ so we may now use Eqs. (3.30) and (3.31). Using Eqs. (A.9), (3.30) and (3.31), $\cos^2\theta$ and

$P_\theta \sin\theta\, P_\theta \sin\theta$ may be expressed in terms of b and J as:

$$\cos^2\theta = -\frac{1}{4}(bb - bb^+ - b^+b + b^+b^+) \quad , \tag{A.10}$$

$$P_\theta \sin\theta\, P_\theta \sin\theta = \frac{1}{16\pi^2}(bJbJ + bJ^2b + Jb^+b^+J + Jb^+Jb^+) \quad . \tag{A.11}$$

Using $[J_\theta, e^{\pm i2\pi w_\theta}] = \pm 2\pi\hbar\, e^{\pm i2\pi w_\theta}$, we have the following useful commutators:

$$[b,J] = 2\pi\hbar b \quad , \tag{A.12}$$

$$[b^+,J] = -2\pi\hbar b^+ \quad , \tag{A.13}$$

$$[J,bb^+] = [J,b^+b] = 0 \quad . \tag{A.14}$$

Using Eqs. (A.12)-(A.14) with Eq. (A.11) we obtain after manipulation:

$$\begin{aligned} P_\theta \sin\theta\, P_\theta \sin\theta = \frac{1}{32\pi^2}[&J(J + 2\pi\hbar)bb + bbJ(J + 2\pi\hbar) - 8\pi^2\hbar^2 bb \\ &+ J(J + 2\pi\hbar)b^+b^+ + b^+b^+J(J + 2\pi\hbar) - 8\pi^2\hbar^2 b^+b^+ \\ &+ 2(J + 2\pi\hbar)^2 bb^+ + 2J^2b^+b] \quad . \end{aligned} \tag{A.15}$$

Combining Eqs. (A.10) and (A.15) we have part of the RHS of Eq. (A.8):

$$\begin{aligned} P_\theta \sin\theta\, P_\theta \sin\theta - \frac{5}{4}\hbar^2\cos^2 = \frac{1}{32\pi^2}[&(J + \pi\hbar)^2 bb + bb(J + \pi\hbar)^2 \\ &+ (J + \pi\hbar)^2 b^+b^+ + b^+b^+(J + \pi\hbar)^2 \\ &+ 2(J^2 + 4\pi\hbar J - \pi^2\hbar^2)bb^+ \\ &+ 2(J^2 - 5\pi^2\hbar^2)b^+b] \quad . \end{aligned} \tag{A.16}$$

Continuing to rewrite the RHS of Eq. (A.8), we multiply $\cos^2\theta$ by $(L^2 + \frac{1}{4}\hbar^2)$ and use Eq. (A.10) to form:

$$\frac{1}{2}\,(\cos^2\theta(L^2 + \tfrac{1}{4}\hbar^2) + (L^2 + \tfrac{1}{4}\hbar^2)\cos^2\theta) \;=\; -\frac{1}{8}\,\{(L^2 + \tfrac{1}{4}\hbar^2)bb$$

$$+ bb(L^2 + \tfrac{1}{4}\hbar^2) + (L^2 + \tfrac{1}{4}\hbar^2)b^+b^+ + b^+b^+(L^2 + \tfrac{1}{4}\hbar^2)$$

$$- (L^2 + \tfrac{1}{4}\hbar^2)bb^+ - bb^+(L^2 + \tfrac{1}{4}\hbar^2) - (L^2 + \tfrac{1}{4}\hbar^2)b^+b$$

$$- b^+b(L^2 + \tfrac{1}{4}\hbar^2)\} \quad . \tag{A.17}$$

If we add Eq. (A.17) to Eq. (A.16) we obtain the right hand side of Eq. (A.8) in terms of L^2, J, b, and b^+:

$$P_\theta \sin\theta\, P_\theta \sin\theta - \tfrac{5}{4}\hbar^2\cos^2\theta + \tfrac{1}{2}\,[\cos^2\theta(L^2 + \tfrac{1}{4}\hbar^2) + (L^2 + \tfrac{1}{4}\hbar^2)\cos^2\theta]$$

$$= \frac{1}{32\pi^2}\,[-4\pi^2(L^2 + \tfrac{1}{4}\hbar^2) + (J + \pi\hbar)^2]bb + bb[-4\pi^2(L^2 + \tfrac{1}{4}\hbar^2)$$

$$+ (J + \pi\hbar)^2] + [-4\pi^2(L^2 + \tfrac{1}{4}\hbar^2) + (J + \pi\hbar)^2]b^+b^+$$

$$+ b^+b^+[-4\pi^2(L^2 + \tfrac{1}{4}\hbar^2) + (J + \pi\hbar)^2] + [4\,^2(L^2 + \tfrac{1}{4}\hbar^2)$$

$$+ 2(J^2 + 4\pi\hbar J - \pi^2\hbar^2)]bb^+ + [4\pi^2(L^2 + \tfrac{1}{4}\hbar^2) + 2(J^2 - 5\pi^2\hbar^2)]b^+b$$

$$+ bb^+[4\pi^2(L^2 + \tfrac{1}{4}\hbar^2)] + b^+b[4\pi^2(L^2 + \tfrac{1}{4}\hbar^2)] \quad . \tag{A.18}$$

Before simplifying Eq. (A.18) it is important to know the effect of $f(J_\theta, J''_\phi)e^{\pm i2\pi w_\theta}$ and of $e^{\pm i2\pi w_\theta} f(J_\theta, J''_\phi)$ on states $|J'_\theta, J'_\phi\rangle$. We have required that the following boundary condition be satisfied by $\langle w'|J'\rangle$ for action-angle coordinates:

$$\langle w' + 1|J'\rangle \;=\; \langle w'|J'\rangle \quad . \tag{A.19}$$

Under this boundary condition it follows that (4) we have for Hermitian J:

$$J = \frac{\hbar}{i} \frac{\partial}{\partial w} \tag{A.20}$$

and also that (4):

$$\langle w'|J|J'\rangle = \frac{\hbar}{i} \frac{\partial}{\partial w'} \langle w'|J'\rangle \quad , \tag{A.21}$$

$$= J'\langle w'|J'\rangle \quad . \tag{A.22}$$

Using Eqs. (A.19), (A.21) and (A.22) we have:

$$\langle w'|J'\rangle = e^{iJ'w'/\hbar} \tag{A.23}$$

$$J' = 2\pi\hbar n \qquad n = 0,\pm1,\pm2, \ldots \quad .$$

Using Eq. (A.23) we have the following:

$$\langle w'|e^{\pm i2\pi w'}|J'\rangle = e^{\pm i2\pi w'} \langle w'|J'\rangle$$

$$= \langle w'|J' \pm 2\pi\hbar\rangle \quad . \tag{A.24}$$

From Eq. (A.25) it follows that:

$$e^{\pm i2\pi w}|J'\rangle = |J' \pm 2\pi\hbar\rangle \quad . \tag{A.25}$$

Also

$$f(J)|J'\rangle = f(J')|J'\rangle \quad . \tag{A.26}$$

Using Eqs. (A.25) and (A.26) we evaluate $f(J)e^{i2\pi w}$:

$$\langle w'|f(J)e^{\pm i2\pi w}|J'\rangle = \langle w'|f(J)|J' \pm 2\pi\hbar\rangle$$

$$= f(J' \pm 2\pi\hbar)\langle w'|J' \pm 2\pi\hbar\rangle \quad . \tag{A.27}$$

We also evaluate $e^{\pm i2\pi w} f(J \pm 2\pi\hbar)$:

$$\langle w'|e^{\pm i2\pi w} f(J \pm 2\pi\hbar)|J'\rangle = f(J' \pm 2\pi\hbar)\langle w'|e^{\pm i2\pi w}|J'\rangle$$
$$= f(J' \pm 2\pi\hbar)\langle w'|J' \pm 2\pi\hbar\rangle \quad . \quad (A.28)$$

Comparing Eqs. (A.27) and (A.28) it follows that:

$$e^{\pm i2\pi w} f(J \pm 2\pi\hbar) = f(J)\, e^{\pm i2\pi w} \quad . \quad (A.29)$$

Equation (A.29) is a general result which is valid without respect to the specific type of action-angle variables under consideration (i.e., without respect to J_θ, J_ϕ, w_θ, w_ϕ, etc.).

Equation (A.29) can now be used to reduce the RHS of Eq. (A.18), since bb, b^+b^+, b^+b bb^+ may now be simplified. For example, bb is:

$$bb = e^{-i2\pi w_\theta} f(J_\theta, J''_\phi)\, e^{-i2\pi w_\theta} f(J_\theta, J''_\phi) \quad . \quad (A.30)$$

Using Eq. (A.29) in Eq. (A.30) we obtain:

$$bb = e^{-i4\pi w_\theta} f(J_\theta - 2\pi\hbar,\, J''_\phi)\, f(J_\theta, J''_\phi) \quad . \quad (A.31)$$

Similarly, b^+b^+, b^+b and bb^+ become:

$$b^+b^+ = f^+(J_\theta, J''_\phi)\, f^+(J_\theta - 2\pi\hbar,\, J''_\phi)\, e^{i4\pi w_\theta} \quad , \quad (A.32)$$

$$bb^+ = f(J_\theta + 2\pi\hbar,\, J''_\phi)\, f^+(J_\theta + 2\pi\hbar,\, J''_\phi) \quad , \quad (A.33)$$

$$b^+b = f^+(J_\theta, J''_\phi)\, f(J_\theta, J''_\phi) \quad , \quad (A.34)$$

Now, the left side of Eq. (A.18) is equal to $L^2 - P'^2_\phi$ from Eq. (A.8). One of our goals has been to find L^2 as a function of J_θ only, and hence

L^2 must be independent of w_θ. Since $P_\phi'^2 = J_\phi'^2/4\pi^2$, this independence will occur only if the right hand side of Eq. (A.18) is independent of w_ϑ. Referring to Eqs. (A.31-(A.34), the right hand side will be independent of w only if the coefficients of all terms containing bb or b^+b^+ are zero. This condition yields:

$$L^2 + \frac{1}{4}\hbar^2 = \frac{1}{4\pi^2}(J_\theta + J_\phi'' + \pi\hbar)^2$$

$$= \frac{1}{4\pi^2}(J + \pi\hbar)^2 \quad . \tag{A.35}$$

Thus we have now found L^2 as a function of J_θ which was one of our goals.

We will now use $L^2(J_\theta)$ to find the form of f. Once we have found the form of f, we will have specified the transformation equations. Using Eq. (A.35) to reduce Eq. (A.18), and then substituting Eq. (A.18) into the RHS of Eq. (A.8) we obtain:

$$L^2 - P_\phi'^2 = \frac{1}{8\pi^2}[(J^2 + 3\pi\hbar J)bb^+ + (J + 2\pi\hbar)(J - \pi\hbar)b^+b] \tag{A.36}$$

where bb^+ and b^+b are given in Eqs. (A.33) and (A.34). From the rotor we have:

$$J_\phi'/2\pi = P_\phi' \tag{A.27}$$

where $|J_\phi'| = J_\phi''$ so that $J_\phi'^2 = J_\phi''^2$. Using $L^2(J_\theta)$, Eq. (A.35), the expressions for bb^+ and b^+b, and Eq. (A.37), one obtains from Eq. (A.36):

$$\frac{1}{4\pi^2}(J + \pi\hbar)^2 - \frac{1}{4}\hbar^2 - \frac{J_\phi''^2}{4\pi^2} = \frac{1}{8\pi^2}[(J^2 + 3\pi\hbar J)\, f(J_\theta + 2\pi\hbar)\, f^+(J_\theta + 2\pi\hbar)$$

$$+ (J + 2\pi\hbar)(J - \pi\hbar) f^{+}(J_\theta) f(J_\theta)] \quad . \text{(A.38)}$$

Equation (A.38) cannot be simplified without additional information. The additional information which we use is the commutator:

$$[P_\theta \sin\theta, \cos\theta] = -\frac{\hbar}{i}(1 - \cos^2\theta) \qquad \text{(A.39)}$$

which must be satisfied if our transformation equations are to be considered valid (condition C). We use this commutator to determine the form of $f(J_\theta, J''_\phi)$ by substituting the expressions for $P_\theta \sin\theta$ and $\cos\theta$ (in terms of b and b^+) as given by the transformation equations (3.30) and (3.31). From this commutator we find a relation between bb^+ and b^+b which determines $f(J_\theta, J''_\phi)$. One obtains from the commutator:

$$(J + 3\pi\hbar)bb^+ = 4\pi\hbar + (J - \pi\hbar)b^+b \quad . \qquad \text{(A.40)}$$

Putting Eq. (A.40) into Eq. (A.38) (which we could not simplify earlier) one finds:

$$\frac{1}{4\pi^2}[(J + \pi\hbar)^2 - \pi^2\hbar^2 - J''^2_\phi] = \frac{1}{4\pi^2}[2\pi\hbar J + (J + \pi\hbar)(J - \pi\hbar)]b^+b$$

$$= \frac{1}{4\pi^2}[2\pi\hbar J + (J + \pi\hbar)(J - \pi\hbar)]$$

$$\times f^{+}(J_\theta, J'_\phi)\, f(J_\theta, J'_\phi) \quad . \qquad \text{(A.41)}$$

The left side of Eq. (A.41) will be equal to the right side of Eq. (A.41) only if $f^{+}(J_\theta, J''_\phi) f(J_\theta, J''_\phi)$ has the form:

$$f^{+}f = \frac{J^2 - J''^2_{\phi}}{J^2 - \pi^2\hbar^2} \tag{A.42}$$

$$= \frac{(J_\theta + J''_\phi)^2 - J''^2_\phi}{(J_\theta + J''_\phi)^2 - \pi^2\hbar^2} \quad . \tag{A.43}$$

We now consider the eigenvalue spectrum. First Eq. (A.43) may be evaluated for a state $|J'_\theta, J'_\phi\rangle$:

$$f^{+}(J_\theta, J''_\phi) f(J_\theta, J''_\phi) |J'_\theta, J'_\phi\rangle = f^{+}(J'_\theta, J''_\phi) f(J'_\theta, J''_\phi) |J'_\theta, J'_\phi\rangle \tag{A.44}$$

$$= \frac{(J'_\theta + J''_\phi)^2 - J''^2_\phi}{(J'_\theta + J''_\phi)^2 - \pi^2\hbar^2} |J'_\theta, J'_\phi\rangle \quad . \tag{A.45}$$

Equating Eqs. (A.44) and (A.45) we have the product $f^{+}f$ expressed in terms of the eigenvalue J'_θ:

$$f^{+}(J'_\theta, J''_\phi) f(J'_\theta, J''_\phi) = \frac{(J'_\theta + J''_\phi)^2 - J''^2_\phi}{(J'_\theta + J''_\phi)^2 - \pi^2\hbar^2} \tag{A.46}$$

(where $J''_\phi \geq 0$).

Before we take a square root in Eq. (A.46) and obtain $f(J'_\theta, J''_\phi)$ it is important to consider the spectrum of values which J'_θ may have. The left hand side of Eq. (A.46) is a positive definite quantity and hence is positive. The right hand side of Eq. (A.46) is positive only for those states having $J'_\theta \geq 0$ or $J'_\theta \leq -2J''_\phi$. We choose those states having $J'_\theta \geq 0$ as the physical Hilbert space because in the classical limit we require that J'_θ be a positive quantity (since $J_{\theta c}$ is a positive quantity as is discussed in Chapter III, Section C). In the classical limit with

$J'_\theta \leq -2J''_\phi$, J'_θ becomes a negative quantity which we regard as unphysical. Thus, the physical Hilbert space consists of those states having $J'_\theta \geq 0$ (For a related and more comprehensive discussion see Ref. 17.).

For the allowed or physical Hilbert space $f^+(J'_\theta, J''_\phi) f(J'_\theta, J''_\phi)$ is greater than zero and $f(J'_\theta, J'_\phi)$ is real. Thus we define $f(J_\theta, J''_\phi)$ for the physical Hilbert space as:

$$f(J_\theta, J''_\phi) = \left[\frac{(J_\theta + J''_\phi)^2 - J''^2_\phi}{(J_\theta + J''_\phi)^2 - \pi^2\hbar^2} \right]^{1/2} , \qquad (A.47)$$

and have:

$$f(J_\theta, J''_\phi) = f^+(J_\theta, J''_\phi) \quad .$$

Having restricted the Hilbert space and determined the form of $f(J_\theta, J''_\phi)$, we can now verify the commutator of P_θ sinθ with cosθ, Eq. (A.39). After manipulating this commutator (A.40) was found:

$$(J + 3\pi\hbar) bb^+ = 4\pi\hbar + (J - \pi\hbar) b^+ b \quad . \qquad (A.40)$$

Using the form of f which we have found, and the definitions of b and b^+ we have after manipulation of Eq. (A.40):

$$(J + 3\pi\hbar) f(J_\theta + 2\pi\hbar, J''_\phi) f^+(J_\theta + 2\pi\hbar, J''_\phi) = 4\pi\hbar + (J - \pi\hbar) ff^+ \quad . (A.48)$$

Using the form of f we have:

$$(J + 3\pi\hbar)\left[\frac{(J + 2\pi\hbar) - J''^2_\phi}{(J + 2\pi\hbar) - \pi^2\hbar^2} \right] = 4\pi\hbar + (J - \pi\hbar)\left[\frac{J^2 - J''^2_\phi}{J^2 - \pi^2\hbar^2} \right] \quad . \quad (A.49)$$

From Eq. (A.49) one finds:

$$\frac{(J + 2\pi\hbar)^2 - J''^2_\phi}{J + \pi\hbar} = 4\pi\hbar + \frac{J^2 - J''^2_\phi}{J + \pi\hbar}$$

$$= \frac{J^2 + 4\pi\hbar + 4\pi^2\hbar^2 - J''^2_\phi}{J + \pi\hbar} \quad . \qquad (A.50)$$

Clearly, both sides of Eq. (A.50) are equal and the commutator of $P_\theta \sin\theta$ with $\cos\theta$ is verified for the physical Hilbert space. This is condition C.

The six conditions imposed on a set of transformation equations have been verified for the restricted Hilbert space. In this space the eigenvalues of L^2 may be found using Eq. (A.35):

$$L^2|J'_\theta, J'_\phi\rangle = \frac{1}{4\pi^2}((J'_\theta + J''_\phi + \pi\hbar)^2/4\pi^2 - \frac{1}{4}\hbar^2)|J'_\theta, J'_\phi\rangle \quad . \qquad (A.51)$$

Defining $J'_\theta + J''_\phi \equiv \ell 2\pi\hbar = 2\pi\hbar(n_\theta + m'')$ the eigenvalues of L^2 are:

$$L^{2'} = (\hbar^2(\ell + \frac{1}{2})^2 - \frac{1}{4}\hbar^2) = \hbar^2\ell(\ell + 1) \quad . \qquad (A.52)$$

Since both n_θ and m'' have allowed values: 0, 1, 2, ..., it follows that ℓ has allowed values: 0, 1, 2, ... and L^2 has the spectrum:

$$L^{2'} = \hbar^2\ell(\ell + 1) = \hbar^2(0, 2, 6, 12, \ldots) \quad . \qquad (A.53)$$

Having found the eigenvalues of L^2 and the transformation equations from P_θ and θ to J_θ and w_θ, the problem is completed. As in the harmonic oscillator and rotor, the procedure was to use the classical transformation equations to deduce the quantum equations and to verify

that the transformation equations and Hamiltonian, H(J), have certain properties. On the physical Hilbert space the eigenvalues of H(J) (or $L^2(J_e)$ in this case) were finally determined.

VII. APPENDIX B: TWO-DIMENSIONAL HARMONIC OSCILLATOR

The planar oscillator is easily done using the procedure employed for the three-dimensional oscillator. The classical Hamiltonian and transformation equations are: (2m = 1)

$$H_c = P_c^2 + \frac{P_{\phi c}^2}{\rho^2} + \frac{1}{4}\omega^2\rho^2 \qquad (B.1)$$

$$= \frac{\omega}{2\pi}(2J_{\rho c} + J''_{\phi c}) \quad ,$$

$$P_{\phi c} = \frac{J_{\phi c}}{2\pi} \text{ (Rotor)} \quad , \qquad (B.2)$$

where $J''_\phi \equiv \sqrt{J'^2_\phi} \geq 0$, real for J'_ϕ real

$$\phi_c = 2\pi w_{\phi c} \text{ (Rotor)} \quad , \qquad (B.3)$$

$$P_{c\rho} = \frac{1}{2\pi}[(2J_{\rho c} + J_{\phi c})^2 - J_{\phi c}^2]^{1/2}\cos(2\pi w_{\rho c}) \quad , \qquad (B.4)$$

$$\omega\rho^2/2 = \frac{1}{2\pi}[(2J_{\rho c} + J_{\phi c})^2 - J_{\phi c}^2]^{1/2}\sin(2\pi w_{\rho c}) + H(J_{\rho c}, J_{\phi c})/\omega \quad . \qquad (B.5)$$

In analogy with the three-dimensional harmonic oscillator $J_{\rho c}$ is defined as:

$$J_{\rho c} = \frac{1}{2}\left\{\frac{2\pi}{\omega} H_c - \sqrt{P^2_{\phi c}}\right\} \quad .$$

The action variable $J_{\rho c}$ is defined using the branch of P_c which is pictured in Figure 1, positive along the bottom of the cut. The direction of integration is chosen to be counterclockwise and, hence, $J_{\rho c}$

is a non-negative quantity. The sign of the square root of $P_{\phi c}^2$ is chosen to be positive which is consistent with the branch of P_c chosen, and with the interpretation of $[P_{\phi c}^2]^{1/2}$, as the length of the angular momentum vectors. For these choices of sign it follows that H_c is positive which is consistent with (B.1) (where P_c, ρ and $P_{\phi c}$ are real quantities).

The quantum Hamiltonian is: $(2m = 1)$

$$H = \frac{1}{\rho} P_\rho P + \frac{P_\phi'^2}{\rho^2} + \frac{1}{4}\omega^2\rho^2 \qquad \text{(B.6)}$$

where P_ϕ' is the eigenvalue of P_ϕ, the rotor momentum, in a state $\langle\phi'|P_\phi' = \hbar m\rangle$ where $m = 0,\pm1,\pm2, \ldots$.

Furthermore, from the quantum rotor we also have: $J_\phi'' = 2\pi P_\phi'$. In analogy to the classical $J_{\phi c}''$ we introduce the quantum J_ϕ'':

$$J_\phi'' = + \sqrt{J_\phi'^2} = 2\pi \sqrt{P_\phi'^2} \quad . \qquad \text{(B.7)}$$

From the rotor the eigenvalues of J_ϕ'' are $2\pi\hbar m''$, where $m'' = 0,1,2,3, \ldots$. The introduction of J_ϕ'' is necessary because P_ϕ' enters in the Hamiltonian (B.6) as $P_\phi'^2/\rho^2$. "$P_\phi'^2$" is a positive quantity. Thus, J_ϕ'' is the square root of a positive quantity. We choose the plus sign for this square root by analogy to the plus sign chosen in the corresponding classical expression.

Given the quantum Hamiltonian (B.6) and the classical transformation equations (B.1)-(B.5) we can now obtain the quantum transformation equations. By analogy to Eq. (B.4), Eq. (B.5) and the three-dimensional

harmonic oscillator, we assert that the quantum transformation equations are:

$$P\rho = \frac{1}{2}(d^{+} + d) \tag{B.8}$$

$$\frac{\omega}{2}\rho^{2} = \frac{1}{2i}(d^{+} - d) + \frac{H(J_{\rho},J''_{\phi})}{\omega} \tag{B.9}$$

$$\begin{aligned} d^{+} &= f^{+}\, e^{i2\pi w_{\rho}} \\ d &= e^{-i2\pi w_{\rho}}\, f(J_{\rho},J''_{\phi}) \quad . \end{aligned} \tag{B.10}$$

Using the fact that $P\rho$ and ρ are Hermitian planar-polar coordinates, it can be shown that the left-hand side of Eqs. (B.8) and (B.9) are Hermitian. The right-hand side of Eqs. (B.8) and (B.9) are clearly Hermitian. Since d^{+} is of the $f^{+}\, e^{i2\pi w_{\rho}}$, it follows from Eq. (2.41) that both $\langle \omega' | P\rho | J'_{\rho} \rangle$ and $\langle \omega'_{\rho} | \frac{\omega}{2}\rho^{2} | J'_{\rho} \rangle$ are invariant under $\langle \omega'_{\rho} | \rightarrow \langle \omega'_{\rho} + 1 |$. Similarly Eqs. (B.8) and (B.9) are invariant under $\omega_{\rho} \rightarrow \omega_{\rho} \div 1$. Equations (B.8) and (B.9) will have the correct classical limit if

$$f(J_{\rho},J''_{\phi}) \xrightarrow{\hbar \rightarrow 0} \frac{1}{2\pi}\left[(2J_{\rho c} \div J''_{\phi c})^{2} - J''^{2}_{\phi c}\right]^{1/2} \quad . \tag{B.11}$$

Since as shown in the rotor, J'_{ϕ} has $J_{\phi c}$ as its classical limit we assert that $f(J_{\rho},J''_{\phi})$ has the form:

$$f(J_{\rho},J''_{\phi}) = \frac{1}{2\pi}\left[(2J_{\rho} + J''_{\phi})^{2} - J''^{2}_{\phi}\right]^{1/2} \quad . \tag{B.12}$$

We will consider Eq. (B.12) correct if all of the conditions demanded of a set of transformation equations in Chapter II are satisfied.

Having asserted f as in Eq. (B.12), both Eqs. (B.8) and (B.9) now have the correct classical limits.

Using Eqs. (B.8) and (B.9), $H(J_\rho, J_\phi'')$ may now be calculated. We begin by rewriting the quantum Hamiltonian (B.6) so that it is a function of P_ρ and $\frac{\omega}{2}\rho^2$. We multiply Eq. (B.6) by ρ on both sides:

$$\rho H_\rho = P_\rho P_\rho + P_\phi'^2 + \frac{1}{4}\omega^2\rho^4$$

$$\rho H_\rho = (P_\rho)^2 + P_\phi'^2 + \frac{\omega^2}{4}\rho^4 \quad . \tag{B.13}$$

Using $[P,\rho] = \hbar/i$, we have:

$$\frac{1}{2}(\rho^2 H + H\rho^2) + \hbar^2 = \rho H_\rho \quad . \tag{B.14}$$

Combining Eqs. (B.13) and (B.14), we obtain an expression in the desired form:

$$\left(\frac{\omega}{2}\rho^2\right)H + H\left(\frac{\omega}{2}\rho^2\right) + \hbar^2\omega = \omega(P_\rho)^2 + \left(\frac{\omega}{2}\rho^2\right)^2 + \omega P_\phi'^2 \tag{B.15}$$

Note that Eq. (B.15) contains only P_ρ and ρ^2 as needed. Into Eq. (B.15) we substitute the quantum forms of P_ρ and ρ^2, Eqs. (B.8) and (B.9), and find that the left side of Eq. (B.15) is equal to:

$$h^2\omega + \frac{\omega}{2}\rho^2 H + H\frac{\omega}{2}\rho^2 = \frac{1}{2i}[d^+H + Hd^+ - dH - Hd] + 2\frac{H^2}{\omega} + h^2\omega \quad . \tag{B.16}$$

Similarly the right side of Eq. (B.15) is:

$$\omega(P_\rho)^2 + \left(\frac{\omega}{2}\rho^2\right) + \omega P_\phi'^2 = \frac{\omega}{4}(dd + d^+d^+ + dd^+ + d^+d) + \omega P_\phi'^2$$

$$- \frac{\omega}{4} (dd + d^+d^+ - dd^+ - d^+d) + \frac{H^2}{\omega}$$

$$+ \frac{1}{2i} (d^+H + Hd^+ - dH - Hd) \qquad (B.17)$$

$$= \omega P_\phi'^2 + \frac{H^2}{\omega} + \frac{1}{2i} (d^+H + Hd^+ - dH - Hd)$$

$$+ \frac{\omega}{2} (dd^+ + d^+d) \quad . \qquad (B.18)$$

Equating Eqs. (B.17) and (B.18) we find:

$$\frac{H^2}{\omega} + \hbar^2\omega = \omega P_\phi'^2 + \frac{\omega}{2} (dd^+ + d^+d) \quad . \qquad (B.19)$$

From the definition of d, d^+, Eq. (B.10) we have

$$d^+d = f^+(J_\rho, J_\phi'') \, f(J_\rho, J_\phi'') \quad , \qquad (B.20)$$

$$dd^+ = e^{-i2\pi w_\rho} \, ff^+ \, e^{i2\pi w_\rho} \quad . \qquad (B.21)$$

Using Eqs. (B.20) and (B.21) we have:

$$dd^+ = f(J_\rho + 2\pi\hbar, J_\phi'') \, f^+(J_\rho + 2\pi\hbar, J_\phi'') \quad . \qquad (B.22)$$

Putting Eqs. (B.20) and (B.22) into Eq. (B.19) we find:

$$\frac{H^2}{\omega} + \hbar^2\omega = \omega P_\phi'^2 + \frac{\omega}{2} [f(J_\rho + 2\pi\hbar) \, f^+(J_\rho + 2\pi\hbar) + f^+(J_\rho) f(J_\rho)] \quad . (B.23)$$

We can use the definition of f, Eq. (B.12) in Eq. (B.23), once we have found those states for which $f(J_\rho + 2\pi\hbar)$ and $f(J_\rho)$ are real or imaginary. This determination is made with fixed J_ϕ'. We allow f to act on a state $|J_\phi', J_\phi'\rangle$.

$$f(J_\rho)|J'_\rho,J'_\phi\rangle = \frac{1}{2\omega}\left[(2J'_\rho + J''_\phi)^2 - J''^2_\phi\right]^{1/2}|J'_\rho,J'_\phi\rangle \qquad (B.24)$$

$$f(J_\rho + 2\pi\hbar)|J'_\rho,J'_\phi\rangle = \frac{1}{2\omega}\left[(2J'_\rho + 4\pi\hbar + J''_\phi)^2 - J''^2_\phi\right]^{1/2}|J'_\rho,J'_\phi\rangle \quad . \qquad (B.25)$$

From Eqs. (B.24) and (B.25), with $J''_\phi \geq 0$, we have:

$$\begin{aligned} J'_\rho \geq 0: \quad & f(J'_\rho) \quad \text{real if} \quad J'_\rho \geq 0 \ \text{ or } \ J'_\rho \leq -J''_\phi \quad , \\ & f(J'_\rho + 2\pi\hbar) \quad \text{real if} \quad J'_\rho \geq -2\pi\hbar \ \text{ or } \ J'_\rho \leq -(J''_\phi + 2\pi\hbar) \quad . \end{aligned} \qquad (B.26)$$

For states not covered in Eq. (B.26), $f(J'_\rho)$ and $f(J'_\rho + 2\pi\hbar)$ are pure imaginary. Since $f(J'_\rho)$ and $f(J'_\rho + 2\pi\hbar)$ are not always both real or imaginary, with respect to a state $|J'_\rho,J'_\phi\rangle$ we have four possibilities: both real, both imaginary or one real and the other imaginary. With respect to these possibilities we have from Eq. (B.12):

$f(J'_\rho)$ real:
$$ff^+ = \frac{1}{4\pi^2}\left[(2J_\rho + J''_\phi)^2 - J''^2_\phi\right] \quad , \qquad (B.27)$$

$f(J'_\rho)$ imaginary:
$$ff^+ = -\frac{1}{4\pi^2}\left[(2J_\rho + J''_\phi)^2 - J''^2_\phi\right] \quad , \qquad (B.28)$$

$f(J'_\rho + 2\pi\hbar)$ real:
$$f(J_\rho + 2\pi\hbar)f^+(J_\rho + 2\pi\hbar) = \frac{1}{4\omega^2}\left[(2J_\rho + 4\pi\hbar + J''_\phi)^2 - J''^2_\phi\right] \quad . \qquad (B.29)$$

$f(J'_\rho + 2\pi\hbar)$ imaginary:
$$f(J_\rho + 2\pi\hbar)f^+(J_\rho + 2\pi\hbar) = -\frac{1}{4\omega}\left[(2J_\rho + 4\pi\hbar + J''_\phi)^2 - J''^2_\phi\right] . \qquad (B.30)$$

For the four cases we now use Eq. (B.7), $J''_\phi = 2\pi(P'_\phi)^{1/2}$, and Eqs. (B.27) -(B.30) in Eq. (B.23) to find H.

Case 1: both $f(J_\rho')$ and $f(J_\rho' + 2\pi\hbar)$ real:

$$\frac{H^2}{\omega} + h^2\omega = \omega P_\phi'^2 + \frac{\omega}{8\pi^2}\left[(2J_\rho + J_\phi'')^2 - J_\phi''^2 + (2J_\rho + 4\pi\hbar + J_\phi'')^2 - J_\phi''^2\right] . \tag{B.31}$$

Solving Eq. (B.31) for H we have:

$$H = \pm \frac{\omega}{2\pi}(2J_\rho + J_\phi'' + 2\pi\hbar) . \tag{B.32}$$

Case 2: both $f(J_\rho')$ and $f(J_\rho' + 2\pi\hbar)$ imaginary:

$$\frac{H^2}{\omega} + h^2\omega = \omega P_\phi'^2 - \frac{\omega}{8\pi^2}\left[(2J_\rho + J_\phi'')^2 - J_\phi''^2 + (2J_\rho + 4\pi\hbar + J_\phi'')^2 - J_\phi''^2\right] . \tag{B.33}$$

From Eq. (B.33) we find:

$$H = \pm \frac{i\omega}{2\pi}\left\{(2J_\rho + J_\phi'' + 2\pi\hbar)^2 - 2J_\phi''^2 + 8\pi^2\hbar^2\right\}^{1/2} . \tag{B.34}$$

Case 3: $f(J_\rho')$ real with $f(J_\rho' + 2\pi\hbar)$ imaginary:

$$\frac{H^2}{\omega} + h^2\omega = \omega P_\phi'^2 + \frac{\omega}{8\pi^2}\left[(2J_\rho + J_\phi'')^2 - J_\phi''^2 - (2J_\rho + 4\pi\hbar + J_\phi'')^2 + J_\phi''^2\right] , \tag{B.35}$$

From Eq. (B.35) we obtain:

$$H = \pm \frac{\omega}{2\pi}\left\{-4\pi\hbar(2J_\rho + J_\phi'') - 2\pi^2\hbar^2 + J_\phi''^2\right\}^{1/2} . \tag{B.36}$$

Case 4: $f(J_\rho')$ imaginary but $f(J_\rho' + 2\pi\hbar)$ real:

$$\frac{H^2}{\omega} + h^2\omega = \omega P_\phi'^2 + \frac{\omega}{8\pi^2}\left[-(2J_\rho + J_\phi'')^2 + J_\phi''^2 + (2J_\rho + 4\pi\hbar + J_\phi'')^2 - J_\phi''^2\right] . \tag{B.37}$$

From Eq. (B.37) we find:

$$H = \pm \frac{\omega}{2\pi} \{4\pi\hbar(2J_\rho + J''_\phi) + 4\pi^2\hbar^2 + J''^2_\phi\}^{1/2} \quad . \tag{B.38}$$

In the classical limit where $\hbar \to 0$ and $J'_\rho \to J_{\rho c}$, $J''_\phi \to J''_{\phi c}$, H must become H_c as given by Eq. (B.1). Cases 2, 3, and 4 all fail this test. Hence, we choose Eq. (B.32) as the Hamiltonian:

$$H = \pm \frac{\omega}{2\pi} (2J_\rho + J''_\phi + 2\pi\hbar) \tag{B.39}$$

where $f(J'_\rho)$ and $f(J'_\rho + 2\pi\hbar)$ are both real. For this choice of the Hamiltonian we have the right classical limit and have a Hamiltonian which is independent of w_ρ. Thus, conditions D and E in Chapter II are verified.

The Hamiltonian as given by Eq. (B.32) has not been completely specified since an overall sign has not been chosen. In order to choose this sign, we refer to the quantum Hamiltonian (B.6):

$$H = \frac{1}{\rho} P_\rho P + \frac{P'^2_\phi}{\rho^2} + \frac{1}{4}\omega^2\rho^2 \quad . \tag{B.6}$$

This Hamiltonian may be rewritten in the form:

$$H = \Lambda\Lambda^+ + \alpha\alpha^+ + \beta\rho^+ \tag{B.40}$$

where

$$\Lambda = \frac{1}{\rho} P_\rho \quad ,$$

$$\alpha = \frac{\sqrt{P'^2_\phi}}{\rho} \quad ,$$

$$\beta = \frac{1}{2}\omega\rho \quad .$$

Written in this form, $H(P,\rho)$ is the sum of three terms each of which is positive definite and hence each of which will have positive eigenvalues. Hence, $H(P,\rho)$ will have positive eigenvalues.

$H(J_\rho, J''_\phi)$, as given in Eq. (B.32), must also have positive eigenvalues if we are to conclude that we have made a valid cononical transformation. From Eq. (B.26) we have restricted our Hilbert space to states $|J'_\rho, J'_\phi\rangle$ such that:

$$J' \geq 0 \quad \text{or} \quad J'_\rho \leq -(J''_\phi + 2\pi\hbar) \quad . \tag{B.41}$$

Allowing $H(J_\rho, J''_\phi)$ to act on states of satisfying Eq. (B.41) we have:

$$H(J_\rho, J''_\phi)\,|J'_\rho, J'_\phi\rangle = \pm\frac{\omega}{2\pi}(2J'_\rho + J''_\phi + 2\pi\hbar)\,|J'_\rho, J'_\phi\rangle \quad . \tag{B.42}$$

Putting the values of Eq. (B.41) into Eq. (B.42) we find that the positive sign must be chosen for $J'_\rho \geq 0$ and the negative sign must be chosen for $J'_\rho \leq -(J''_\phi + 2\pi\hbar)$:

$$H(J_\rho, J''_\phi) = +\frac{\omega}{2\pi}(2J_\rho + J''_\phi + 2\pi\hbar) \quad \text{for} \quad J'_\rho \geq 0 \tag{B.43}$$

$$H(J_\rho, J''_\phi) = -\frac{\omega}{2\pi}(2J_\rho + J''_\phi + 2\pi\hbar) \quad \text{for} \quad J'_\rho \leq -(J''_\phi + 2\pi\hbar) \quad . \tag{B.44}$$

In order to make a choice between Eqs. (B.43) and (B.44) we need one more physical condition. For this we will use the commutator of $P\rho$ with $\frac{\omega}{2}\rho^2$.

The commutator of $P\rho$ with $\frac{\omega}{2}\rho^2$ is calculated using $[P,\rho] = \hbar/i$ and is:

$$[P\rho\ ,\ \frac{\omega}{2}\rho^2] \ = \ \frac{2\hbar}{i}\ (\frac{\omega}{2}\rho^2) \qquad . \tag{B.45}$$

Satisfying Eq. (B.45) using the transformation equations (B.8), (B.9), (B.10) and (B.2) will verify condition C (commutation of the transformation equations) and will further restrict the Hilbert space and thus make a choice between the Hamiltonians given in Eqs. (B.43) and (B.44). Substituting the transformation equations into Eq. (B.45) (with both $f(J'_\rho)$ and $f(J'_\rho + 2\pi\hbar)$ real) we find:

$$[\ \frac{1}{2}\ (d^+ + d),\ \frac{1}{2i}\ (d^+ - d) + \frac{1}{\omega}\ H(J_\rho, J''_\phi)\ ] \ = \ \frac{2\hbar}{i}\ [\ \frac{1}{2i}\ (d^+ - d) + \frac{1}{\omega}\ H(J_\rho, J''_\phi)\ ] \qquad . \tag{B.46}$$

From Eq. (B.46) we obtain:

$$-\ \frac{1}{2i}\ [d^+, d] + \frac{1}{2\omega}\ [d^+, H] + \frac{1}{2\omega}\ [d, H] \ = \ -\ \hbar d^+ + \hbar d + \frac{2\hbar}{i\omega}\ H \qquad . \tag{B.47}$$

Using the definitions of d, d^+ and H we can calculate each term on the left of Eq. (B.47). We now use the Hamiltonian as given in Eq. (B.32) with both signs and the definition of d^+, Eq. (B.10), to find:

$$\begin{aligned} \frac{1}{2\omega}\ [d^+, H] \ &= \ [f^+(J_\rho)\ e^{i2\pi w_\rho},\ \pm\ \frac{\omega}{2\pi}\ (2J_\rho + J'_\phi + 2\pi\hbar)\ ] \\ &= \ \pm\ f^+(J_\rho)[e^{i2\pi w_\rho},\ J_\rho] \\ &= \ \pm\ \hbar d^+ \qquad . \end{aligned} \tag{B.48}$$

Similarly, we find:

$$\frac{1}{2\omega}\ [d, H] \ = \ \pm\ \hbar d \qquad . \tag{B.49}$$

Finally, we calculate $-\frac{1}{2i}[d^+,d]$ using the definitions of d and d^+, Eq. (B.10):

$$-\frac{1}{2i}[d^+,d] = -\frac{1}{2i}\{f^+(J_\rho)f(J_\rho) - e^{-i2\pi w_\rho} f^+(J_\rho)f(J_\rho)\, e^{i2\pi w_\rho}\} \quad . \tag{B.50}$$

Using Eq. (B.28), $f(J\ )e^{i2\pi w} = e^{i2\pi w}\, f(J + 2\pi\hbar)$, Eq. (B.50) becomes:

$$-\frac{1}{2i}[d^+,d] = -\frac{1}{2i}\ f^+(J_\rho)f(J_\rho) - f^+(J_\rho + 2\pi\hbar)f(J_\rho + 2\pi\hbar) \quad . \tag{B.51}$$

We have restricted ourselves to states for which both $f(J_\rho)$ and $f(J_\rho + 2\pi\hbar)$, and we thus obtain:

$$-\frac{1}{2i}[d^+,d] = -\frac{1}{2i}\left(\frac{1}{4\pi^2}\right)\{(2J_\rho + J''_\phi)^2 - J''^2_\phi - (2J_\rho + 4\pi\hbar + J''_\phi)^2 + J''^2_\phi\}$$

$$= -\frac{\hbar}{\pi i}\{2J_\rho + J''_\phi + 2\pi\hbar\} \quad . \tag{B.52}$$

We have now calculated the three terms on the left side of Eq. (B.47). We now substitute Eqs. (B.48), (B.49) and (B.52) into their respective positions in Eq. (B.47) and find:

$$\mp\hbar d^+ \pm \hbar d - \frac{\hbar}{\pi i}\{2J_\rho + J''_\phi + 2\pi\hbar\} = -\hbar d^+ + \hbar d + \frac{2\hbar}{i\omega} H \quad . \tag{B.53}$$

The left side of Eq. (B.53) will equal the right side of Eq. (B.53) providing we choose the plus sign in Eq. (B.32) and hence choose Eq. (B.43) but reject Eq. (B.44) for the Hamiltonian:

$$H(J_\rho,J''_\phi) = +\frac{\omega}{2\pi}(2J_\rho + J''_\phi + 2\pi\hbar) \quad \text{for states with } J'_\rho \geq 0 \quad . \tag{B.43}$$

Thus the commutator of $P\rho$ with $\frac{\omega}{2}\rho^2$ will be satisfied if and only if the Hamiltonian is chosen as in Eq. (B.43) and the Hilbert space is restricted to those states having $J' \geq 0$.

Satisfying this commutator completes the verification of conditions A-F as given in Chapter II. We conclude, then, that the transformation equations (B.8), (B.9), (B.10) and (B.12) define a valid transformation from P and ρ to J_ρ and ω_ρ for the restricted or physical Hilbert space. Having completed our treatment of the transformation equations, we can now find the energy levels of $H(J_\rho, J''_\phi)$.

We find the energy levels of $H(J_\rho, J''_\phi)$ using Eq. (B.43). Allowing $H(J_\rho, J''_\phi)$ to act on a state $|J'_\rho, J'_\phi\rangle$, we have:

$$H(J_\rho, J''_\phi)|J'_\rho, J'_\phi\rangle = \frac{\omega}{2\pi}(2J'_\rho + J''_\phi + 2\pi\hbar)|J'_\rho, J'_\phi\rangle$$

$$= E'_n|J'_\rho, J'_\phi\rangle \qquad \text{(B.54)}$$

where $J'_\rho = 2\pi\hbar n_\rho$, $n_\rho = 0,1,2, \ldots$ and $J''_\phi = 2\pi\hbar m''$, $m'' = 0,1,2, \ldots$. Hence, the energy levels are:

$$E'_n = \hbar\omega(2n_\rho + m'' + 1) \quad . \qquad \text{(B.55)}$$

Gathering together the transformation equations, Hamiltonian, energy levels and Hilbert space we have:

$$P\rho = \frac{1}{2}(d^+ + d) \quad ,$$

$$\frac{\omega}{2}\rho^2 = \frac{1}{2i}(d^+ - d) + \frac{H(J_\rho, J''_\phi)}{\omega} \quad ,$$

$$d^{+} = \frac{1}{2\pi}\left[(2J_{\rho} + J''_{\phi})^{2}\right]^{1/2} e^{i2\pi w_{\rho}} ,$$

$$J''_{\varphi} = + \sqrt{J'^{2}_{\phi}} = + \frac{1}{2\pi}\sqrt{P'^{2}_{\phi}} ;$$

$$H(P,\rho) = \frac{1}{\rho} P\rho P + \frac{P'^{2}_{\phi}}{\rho^{2}} + \frac{1}{4}\omega^{2}\rho^{2} ,$$

$$H(J_{\rho},J_{\phi}) = \frac{\omega}{2\pi}(2J_{\rho} + |J_{\phi}| + 2\pi\hbar) ;$$

$|J'_{\rho},J'_{\phi}>$ restricted to $J'_{\rho} \geq 0$:

$$J'_{\rho} = 2\pi\hbar n_{\rho} , \quad n_{\rho} = 0,1,2,3, \ldots ,$$

$$J''_{\phi} = 2\pi\hbar m'' , \quad m'' = 0,1,2,3, \ldots ;$$

$$E_{n} = h\omega(2n_{\rho} + m'' + 1) .$$

This completes the treatment of the planar harmonic oscillator. All six conditions placed on a set of transformation equations have been verified. The Hamiltonian $H(J_{\rho},J'_{\phi})$ is independent of all coordinates and its energy levels have the trivial form (B.55) which agrees with normal quantum calculations. This calculation does show that it is possible to carry out the $(p,q) \rightarrow (J,w)$ transformation for a simple planar system.

VIII. APPENDIX C: LOCATION OF POLES OF $p^*(z',E')$ USING ZEROS OF THE WAVEFUNCTION

In order to evaluate the integral for J(E'), it is helpful to know as much as possible about the location of the singularities of $p^*(z',E')$. This is most easily done by retreating to our knowledge of the wavefunction $\langle z'|E'\rangle$ since, e.g., a zero of the wavefunction will be located at the same place as a pole of $p^*(z',E')$. This may be seen by noting that $p^*(z',E')$ is defined via $W_0(z',E')$ where:

$$\langle z'|E'\rangle \quad e^{iW_0(z',E')/\hbar} \quad , \tag{C.1}$$

$$p^*(z',E') \quad \frac{dW_0(z',E')}{dz'} \quad . \tag{C.2}$$

Using Eqs. (C.1) and (C.2) we have:

$$p^*(z',E') = \left(\frac{\hbar}{i}\right) \frac{1}{\langle z'|E'\rangle} \frac{d}{dz'} \left(\langle z'|E'\rangle\right) \quad . \tag{C.3}$$

From Eq. (C.3) it is clear that if $\langle z'|E'\rangle$ is analytic at a point z'_0, has nonzero derivatves and is itself zero at that point, then $p^*(z'_0,E')$ will have a pole at z'_0 with residue $\hbar/i$.

The advantage of studying the zeros of $\langle z'|E'\rangle$ instead of $p^*(z',E')$ itself is that the wavefunction satisfies a second-order differential equation. The problem of locating the zeros of solutions of second-order differential equations has been studied extensively and we need only refer to the relevant theorems. The mathematical discussion below follows in Ince (19) (see especially Chapter 21). The reader is referred to that source for a more complete treatment.

Any "self-adjoint" equation of the form:

$$\frac{d}{dS}\left[h(S)\frac{dw}{dS}\right] + k(S)w = 0 \qquad (C.4)$$

can be transformed to:

$$\frac{d^2}{dh^2}w + D(h)w = 0 \qquad (C.5)$$

where $dS = hdh$ and

$$d(h) - h(S)k(S) \quad . \qquad (C.6)$$

The theorems which we will use as invariant under such a transformation are written for equations of the form (C.5). As we will later discuss, this general form of the differential equation (C.5) is very useful to physicists since most Schrödinger's equations can be put in that form. Thus, the locations of many of the zeros of solutions of Schrödinger's equations may be found using the methods which we are now presenting.

We now quote from Ince (19), Chapter 21 (pp. 513-515) three theorems which depend only on D(z) and the properties of w(z). For proofs and background material on these theorems, the reader is referred to the above reference. These mathematical results are reproduced here as a convenience to the reader for the discussions which follow.

Four theorems which depend only on D(z) and properties of w(z) are:

Theorem A: "If w(z) is a solution which is real on a segment (a,b) of the real axis; if, further, T is a region symmetrically situated with respect to the real axis, and such that every

line perpendicular to the real axis which cuts the region cuts its boundary in two points and meets (a,b) in an interior point; and if finally $Re\{D(x)\} \geq 0$ throughout T, then w(z) can have no complex zero or extremum (i.e., $w\, dw/dz \neq 0$) in T."

Theorem B: "On the real axis, if throughout the interval (a,b), either $ReD(z) \leq 0$ or ImD(z) does not change sign, then there can be at most one zero of $w \frac{dw}{dz}$ in that interval (where w is a real function of z)."

Theorem C: "Let the region T be as before, and let w(z) be a solution, real on the segment (a,b) and such that in (a,b) $w \frac{dw}{dz}$ has a fixed sign; let $Im\{D(z)\}$ have this sign throughout that part of the region T which lies above the real axis, then w(z) can have no complex zero on extrememm in T."

The following theorem is a direct result of theorem C:

Theorem D: Let the region T be as before, and let w(z) be a solution, real on the segment (a,b) such that in (a,b) $w \frac{dw}{dz}$ has a fixed sign; let $Im\{D(z)\}$ have the opposite of this sign throughout that part of the region T which lies below the real axis, then w(z) can have no complex zero or extremum in T.

The final theorem which we will quote here deals with "the zero-free star." We consider a point a at which D(z) is regular but not zero. We define (following Ince (19)):

$$z = a + r e^{i\theta} \quad , \tag{C.7}$$

$$(z-a)^2 D(z) = P(z) + iQ(z) \quad , \tag{C.8}$$

$$D(z) = g_1(z) + ig_2(z) \quad , \tag{C.9}$$

where P, Q, g_1 and g_2 are real functions of z.

The curves P(z) = 0, Q(z) = 0 intersect at a with tangents having angles θ_1 and θ_2, with respect to the real axis given by:

$$P = 0: \quad g_1(a)\cos 2\theta_1 - g_2(a)\sin 2\theta_1 = 0 \quad ,$$

$$Q = 0: \quad g_2(a)\cos 2\theta_2 + g_1(a)\sin 2\theta_2 = 0 \quad . \tag{C.10}$$

Following Ince (19), the star originating at a is the set of straight line segments (rays) from a to p(θ) where p(θ) is defined as follows. Starting at the point a, move in the direction θ along a ray until Q changes sign. If along the ray P(z) has been positive or changed sign, then p(θ) is the point at which Q changes sign. If P(z) has been negative only, then one continues along the ray until P(z) changes sign and that point is defined as p(θ). If a singular point or zero of D(z) is located within the star, then it is excluded by a rectilinear cut going away from a. Given the above, the region of the plane which is excluded from the star consists of at least those points with P > 0 which lie between the branch of Q = 0 in P > 0 and the tangent to Q = 0 at z = a. This is illustrated in Figure 3. The theorem relating to the star is:

Theorem E: "If z = a is a zero of $w \frac{dw}{dz}$, then this product does not vanish at any point of the star belonging to a, including the nonsingular points of its boundary."

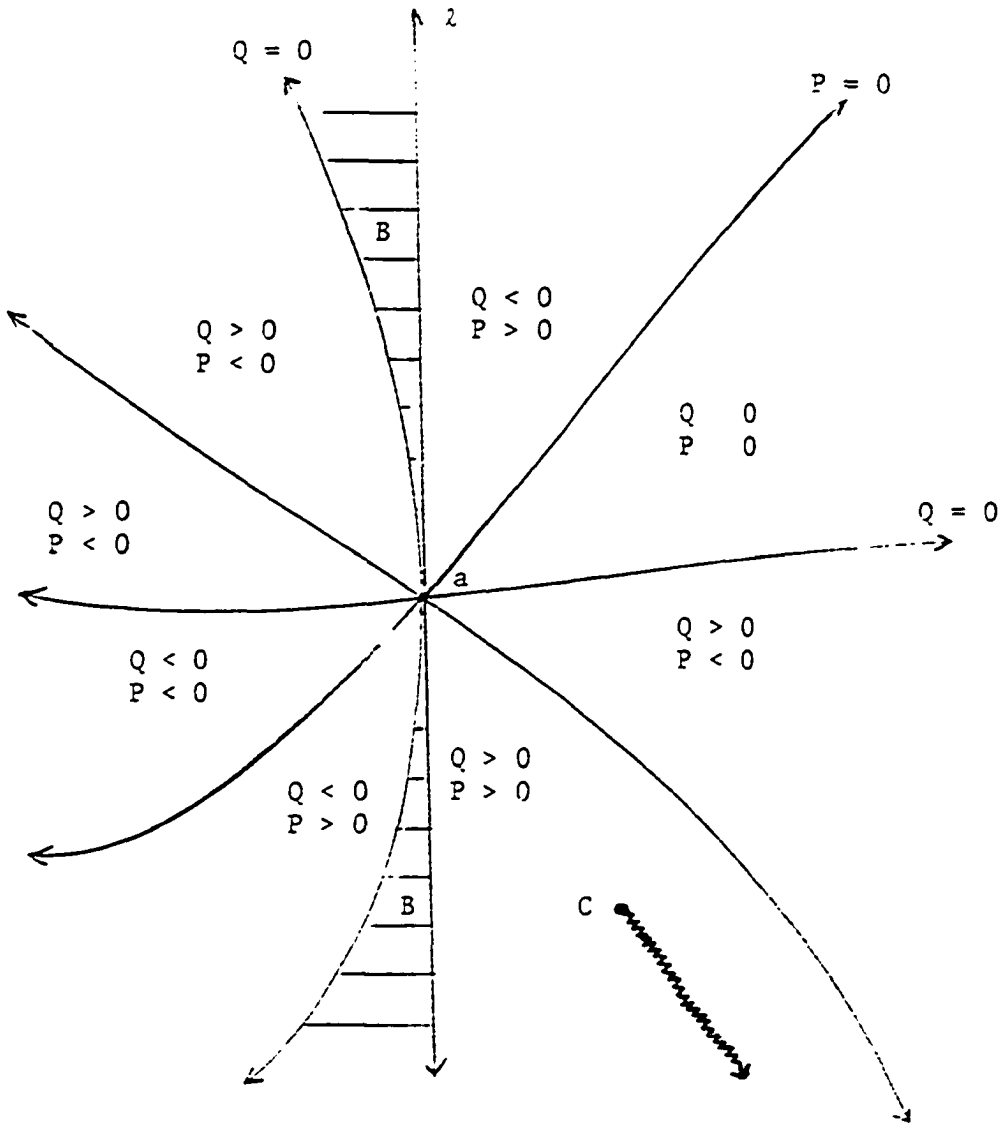

Figure 3. Illustration of a star. The line, ℓ, is the tangent to the curve, Q = 0, in the region having P > 0. The shaded region, B, is excluded from the star. The cut, C, begins at a singular point or zero of D(z) and is also excluded from the star

The importance of these theorems to physicists lies in the fact that virtually all one-dimensional Hamiltonians can be written in the form of Eq. (C.4) and transformed to the form (C.5): $2m = 1$

$$\frac{d^2}{dz^2} w + \frac{1}{\hbar^2} (E - V(z))w = 0 \quad , \tag{C.11}$$

$$D(z) = \frac{1}{\hbar^2} (E - V(z)) \quad . \tag{C.12}$$

From Eq. (C.11) for real E we have:

$$\mathrm{Re}\{D(z)\} = \frac{1}{\hbar^2} (E - \mathrm{Re}\ V(z)) \quad ,$$

$$\mathrm{Im}\{D(z)\} = -\frac{1}{\hbar^2} \mathrm{Im}\ V(z) \quad . \tag{C.13}$$

Knowing the potential allows one to apply the theorems. First, normally, physical potentials are real on the real axis. From this fact we have that solutions of Eq. (C.11) can be found which are real. Also we have ($z = x + iy$):

$$\mathrm{Im}\ D(z) = 0 \quad \text{for} \quad y = 0,\ z = x \quad , \tag{C.14}$$

$$\mathrm{Re}\ D(z) = \frac{1}{\hbar^2} (E - V(x)) \quad \text{for} \quad y = 0 \quad . \tag{C.15}$$

On the real axis we can use Eq. (C.15) to denote two regions for a potential as illustrated in Figure 4: the classical region for which $E \geq V$ and the nonclassical region in which $V > E$. Using Theorem B, in the nonclassical region, on the real axis, the wavefunction $w(z)$ (where $w(z) \equiv \langle z' | E' \rangle$, $z \equiv z'$) can have at most one zero or extremum,

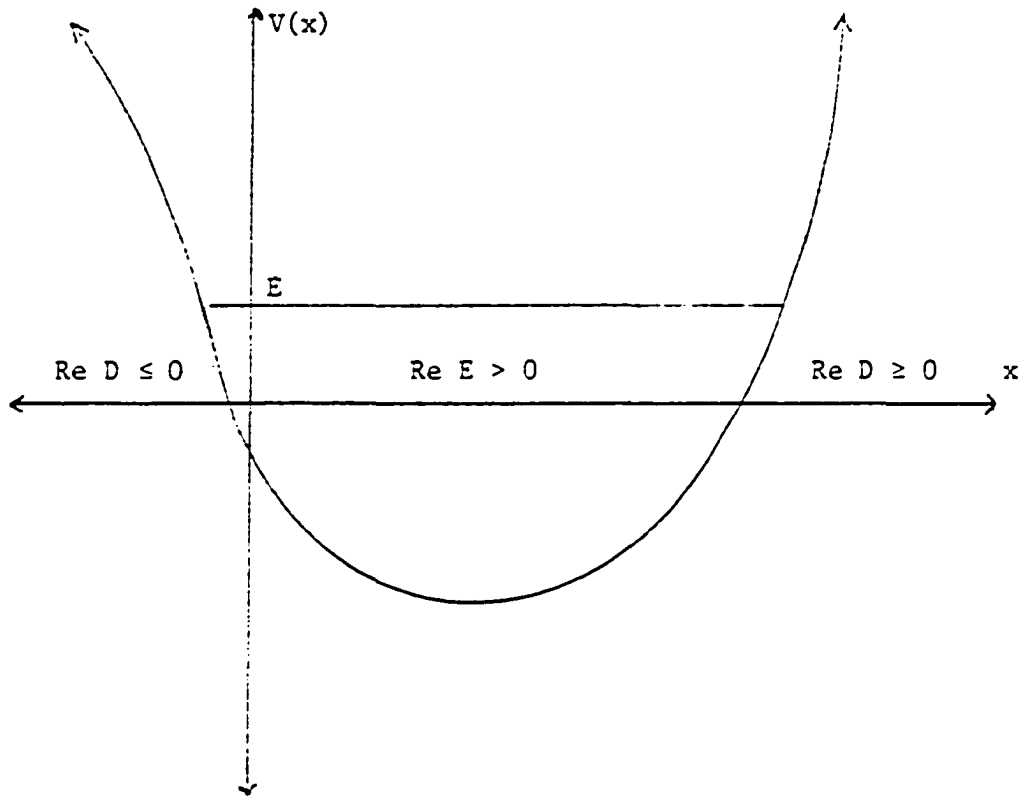

Figure 4. A typical simple potential

that is one zero of $w(x)\frac{dw}{dz}$ is at x = infinity (Ref. 22). It follows, then, that for an eigenstate, $w\frac{dw}{dz}$ does not change sign in a nonclassical region. Also, for an eigenstate (of a potential as in Figure 4) in the right nonclassical region, $w\frac{dw}{dz}$ is negative and in the left nonclassical region $w\frac{dw}{dz}$ is positive (where we have assumed that the zero of $w\frac{dw}{dz}$ is at x = infinity).

For a real potential, we see that Eq. (C.14) has Im D(z) = 0 on the real axis, for E real. Let us suppose that in the right nonclassical region Im D(z) < 0 for y > 0 and Im D(z) > 0 for y < 0 (i.e., Im D(z) < 0 above the real axis and Im D > 0 below the real axis). From Theorems C and D it follows that there are no zeros in this nonclassical region above or below the real axis, for any eigenstate of the system. Similar statements can be made about the left nonclassical region (i.e., above and below the real axis) as will be seen when we analyze the harmonic oscillator.

These and other ideas are most easily illustrated with some examples. The first one which we will consider is the harmonic oscillator. For this potential we have:

$$\frac{d^2w}{dz^2} + (E - \frac{1}{4}\omega^2 z^2)w = 0 \quad , \tag{C.16}$$

where 2m = 1, $\hbar$ = 1, and where E is real and positive. From Eq. (C.16) we have:

$$D = E - \frac{1}{4}\omega^2 z^2 \tag{C.17}$$

$$\text{Re } D = E - \frac{1}{4}\omega^2(x^2 - y^2) \tag{C.18}$$

$$\text{Im } D = -\frac{1}{2}\omega^2 xy \quad . \tag{C.19}$$

The various D regions are illustrated in Figures 5 and 6.

Let us assume that Eq. (C.16) has been solved for real w(z). Then, using Theorem A, it follows from Figure 6 and Eq. (C.18) that the region T_0 has no complex zeros or extremum for any energy, E. Applying Theorems C and D to regions T_1, T_2, T_3 and T_4 (see Figures 5 and 6), it follows that at an eigenstate these regions have no zeros of $w\frac{dw}{dz}$. From Theorem B, it follows that at an eigenstate on the real axis with $|\text{Re}| \geq (4E/w^2)^{1/2}$, the only zeros are at Re(z) = infinity. Thus, at an eigenstate the zeros of w(z) are restricted to be at Re(z) = infinity and on the real axis in the interval $((4E/w^2)^{1/2}, -(4E/w^2)^{1/2})$. There are no other zeros in the complex plane. Hence, form Eq. (C.3) $p^*(z',E')$ may have poles only at Re(z) = infinity and on the real axis in the classical region. When one is not at an eigenstate of the system, $p^*(z',E')$ is allowed to have poles off the real axis in regions T_1, T_2, T_3 and T_4 of Figure 6. Thus, an eigenstate has a simpler singularity for $p^*(z',E')$.

An example in which the "star" technique is useful is the Coulomb potential. When placed in the form of Eq. (C.5), Schrödinger's equation for the radial coordinate is:

$$\frac{d^2w}{dz^2} + (E - \frac{L}{z^2} + \frac{g}{z})w = 0 \quad , \tag{C.20}$$

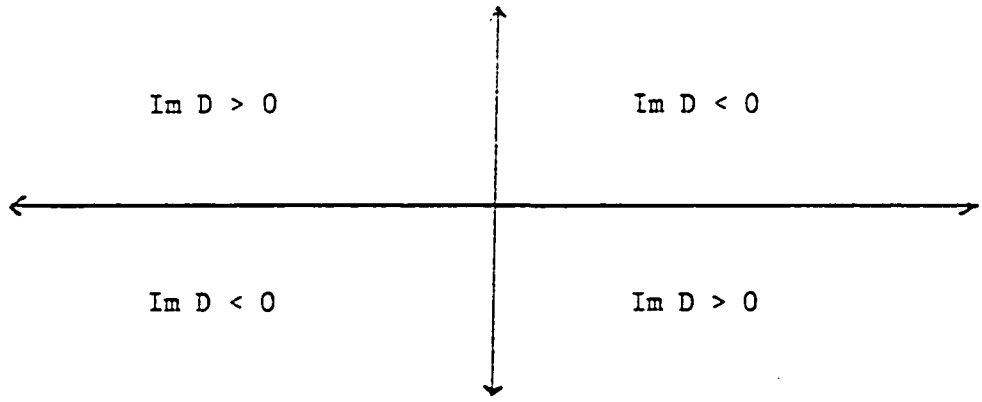

Figure 5. Regions of Im D as given by Eq. (C.19). Note that the lines $x = 0$ and $y = 0$ have Im D = 0

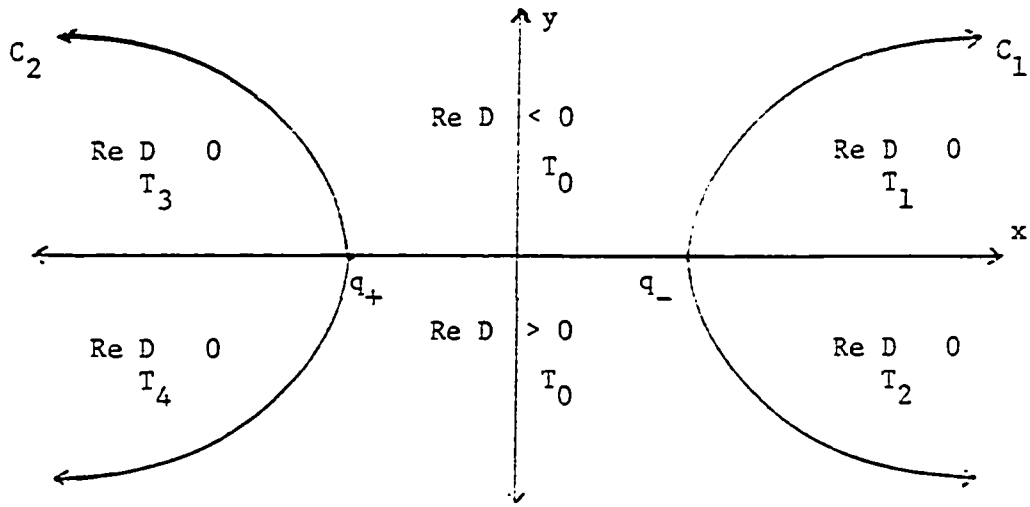

Figure 6. Regions of Re D as given by Eq. (C.18). Note that the curves C_1 and C_2 have Re D = 0. The points, q_+ and q_-, are the classical turning points where $q_\pm = \pm(4E/\omega^2)^{1/2}$

where E is real, $2m = 1$, $\hbar = 1$, $g > 0$ (and real), and where $L = \ell(\ell + 1)$, ($\ell = 0, 1, 2, \ldots$). The real and imaginary parts of D(z) are:

$$\text{Re } D = E - \frac{L(z^2 - y^2)}{(x^2 + y^2)^2} + \frac{gx}{x^2 + y^2} \quad ,$$

$$= E - \frac{L \cos(2\theta)}{r^2} + \frac{g \cos\theta}{r} \qquad (z = r\, e^{i\theta}) \quad , \tag{C.21}$$

$$\text{Im } D = \frac{2L\, xy}{(x^2 + y^2)^2} - \frac{gy}{x^2 + y^2} \quad ,$$

$$= \frac{2L \cos\theta \sin\theta}{r^2} - \frac{g \sin\theta}{r} \quad . \tag{C.22}$$

For $E < 0$, there are two classical turning points on the real axis, z_1 and z_+ ($z_+ > z_-$), where $D(z_+) = D(z_-) = 0$. Between z_- and z_+, Re D > 0, and Re $D \leq 0$ for all other points on the real axis (excluding the point $z = 0$). In the region on the real axis having $z > z_+$ (to the right of z^+), Re $D \leq 0$ and Theroem B tells us that $w \frac{dw}{dz}$ will have at most one zero. Let us assume that this zero is at $z = a$ (on the real axis). From the definition of the star using Eqs. (C.8) and (C.9) and the equations for Re D and Im D, Eqs. (C.21) and C(.22), the star for the Coulomb problem is defined by:

$$(z - a)^2 \{E - \frac{L}{z^2} + \frac{g}{z}\} = P(z) + iQ(z) \quad . \tag{C.23}$$

From Eq. (C.23) we find:

$$P(z) = E[(x-a)^2 - y^2] - \frac{L}{r^4} (x^2(r-a)^2 - x^2y^2 + 4xy^2(x-a) + y^4 - y^2(x-a)^2)$$

$$+ \frac{g}{r^2}\left[x(x-a)^2 - xy^2 + 2y^2(x-a)\right] \quad , \tag{C.24}$$

$$Q(z) = 2Ey(x-a) - \frac{L}{r^4}\left[2xy^3 - 2xy(x-a)^2 + 2x^2y(x-a) - 2y^3(x-a)\right]$$

$$+ \frac{g}{r^2}\left[y^3 - y(x-a)^2 + 2xy(x-a)\right] \quad . \tag{C.25}$$

The star originating at $x = a$ as generated by Eqs. (C.24) and (C.25) is pictured in Figure 7. Referring to Theorem E, we see that there are no zeros of we to the left or right of the shaded regions in Figure 7, excluding the cut on the real axis which begins at z_+ where $D(z_+) = 0$. At an eigenstate $a \to +\infty$, and there are no zeros of w off the real axis in the finite z plane. At an eigenstate the only zeros of w are on the real axis between z_- and z_+, i.e., in the classical region.

On the real axis, the intervals from z_+ to $+\infty$ and from z_- to $-\infty$ each have Re $D \leq 0$ (see (Eq. (C.21)). In these intervals w(z) has at most one zero. The zeros of w are at $z = 0$ and $z = a = +\infty$ for an eigenstate. Thus, the zeros of $w \frac{dw}{dz}$ and the poles of $p^*(z',E')$ in the finite z'-plane are only allowed on the real axis between z_- and z_+, at $z = 0$ and at $z = a = +\infty$ at an eigenstate.

The point $z = a = +\infty$ can be studied more closely in order to verify that there are no zeros of $w \frac{dw}{dz}$ "above" or "below" that point. This is done by transforming Schrödinger's euqation (C.20), using $z' = S^{-1}$:

$$\frac{d^2w}{dS^2} + \left\{ \frac{E}{S^4} - \frac{L}{S^2} + \frac{g}{S^3} \right\} w = 0 \quad . \tag{C.27}$$

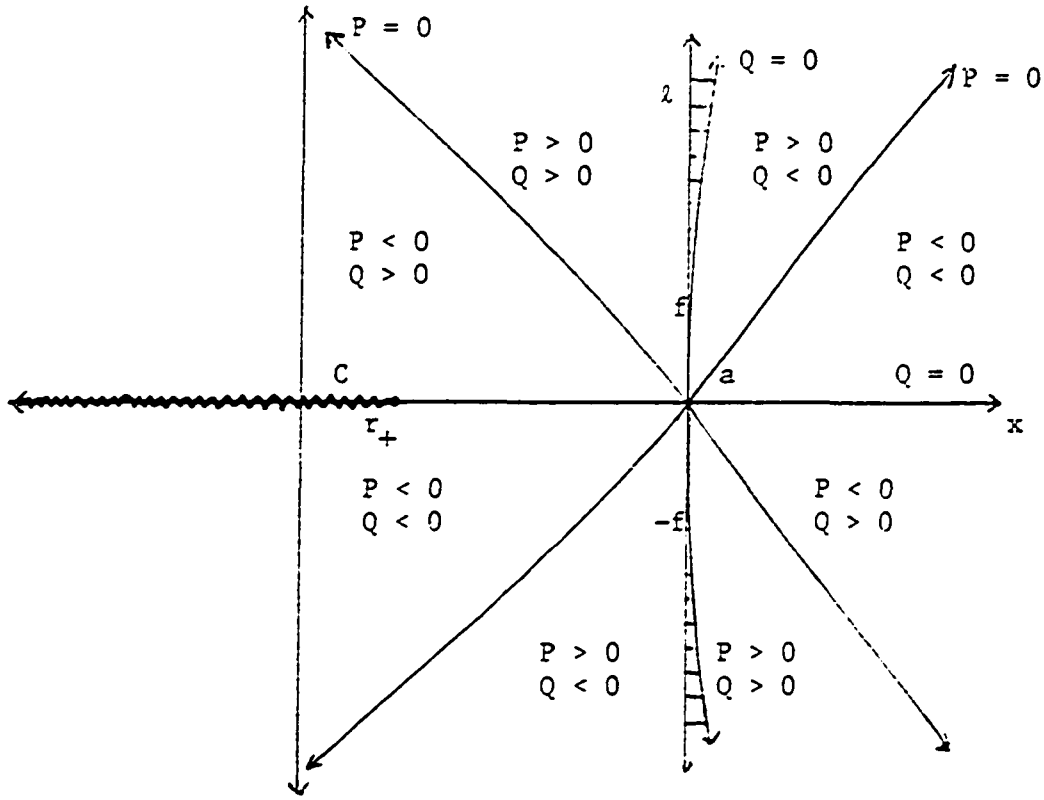

Figure 7. Illustration of the star at the zero, x = a, for the radial Coulomb problem with $0 > E > -(g^2/4L)$. The cut, C, which begins at the right classical turning point, r_+, and the shaded region are excluded from the star. The line, ℓ, is the tangent to Q = 0 at z = a (in the region having P > 0)

$$\text{Re } D(S) = t^{-4} E \cos 4\theta - Lt^{-2} \cos 2\theta + gt^{-3} \cos 3\theta \quad , \qquad \text{(C.28)}$$

$$\text{Im } D(S) = - t^{-4} E \sin 4\theta + Lt^{-2} \sin 2\theta - gt^{-3} \cos 3\theta \quad . \qquad \text{(C.29)}$$

At $S = 0$, we have Im $D(S) > 0$ for $\theta = \pi/2$ and Im $D(S) < 0$ for $\theta = -\pi/2$. On the real axis the sign of $w \frac{dw}{dz}$ is negative for $z \to \pm\infty$. Thus, at $S = 0$, the sign of $w \frac{dw}{dz}$ is thus negative since it is negative in the limit of $S \to +0$ and $S \to -0$ (i.e., $z \to \pm\infty$). The sign of $w \frac{dw}{dz}$ is given by: $w \frac{dw}{dz} = - S^2 w \frac{dw}{dS}$. Thus, $w \frac{dw}{dS}$ is positive at $S = 0$. With this assignment of the sign of $w \frac{dw}{dS}$ and Theorems C and D, there are no zeros of $w \frac{dw}{dS}$ on the line through $S = 0$ with $\theta = \pm\pi/2$, at an eigenstate of the system. This completes the specification of the zeros of $w \frac{dw}{dz}$ at an eigenstate. Thus, all of the zeros of $w \frac{dw}{dz}$ for the attractive Coulomb potential at an eigenstate are limited to the real axis in the classical region, plus one at $z = 0$ and one at $x = +\infty$ ($S = 0$).

This completes our treatment of the Coulomb problem. Other problems and potentials are similarly handled. If severe difficulties arise, a reference to consult is Ince (19), Chapter 21. While we do not say that for all physical potentials, eigenstates have all zeros of $w \frac{dw}{dz}$ on the real axis, a trend does seem to exist and a proof of such a proposition would be quite convenient when one attempts to evaluate the contour integrals which define $J'(E')$ at an eigenstate.

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