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Hamilton-Jacobi/action-angle quantum mechanics

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A quantum mechanics is constructed which is patterned on classical Hamilton-Jacobi theory. The dynamical basis of the theory is a quantum Hamilton-Jacobi equation with accompanying physical boundary conditions. Basic objects of the formulation are quantum Hamilton's principal and characteristic functions. As an application of the formalism a theory of quantum action-angle variables is set up. The central feature of this theory is the definition of the quantum action variable which permits the determination of the bound-state energy levels without solving the dynamical equation.

I. INTRODUCTION/OVERVIEW

The theory of transformations from one set of canonically conjugate coordinates and momenta to another set is well developed in classical mechanics. In quantum mechanics, however, it is only somewhat recently that transformation theory has been extensively examined.

Quantum canonical transformation theory appears to have its start in papers by Jordan[1] and Dirac.[2] Jordan invents the notion of a well-ordered operator by which he is able to cast quantum transformation equations in the same form as the corresponding classical equations. Dirac's approach to quantum transformation theory is based upon his interpretation of the quantity $(\xi' \mid \alpha')$ as the "transformation function" which connects the ξ representation to the α representation. By defining S via $(\xi' \mid \alpha')=\exp(iS/\hbar)$ he demonstrates that quantum transformation equations obtain which have the same form as the classical equations.[2] In later papers[3] and in his text[4] Dirac interprets the S defined via the transformation function as the quantum analog of the classical action function.

The next developments in quantum transformation theory appear later in the investigations of Feynman and Schwinger. It is possible to characterize the path-integral formulation of quantum mechanics[5-7] as a transformation theory, and there are close correspondences between the path integrals and the transformation theories of Dirac and of Schwinger. For example, writing Feynman's principle as $(x' \mid x)=\sum \exp[iS_c(x',x)/\hbar]$, where S_c is the classical action and $\sum$ is a sum over all paths between x and x', one sees the correspondence between this principle and the Dirac definition of a quantum S.

The most complete examination of transformation theory in a quantum context is Schwinger's monograph[8] in which variations of states, eigenvalues, and operators are used as a basis for constructing a quantum transformation theory. For transformations through time, Schwinger's action principle is[6-8]

$$\delta(x_2' \mid x_1')=(i/\hbar)(x_2' \mid \delta S(x_2,x_1) \mid x_1') ,$$

where the dynamical postulate is that the operators δS can be obtained by variation of one operator S. Putting S in a well-ordered form, the action principle can be integrated[7,8] to give $(x_2' \mid x_1')=\exp(iS(x_2',x_1')/\hbar)$ which is of the same form as Dirac's original expression; this shows the correspondence between the action principle and the Dirac definition of S.

Quantum transformation theory, as developed in this paper, is a generalization of classical Hamilton-Jacobi theory. This transformation theory is a formulation of quantum mechanics in the same sense that classical Hamilton-Jacobi theory is a formulation of classical mechanics. The basis of the theory is a quantum Hamilton-Jacobi equation. This Hamilton-Jacobi equation, with its accompanying physical boundary condition, is a dynamical equation equivalent in physical content to the Schrödinger equation, to the Heisenberg equations of motion, or to the more recent quantum dynamical principles. The solutions of the Hamilton-Jacobi equation are quantum Hamilton's principal and characteristic functions; these complex functions describe the system motion, and, in addition, enable one to complete Hamilton's original program of associating a (now true) wave with a particle motion.

While the quantum Hamilton-Jacobi theory is general, the central application in this paper is to a theory of the stationary state. By focusing upon Hamilton's characteristic function a quantum theory of action-angle variables is constructed. The basic object of this theory is the quantum action variable which is defined as an integral of a quantum momentum function. The quantum action variable gives the energy levels of the system directly; it is not necessary to solve the equation of motion. This powerful result is analogous to the classical action variable giving the frequencies of the system directly.

The quantum action variable can be viewed as completing the program begun by Wilson and Sommerfeld.[9] In the Wilson-Sommerfeld quantization rule the quantum energy levels are given (approximately) by setting the classical action variable equal to an integer multiple of Planck's constant. In the formalism presented here the quantum energy levels are given (exactly) by setting the quantum action variable equal to an integer multiple of Planck's constant.

Section II is an introduction to a quantum Hamilton-Jacobi theory; Sec. III contains the definition of the quantum action variable; the quantum momentum function and physical boundary conditions are defined also; Sec. IV includes an examination of the angle variable function and the characteristic function; Sec. V contains the classical limit of the quantum quantities; Secs. VI and VII give a number of illustrations of the use of the quantum action variable, while Sec. VIII returns to the general Hamilton-Jacobi theory again in connection with dynamics. Appendices A—D contain A: Operators, B: Semiclassical Forms, C: The Connection between the Hamilton-Jacobi and WKB Formalisms, and D: Momentum Function Poles.

II. HAMILTON-JACOBI THEORY

Hamilton-Jacobi theory has four parts: the transformation equations, the Hamilton-Jacobi equation, the definition of the new momenta, and the temporal aspects of the theory.[10] All four parts are considered here, but the dynamics is examined in more detail in Sec. VIII.

We concentrate on systems which are governed by a Hamiltonian that is independent of the time. For systems with a Hamiltonian free of the time one can choose as the generating function either Hamilton's principal function or Hamilton's characteristic function.[10] Hamilton's characteristic function is examined first.

The system considered first is a particle moving on a straight line under the influence of a potential V. In the Schrödinger representation the Hamiltonian is[11]

$$\begin{aligned}&\hat{H}\equiv H(\hat{x},\hat{p})=\hat{p}^2+V(\hat{x})\ ,\\&\hat{x}=x,\ \ \hat{p}=(\hbar/i)\partial/\partial x\ ,\end{aligned}\tag{2.1}$$

where $\hat{x}$ is the linear coordinate operator and $\hat{p}$ is the momentum operator conjugate to $\hat{x}$.

For the system defined by (2.1) a quantum canonical transformation to a new set of coordinates $\hat{Q},\hat{P}$ is sought such that the transformed Hamiltonian is free of $\hat{Q}$. We stress eigenvalues instead of operators; thus, we write the theory in terms of the eigenvalues and functions of eigenvalues x, p, Q, P, and E instead of in terms of the corresponding operators $\hat{x}$, $\hat{p}$, $\hat{Q}$, $\hat{P}$, and $\hat{H}$.[12] Using these quantities, the *quantum canonical transformation* has the same form as the classical transformation, i.e.,[1–3,10]

$$\begin{aligned}&p=\partial W(x,E(P))/\partial x\ ,\\&Q=\partial W(x,E(P))/\partial P\ .\end{aligned}\tag{2.2}$$

We interpret the quantity $W(x,E(P))$ as the *quantum Hamilton's characteristic function.*

Given the transformation relationships (2.2) it is possible to construct the quantum form of the Hamilton-Jacobi equation; this equation defines the quantum characteristic function $W(x,E(P))$. Given (2.1) and (2.2), and following the classical theory, the *quantum Hamilton-Jacobi equation* is postulated as[13]

$$\frac{\hbar}{i}\frac{\partial^2 W(x,E)}{\partial x^2}+\left[\frac{\partial W(x,E)}{\partial x}\right]^2=E-V(x)\ ,\tag{2.3}$$

where $W(x,E)$ is the generating function of (2.2), $V(x)$ is the potential of (2.1), and E is the energy eigenvalue.

Physical arguments lead to boundary conditions which $W(x,E)$ must satisfy and which complete its definition. We leave the specification of the boundary conditions and a detailed discussion of the quantum Hamilton-Jacobi equation to following sections.

The third ingredient in a quantum Hamilton-Jacobi theory is the definition of the new momentum P. In the context of the theory, one is free to choose any definition of P provided P is defined only in terms of E; a particular example, the action variable, is given in Sec. III. We write the defining relationship between the eigenvalues P and E as

$$P=P(E)\ \text{or}\ E=E(P)\ ,\tag{2.4}$$

and (2.4) can be used in (2.2) to complete the canonical transformation equations.[14] Equations (2.4) are independent of the rest of the theory.

Equations (2.1) to (2.4) form an outline of the first three parts of a quantum theory based upon a quantum Hamilton's characteristic function. The time is absent from the formalism, and we turn now to the time dependence to put the theory in perspective. Following the classical theory again, and using (2.3) as a guide, the *quantum Hamilton-Jacobi equation for Hamilton's principal function* S is postulated as[13]

$$\frac{\hbar}{i}\frac{\partial^2 S}{\partial x^2}+\left[\frac{\partial S}{\partial x}\right]^2=-\frac{\partial S}{\partial t}-V(x)\ ,\tag{2.5}$$

where $V(x)$ is the potential of (2.1) and t is the time. Equation (2.5) is the temporal analog of (2.3). The transformations generated by S are different in character than those generated by W. There is one case, however, where there is a relation between S and W. For states of definite energy E one can separate off the time by writing

$$S=W-Et\ ,\tag{2.6}$$

where W does not depend upon t. Use of the special form (2.6) in (2.5) yields (2.3) immediately. We conclude that the time-independent Hamilton-Jacobi theory based upon Hamilton's characteristic function W is a quantum theory of stationary states in that the transformation defined by the theory is time independent, and takes place for states of definite energy.

The generalization of the Hamilton-Jacobi equation (2.3) to two or three dimensions is

$$-i\hbar\nabla\cdot\nabla W+\nabla W\cdot\nabla W=E-V\ ,\tag{2.7}$$

when the Hamiltonian is the two- or three-dimensional generalization of (2.1); ∇ is the gradient operator. In (2.7) W has as its arguments, e.g., three "old" coordinates and three "new" momenta.

Before returning to an examination of quantum Hamilton-Jacobi theory in Sec. VIII we use (2.1)—(2.4) to construct quantum action-angle variables; these variables $\hat{w},\hat{J}$ are a particular case of the conjugate set $\hat{Q},\hat{P}$ considered in this section.

III. ACTION VARIABLE/MOMENTUM FUNCTION

In this section we define the quantum action variable. We continue to consider the one-dimensional system defined by the Hamiltonian (2.1). Since classical action-angle variables are defined for systems that undergo periodic motion, it is assumed that the potential $V(x)$ is such as to allow periodic motion and that the energy eigenvalues considered are those of bound states.

The classical action variable is defined as the integral over one cycle of a classical momentum function. We assume that a similar integral definition can be constructed in the quantum case. The first of the transformation equations (2.2) can be used to define a momentum function in terms of x and E. Thus, we define a *quantum momentum function* $p(x,E)$ in terms of the quantum characteristic function $W(x,E)$ by[15]

$$p(x,E)\equiv\partial W(x,E)/\partial x \ . \tag{3.1}$$

Definition (3.1) requires one to know $W(x,E)$; we can avoid the dependence of $p(x,E)$ on $W(x,E)$ by using (3.1) in the quantum Hamilton-Jacobi equation (2.3); this yields

$$\begin{aligned}\frac{\hbar}{i}\frac{\partial p(x,E)}{\partial x}+p^2(x,E)&=E-V(x)\\ &=p_c{}^2(x,E) \ .\end{aligned} \tag{3.2}$$

We call (3.2) the *quantum momentum function equation,* and it specifies $p(x,E)$ once the physical boundary conditions for $p(x,E)$ are established.

We state the boundary conditions which complete the definition of the quantum momentum function $p(x,E)$ in terms of the classical momentum function. The *classical momentum function* $p_c(x,E)$ is defined by Eq. (3.2), and by the following rule: From (3.2) $p_c(x,E)=[E-V(x)]^{1/2}$. The turning points x_1 and x_2 are defined by the vanishing of $p_c(x,E)$, i.e., by $p_c(x_1,E)=p_c(x_2,E)=0$. The complex x plane on which $p_c(x,E)$ is defined is given a cut connecting the two branch points, i.e., a cut from x_1 to x_2. $p_c(x,E)$ is defined as that branch of the square root which is positive along the bottom of the cut. A picture of the cut x plane is shown in Fig. 1(e).

Given the above definition of the classical momentum function $p_c(x,E)$, we state the physical condition which completes the definition of the quantum momentum function $p(x,E)$ as

$$p(x,E)\underset{\hbar\to 0}{\longrightarrow}p_c(x,E) \tag{3.3}$$

for all x, with E fixed. Requirement (3.3) has two interpretations: as a form of the *correspondence principle,* and as a *boundary condition* on $p(x,E)$.

$p_c(x,E)$ is defined above as a particular branch of the square root $(E-V(x))^{1/2}$, while $p(x,E)$ is given by (3.2). In (3.2) the term $(\hbar/i)\partial p(x,E)/\partial x$ acts as a mixer so that, in general, the solutions of (3.2) have the character of both of the branches of the classical $p_c(x,E)$. Thus, viewed as a correspondence principle, it is seen that (3.3) restricts the physical $p(x,E)$ to have a character like the physical $p_c(x,E)$; a character like the unphysical branch of $p_c(x,E)$ is ruled out.

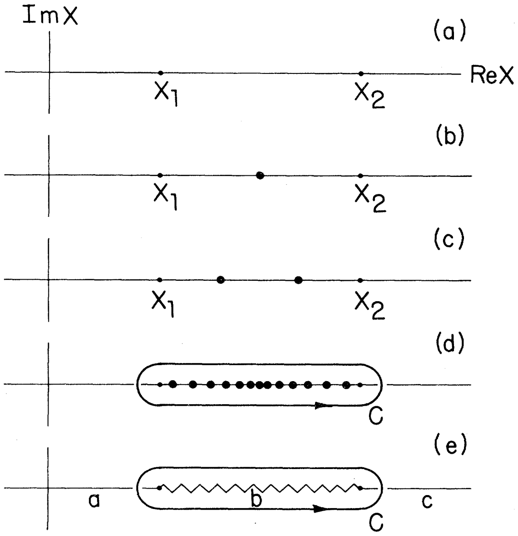

FIG. 1. The complex x plane on which the classical $p_c(x,E)$ and quantum $p(x,E)$ momentum functions are defined. The turning points are x_1 and x_2. The x plane showing (a) no poles of $p(x,E)$ for the ground state, (b) one pole (large dot) of $p(x,E)$ for the first excited state, and (c) two poles (large dots) for the second excited state. (d) The x plane showing the 13 poles (large dots) of $p(x,E)$ for the thirteenth excited state. The contour C enclosing x_1,x_2, and the poles is used in defining the quantum action variable (3.4). (e) The x plane showing the cut (zig-zag line) of the classical momentum function $p_c(x,E)$. The contour C enclosing x_1,x_2, and the cut is used in defining the classical action variable; see Sec. III. The regions designated a, b, and c occur in the discussion of the classical limit of the theory.

The second interpretation of (3.3) is that it is a boundary condition on $p(x,E)$. Consider a point in the x plane, e.g., far out on the real x axis, where the $(\hbar/i)\partial p(x,E)/\partial x$ term in (3.2) is not, usually, important. Then, from (3.2), $p^2(x,E)\simeq p_c{}^2(x,E)$, and the role of (3.3) is to select which sign to take in $p(x,E)\simeq\pm p_c(x,E)$. Equation (3.3) gives $p(x,E)\simeq p_c(x,E)$ at such points. But, since $p_c(x,E)$ is known, the requirement that $p(x,E)\simeq p_c(x,E)$ is a boundary condition because it selects the physical value of $p(x,E)$ at x.

Having defined the quantum momentum function $p(x,E)$, we define the quantum action variable by generalizing the classical definition. The classical action variable can be defined as the integral $(1/2\pi)\int dx\, p_c(x,E)$, where the integral is around a closed contour C. The contour C encloses the cut of $p_c(x,E)$ which runs between the turning points x_1 and x_2; C is shown in Fig. 1(e). Following this definition, we define the *quantum action variable* by

$$J=J(E)\equiv(1/2\pi)\int_C dx\, p(x,E) \ , \tag{3.4}$$

where $p(x,E)$ is the quantum momentum function, and where C is the contour defined immediately above [see Fig. 1(d)]. Definition (3.4) connects the action-variable eigenvalues J to the energy eigenvalues E.

In order to use (3.4) it is necessary to obtain the eigenvalues J. Equations (3.2) and (3.3) imply that $p(x,E)$ has poles of residue $\hbar/i$ on the Rex axis between the turning points x_1 and x_2. For the ground state, first excited state, second excited state,..., $p(x,E)$ has zero, one, two,..., poles, respectively, in the potential well. The number of poles of $p(x,E)$ in the well gives the excitation level of the system. (For further discussion of these poles see Sec. V and Refs. 16 and 17.) Since the poles of $p(x,E)$ are enclosed by the contour C, one has from (3.4)

$$J=n\hbar=J(E)\ , \tag{3.5}$$

where $n=0,1,2,\ldots$, and where E is the energy eigenvalue that is correlated with the value $n\hbar$ for J. The situation leading to (3.5) is illustrated in Figs. 1(a)—1(d).

Equation (3.4) can be inverted. Thus, one has

$$J=J(E) \text{ or } E=E(J)\ , \tag{3.6}$$

where we distinguish between quantities and functions by writing the arguments.[14] Applications of (3.2)—(3.6) are given in Secs. VI and VII.

IV. CHARACTERISTIC FUNCTION/ANGLE VARIABLE

In this section we examine the quantum characteristic function and the angle variable function.[18,19]

In terms of Hamilton's characteristic function $W(x,E(J))$ the canonical transformation equations are, from (2.2),

$$\begin{aligned} p&=\partial W(x,E(J))/\partial x\ ,\\ w&=\partial W(x,E(J))/\partial J\ , \end{aligned} \tag{4.1}$$

where $E(J)$ is given by (3.6). The characteristic function $W(x,E(J))$ is given by the Hamilton-Jacobi equation (2.3), and physical boundary conditions which are yet to be specified. However, an alternative and equivalent method of obtaining $W(x,E)$ is to integrate (3.1); this yields

$$W(x,E)=\int_{x_0}^{x} dx'p(x',E)+W_0(E)\ , \tag{4.2}$$

where the path of integration from x_0 to x in the complex x plane has yet to be specified, and where $W_0(E)$ is some function of the energy eigenvalue E.

In order to construct paths of integration to use in (4.2), it is useful to examine the classical analog of (4.2). The classical characteristic function $W_c(x,E)$ can be specified by an equation of the same form as (4.2) with the quantum $p(x,E)$ replaced by the classical $p_c(x,E)$. $p_c(x,E)$ has a cut from x_1 to x_2 on the Rex axis so the paths of integration should not cross the cut, and, further, should not be allowed to encircle the cut, since multivaluedness would result.

Returning to the quantum characteristic function $W(x,E)$, we follow the classical path restrictions for the integral (4.2). Under these conditions we assert

$$W(x,E)\underset{\hbar\to 0}{\longrightarrow} W_c(x,E) \tag{4.3}$$

for all x, with E fixed. Requirement (4.3) is analogous to (3.3) for the momentum function $p(x,E)$, and can be viewed as a correspondence principle or as a boundary condition. Thus, $W(x,E)$ can be defined either by (4.2) and (4.3), or by (2.3) and (4.3).

Given a definition of $W(x,E)$, and the earlier definition of the action variable $J(E)$ [or $E(J)$], we return to the second of (4.1) and define an *angle variable function* $w(x,J)$ by[20]

$$w(x,J)\equiv\partial W(x,E(J))/\partial J\ . \tag{4.4}$$

In the classical theory the angle variable advances by 2π every time the particle completes one cycle in the potential well. We ask how $w(x,J)$ changes when x changes through one cycle with J fixed. The quantum analog of "x changing through one cycle" is the path C in the complex x plane encircling the segment of the Rex axis between x_1 and x_2; C was used in defining $J(E)$ in (3.4). We define the change in $w(x,J)$ as

$$\Delta w(J)\equiv \int_C dx\ \partial w(x,J)/\partial x=2\pi\ . \tag{4.5}$$

The first of (4.5) defines the change $\Delta w(J)$ as an integral in the x plane, while the second claims that $\Delta w(J)$ is always 2π.

To establish the validity of (4.5) one uses (4.4) and (3.1) to rewrite the integrand of the integral in (4.5); then, changing the order of differentiation, one obtains $(\partial/\partial J)\int dx\, p(x,E)$. The integral is just $2\pi J$ by (3.4); so, one obtains the second of (4.5).

The result that $\Delta w(J)=2\pi$ for all J suggests that $\hat{w}$ is an anglelike quantum coordinate. Since the action variable $\hat{J}$ is conjugate to $\hat{w}$, this suggests that the J eigenvalues are given by $J=n\hbar$ with n integer, as was obtained in Sec. III by more direct means.

V. CLASSICAL LIMIT

Semiclassical expressions for the quantum functions $p(x,E)$ and $W(x,E)$ are used to examine the classical limit of the theory. We continue to consider bound-state motion.

The classical quantities needed in the semiclassical approximation are the classical momentum function $p_c(x,E)$ defined in Sec. III, and the classical characteristic function $W_c(x,E)$. The characteristic function is

$$W_c(x,E)=\int_{x_1}^{x} dx'p_c(x',E)\ . \tag{5.1}$$

For the purposes of this section, the path of integration in (5.1) is below the cut for $p_c(x,E)$ (see also Appendix C).

Three regions in the x plane are of physical interest. Regions a and c are those portions of the x plane immediately surrounding and including the Rex axis to the left of x_1, and to the right of x_2, respectively. Region b is that portion of the x plane immediately below the cut which runs from x_1 to x_2. These regions are marked a, b, and c in Fig. 1(e).

Given the above classical definitions, the semiclassical expressions to order $\hbar$ for the quantum momentum function $p(x,E)$ are

$$p(x,E)\simeq p_c(x,E)+\hbar p_{1c}(x,E) \tag{5.2}$$

in regions a,c, while in region b

$$p(x,E) \simeq i p_c(x,E) \tan(W_c(x,E)/\hbar - \pi/4) + \hbar p_{1c}(x,E) , \tag{5.3}$$

where $p_{1c}(x,E) \equiv i p_c'(x,E)/2p_c(x,E)$ and where the prime means $\partial/\partial x$. Equations (5.2) and (5.3) can be obtained by various methods; one method is described in Appendix B.

Regions a and c can be considered together, since they have the same semiclassical form. It can be verified by direct substitution that (5.2) satisfies the momentum function equation (3.2) to order $\hbar$. Further, (5.2) clearly satisfies the correspondence principle and boundary condition (3.3). Thus, to order $\hbar$, (5.2) is the quantum momentum function for regions a and c. In these regions the quantum $p(x,E)$ is quite close to the classical $p_c(x,E)$, and goes smoothly to $p_c(x,E)$ in the classical limit.

Region b is more interesting than a and c, because in b the quantum momentum function contains a tangent function which is highly nonclassical. It can be verified by direct substitution that (5.3) satisfies the momentum function equation (3.2) to order $\hbar$ as required. However, it is not obvious that (5.3) satisfies the boundary condition (3.3) because of the tangent.

To examine the tangent function in the limit $\hbar \rightarrow 0$, since region b is the area below the cut, one lets x in the argument of the tangent be $x - i\epsilon$ with x real and with ϵ a small positive constant. Expanding the classical characteristic function gives

$$W_c(x - i\epsilon, E) \simeq W_c(x,E) - i\epsilon p_c(x,E) .$$

Thus, the tangent contains exponentials of the form $\exp(\pm \epsilon p_c(x,E)/\hbar)$ where $p_c(x,E)$ is real and positive. In the limit $\hbar \rightarrow 0$ the $+$ exponential becomes infinite, and one has $\tan(W_c/\hbar - \pi/4) \rightarrow -i$. Hence, for region b also, one has $p(x,E) \rightarrow p_c(c,E)$ as $\hbar \rightarrow 0$.[21]

We are now in a position to use (5.3) to gain insight into the quantum momentum function inside the potential well. We neglect the $\hbar p_{1c}(x,E)$ term as it is small and smoothly varying. In the expression

$$p(x,E) \simeq i p_c(x,E) \tan(W_c(x,E)/\hbar - \pi/4) ,$$

both $p_c(x,E)$ and $W_c(x,E)$ are essentially real, positive, and smoothly varying in region b. The tangent has a series of poles whose locations x_k are given by $W_c(x_k,E)/\hbar - \pi/4 = (k + \frac{1}{2})\pi$, with k an integer. If the poles are not too far apart, then the spacing between adjacent poles is approximately $\pi\hbar/p_c(x,E)$. Further, by examining the tangent near a pole at x_k, one can show that $p(x,E) \simeq (\hbar/i)/(x - x_k)$ near the pole. Thus, $p(x,E)$ in the potential well contains a series of poles, each one of which has residue $\hbar/i$, and which are spaced approximately $\pi\hbar/p_c(x,E)$ apart.

The interpretation of each pole of the momentum function $p(x,E)$ is that it is a quantum of momentum. Since each pole of $p(x,E)$ has the same residue, all the poles carry the same amount of momentum. The amount of momentum in a given x region is controlled by the number of poles in that region. As $\hbar \rightarrow 0$ each pole gets weaker since the residue is $\hbar/i$. However, the spacing between poles also shrinks, since it also is proportional to $\hbar$. These two phenomena cooperate in such a way that the series of poles coalesces into the classical $p_c(x,E)$. The poles cause a discontinuity in $p(x,E)$, and this discontinuity becomes the cut of $p_c(x,E)$ in the classical limit. [The classical limit is seen in Fig. 1 as the passage from Fig. 1(d) to 1(e) as more and more poles appear between x_1 and x_2 due to $\hbar \rightarrow 0$.]

Turning now to the characteristic function $W(x,E)$, given, e.g., by (4.2), one can use (5.2) and (5.3) to get semiclassical forms for $W(x,E)$. We concentrate again on region b. Since $W(x,E)$ is the integral of $p(x,E)$, near a pole at x_k one has

$$W(x,E) \simeq (\hbar/i) \int^x dx'/(x' - x_k) = (\hbar/i) \ln(x - x_k) ,$$

neglecting additive terms which are independent of x. In region b, as x increases it passes just below x_k. As x passes x_k, $\mathrm{Re}W(x,E)$ jumps by $\pi\hbar$; $\mathrm{Im}W(x,E)$ fluctuates, but its cummulative change is zero. Thus, in the semiclassical approximation, $\mathrm{Re}W(x,E)$ is a staircaselike function, the stairs of which are $\pi\hbar$ high and $\pi\hbar/p_c(x,E)$ wide, while $\mathrm{Im}W(x,E)$ fluctuates but does not change on the average. In the classical limit $\hbar \rightarrow 0$ the staircase $\mathrm{Re}W(x,E)$ becomes smooth, and $\mathrm{Im}W(x,E)$ vanishes.

For further discussion of semiclassical forms and of the connection between the Hamilton-Jacobi and WKB formalisms see Appendix C.

VI. ILLUSTRATIONS: ONE DIMENSION

The power of the action variable definition (3.4) is illustrated with four one-dimensional systems, and approaches to other systems are discussed.[22]

The one-dimensional harmonic oscillator is defined by Hamiltonian (2.1) with potential $V(x) = x^2$. The oscillator action variable is given by integral (3.4) where the contour C encloses the two turning points $-x_1 = x_2 = +\sqrt{E}$ and the section of $\mathrm{Re}x$ axis between them. The integral (3.4) may be done by distorting the contour, if one knows the location and nature of the singularities of the integrand. It is shown in Appendix D that the only first-order pole of the integrand, besides those of $p(x,E)$ on the $\mathrm{Re}x$ axis between x_1 and x_2, is at $x = \infty$. Thus, the contour may be distorted to enclose the pole at $x = \infty$, and the integral evaluated.

Making the transformation $x = 1/s$ in the integral (3.4) yields $J = (1/2\pi) \int (ds/s^2) p(s,E)$ where the contour C_s in the complex s plane encloses $s = 0$ in a counterclockwise direction. Letting $x = 1/s$ in the momentum equation (3.2) yields

$$\frac{\hbar}{i} \frac{\partial p(s,E)}{\partial s} - p^2(s,E)/s^2 = -E/s^2 + 1/s^4 , \tag{6.1}$$

where $p(s,E)$ obeys boundary condition (3.3). Inspection of (6.1), combined with the fact that we only need the s term of $p(s,E)$, allows us to substitute only the two terms $p(s,E) = a_{-1}s^{-1} + a_1 s + \cdots$ into (6.1). The resulting expressions for the constants are ${a_{-1}}^2 = -1$ and $(\hbar/i)a_{-1} + 2a_{-1}a_1 = E$. The classical momentum function is that branch of the square root $(E - x^2)^{1/2}$ which is positive along the bottom of the cut which runs from x_1

to x_2. With this convention, for large x, $p_c(x,E) \simeq ix = i/s$. Thus, by (3.3), the correct physical solution of $a_{-1}{}^2 = -1$ is $a_{-1} = +i$. The other expansion coefficient is then $a_1 = (E - \hbar)/2i$. Having a_1, the residue theorem can be used to obtain the integral for J; the result is

$$J = E/2 - \hbar/2 \; . \tag{6.2}$$

Result (6.2) holds for the eigenvalues J and E. The eigenvalues J have the values $n\hbar, n = 0,1,2,\ldots$, which correspond to the contour C enclosing $0,1,2,\ldots$, poles of $p(x,E)$. Thus, (6.2) gives the usual oscillator energies.

The second illustration is the one-dimensional "barrier coulomb" system with Hamiltonian (2.1) and potential $V(x) = -g/x + a^2/x^2$ (g and a are positive real constants). The physical motion is defined as taking place only for positive real x. The action variable is given by (3.4) where the contour C encloses the turning points x_1 and x_2 and the section of Rex axis between them. x_1 and x_2 are defined by $E - V(x_1) = E - V(x_2) = 0$.

The integral (3.4) for $J(E)$ may be evaluated by distorting the contour C to enclose the poles of the integrand at $x = 0$ and $x = \infty$. Thus $J = J_0 + J_\infty$ where J_0 and J_∞ are the contributions to J from the poles at $x = 0$ and $x = \infty$, respectively. The evaluation of J_∞ proceeds much like the oscillator case above; the result is $J_\infty = g/2\sqrt{-E}$.

To evaluate J_0 we let $p(x,E) = a_{-1}/x + \cdots$ near $x = 0$, and substitute this form of $p(x,E)$ into (3.2) with $V(x) = -g/x + a^2/x^2$. Collecting coefficients of the $1/x^2$ terms gives $i\hbar a_{-1} + a_{-1}{}^2 = -a^2$ or

$$a_{-1} = -i\hbar/2 \pm i(\hbar^2/4 + a^2)^{1/2}$$

with the square root positive. The classical momentum function near $x = 0$ obeys $p_c(x,E) = -ia/x + \cdots$, so boundary condition (3.3) indicates that the lower sign in a_{-1} is correct:

$$a_{-1} = -i\hbar/2 - i(\hbar^2/4 + a^2)^{1/2} \; .$$

The distorted contour encloses $x = 0$ in the clockwise direction so

$$J_0 = -ia_{-1} = -\hbar/2 - (\hbar^2/4 + a^2)^{1/2} \; .$$

Summing J_0 and J_∞ gives

$$J = -\hbar/2 - (\hbar/4 + a^2)^{1/2} + g/2\sqrt{-E} \; . \tag{6.3}$$

The J eigenvalues are $J = n\hbar$, where $n = 0,1,2,\ldots$, counts the number of poles of $p(x,E)$ in the potential well. Use of $J = n\hbar$ in (6.3) gives the "barrier coulomb" energy levels.

The third one-dimensional illustration is the "barrier oscillator" with Hamiltonian (2.1) and potential $V(x) = a^2/x + x^2$ where a is a positive real constant. The physical motion takes place only for positive real x. For this system there are four turning points:

$$x_1 = [E/2 - (E^2/4 - a^2)^{1/2}]^{1/2} \; ,$$

$$x_2 = [E/2 + (E^2/4 - a^2)^{1/2}]^{1/2} \; ,$$

$x_3 = -x_1$, and $x_4 = -x_2$; x_3 and x_4 are unphysical. The action variable is given by (3.4) with C enclosing x_1 and x_2 and the section of Rex axis between them.

The integral (3.4) is evaluated by distorting the contour C. As in the barrier coulomb problem above, the integrand has poles at $x = 0$ and $x = \infty$; however, in addition, there are poles of $p(x,E)$ on the negative Rex axis between the unphysical turning points x_3 and x_4. Because the potential is symmetric with respect to $x = 0$, for each pole of $p(x,E)$ in the potential well (between x_1 and x_2) there is another pole in the unphysical well (between x_3 and x_4); i.e., $p(x,E)$ is symmetric about $x = 0$ in the number and location of its poles with residue $\hbar/i$. Thus, when C is distorted to enclose the poles between x_3 and x_4 one obtains $J = J_0 + J_\infty - J$ or $2J = J_0 + J_\infty$.

Inspection shows that J_0 is the same as in the barrier coulomb problem while J_∞ is the same as in the harmonic oscillator. Thus, one obtains

$$J = \tfrac{1}{2}[-\hbar - (\hbar^2/4 + a^2)^{1/2} + E/2] \; . \tag{6.4}$$

As in the earlier cases, $J = n\hbar, n = 0,1,2,\ldots$, which, when used in (6.4), gives the system energies.

By applying the residue theorem the exact quantum energy levels for the three systems above are found via (3.4) without obtaining a complete solution for $p(x,E)$. It is necessary only to obtain one or several terms in the expansion of $p(x,E)$ at the locations of the poles of the integrand.

In order to use the residue theorem to do the $J(E)$ integral (3.4) it is necessary to know the location of the singularities of the integrand. Three methods exist for locating these singularities using only the known classical $p_c(x,E) = (E - V(x))^{1/2}$. First, because of (3.2) and (3.3), the fixed poles of $p(x,E)$ are at the same location as the fixed poles of $p_c(x,E)$, while the moving poles of $p(x,E)$ are found along the cuts of $p_c(x,E)$.[23] Examples of "fixed" poles are the poles at $x = 0$ and $x = \infty$ in the barrier Coulomb problem above. Examples of "moving" poles are the poles on the negative Rex axis in the barrier oscillator problem above (these poles move when E is changed).[23] Second, the moving poles of $p(x,E)$, which correspond to the zeros of the wave function,[16] can occur only on or near a line defined by the equation $\int_a^x dx' p_c(x',E) =$ real, where a is a turning point.[24] Third, there exist theorems on the location of zeros of the solutions of differential equations which provide a general method for finding the poles of $p(x,E)$ without solving for $p(x,E)$ (see Appendix D).

As a fourth illustration we consider a system with Hamiltonian (2.1) and potential $V = x^2 + \lambda x^4$, with λ a real positive constant. The system has four turning points:

$$-x_1 = x_2 = \{[-1 + (1 + 4\lambda E)^{1/2}]/2\lambda\}^{1/2}$$

(physical)

and

$$-x_3 = x_4 = i\{[1 + (1 + 4\lambda E)^{1/2}]/2\lambda\}^{1/2}$$

(unphysical).

The action variable is given by (3.4) where the contour C encloses x_1 and x_2 and the section of the Rex axis between them.

As in the pure harmonic oscillator case, the integral (3.4) for $J(E)$ may be evaluated by distorting the contour C. In the present anharmonic system, however, $p(x,E)$ has poles on the Imx axis below x_3 and above x_4 so that when C is distorted it encloses these poles. To compute $J(E)$ one writes $p_c(x,E)$ as

$$p_c(x,E)=\sqrt{\lambda}x_4x(1-x_2^2/x^2)^{1/2}(1-x^2/x_4^2)^{1/2}$$

and expands the square roots, obtaining $p_c(x,E)=\sum\sum b(n,r)\alpha^r x^{1-2n}$ where the first sum is over $r=0$ to ∞ and the second sum is over $n=-r$ to ∞ and where $\alpha\equiv x_2^2/x_4^2$. The quantum momentum function has an expansion of the same form: $p(x,E)=\sum\sum a(n,r)\alpha^r x^{1-2n}$ where the sums are as before. To find the $a(n,r)$ in terms of the $b(n,r)$, the $p(x,E)$ and $p_c(x,E)$ expansions are substituted into the left-hand and right-hand sides of (3.2), respectively. By collecting powers of α and x one obtains an equation for the unknown quantum $a(n,r)$ in terms of the known classical $b(n,r)$.[25]

Once the $a(n,r)$ are known, the action variable follows from the $p(x,E)$ expansion and (3.4); the result is

$$J=i\sum_{r=0}^{\infty}a(1,r)\alpha^r \tag{6.5}$$

which is an asymptotic expansion of $J(E)$ in powers of α. As in the earlier illustrations, the energy levels are given by $J=n\hbar$ where $n=0,1,2,\ldots$, counts the number of poles of $p(x,E)$ in the physical potential well.[25]

We have used (6.5) to find the ground-state energies of systems with $\lambda=0.1$, 0.2, 0.5, and 1.0, and have compared the results with those found by other methods.[26] For these λ values we obtain $E=1.0653$, 1.1183, 1.242, and 1.392, respectively, in agreement with the values in Ref. 26 to the significant figures quoted.

VII. ILLUSTRATIONS: THREE DIMENSIONS

In order to consider motion in three dimensions under, e.g., a spherical potential, one returns to the basic equation (2.7) and writes it in terms of spherical polar coordinates r,θ,ϕ. The resulting equation is separated by letting

$$W(r,\theta,\phi)=W_r(r,E,\lambda)+W_\theta(\theta,\lambda,c)+W_\phi(\phi,c)\ ,$$

where E, λ, and c are the eigenvalues of the W_r, W_θ, and W_ϕ equations, respectively. By using the definitions $p_r(r,E,\lambda)\equiv\partial W_r(r,E,\lambda)/\partial r$ and $p_\theta(\theta,\lambda,c)\equiv\partial W_\theta(\theta,\lambda,c)/\partial\theta$ in the W_r and W_θ equations, respectively, one obtains the r and θ quantum momentum function equations

$$\frac{\hbar}{i}\frac{1}{r^2}\frac{\partial}{\partial r}[r^2p_r(r,E,\lambda)]+p_r^2(r,E,\lambda)=E-V(r)-\lambda/r^2\ , \tag{7.1}$$

$$\frac{\hbar}{i}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}[\sin\theta p_\theta(\theta,\lambda,c)]+p_\theta^2(\theta,\lambda,c)=\lambda-c/\sin^2\theta\ . \tag{7.2}$$

The solutions of (7.1) and (7.2) obey boundary conditions analogous to (3.3). The eigenvalues of the $p_\phi(\phi,c)$ momentum function equation are $\sqrt{c}\equiv J_\phi=n_\phi\hbar,n_\phi=0,\pm1,\pm2,\ldots$, and these are used in (7.2).

Turning first to the θ motion, the integral that gives the desired relation between J_θ and the pair λ,J_ϕ is (3.4), i.e., $J_\theta=(1/2\pi)\int d\theta p(\theta,\lambda,J_\phi)$ where $p(\theta,\lambda,J_\phi)\equiv p_\theta(\theta,\lambda,c)$, and where the contour C encloses the two turning points θ_1 and θ_2 [defined by setting the right-hand side of (7.2) equal to zero] and the section of Reθ axis between θ_1 and θ_2. Because of the periodicity of sinθ in θ, it is convenient to change variables via $y=-\cot\theta$ so that the J_θ integral is

$$J_\theta=(1/2\pi)\int dy\,p(y,\lambda,J_\phi)/(y-i)(y+i)\ .$$

The momentum function $p(y,\lambda,J_\phi)$ is the solution of (7.2) after it has been transformed to the y plane. The integration is around a closed contour C_y which encloses the y plane turning points y_1 and $y_2(-y_1=y_2=+[(\lambda-J_\phi^2)/J_\phi^2]^{1/2})$ and the section of Rey axis between y_1 and y_2.

One evaluates the integral by distorting the contour C_y to enclose the other first-order poles of the integrand. The relevant poles are at $y=\pm i$ and $y=\infty$. The lowest order terms in $p(y,\lambda,J_\phi)$ are obtained at the points $y=\pm i$, ∞ from the $p(y,\lambda,J_\phi)$ equation and the boundary condition, and these are used with the residue theorem to obtain J_θ.

The J_θ integral is

$$J_\theta=[\lambda+(\hbar/2)^2]^{1/2}-\hbar/2-(J_\phi^2)^{1/2}\ , \tag{7.3}$$

where the square roots are positive. The values of J_θ are $n_\theta\hbar,n_\theta=0,1,2,\ldots$, which correspond, respectively, to having $0,1,2,\ldots$, poles of $p_\theta(\theta,\lambda,c)$ in the potential well between θ_1 and θ_2. The values of J_ϕ are $n_\phi,n_\phi\hbar=0,\pm1,\pm2,\ldots$. Inverting (7.3) gives the λ eigenvalue in terms of the action variable eigenvalues as

$$\begin{aligned}\lambda&=(J_\theta+J'_\phi+\hbar/2)^2-(\hbar/2)^2\\&=(n_\theta+n'_\phi)(n_\theta+n'_\phi+1)\hbar^2\ ,\end{aligned}$$

where J'_ϕ is the positive square root $(J_\phi^2)^{1/2}$ and n'_ϕ is the positive square root $(n_\phi^2)^{1/2}$. These results are the same as those obtained in the traditional theories of angular momentum.

The next illustration is the Coulomb radial motion, i.e., the r motion described by the radial momentum function equation (7.1) with potential $V(r)=-g/r$ (g is a positive, real constant). The radial action variable is, from (3.4), $J_r=(1/2\pi)\int dr\,p_r(r,E,\lambda)$, where the contour encloses the two turning points r_1 and r_2 and the section of Rer axis between them. The turning points r_1 and r_2 are found by setting the right-hand side of (7.1) equal to zero.

The radial Coulomb system considered here is much like the one-dimensional "barrier Coulomb" system considered in Sec. VI. The significant difference between the two systems is that the left-hand side of (7.1) contains the term $-i\hbar(2/r)p_r(r,E,\lambda)$ which (3.2) does not have.

As in the "barrier Coulomb" case, inspection of the J_r integral and (7.1) with $V(r)=-g/r$ (see also Appendix D) shows that the only poles of the integrand relevant to evaluating the J_r integral by distorting the contour are those at $r=0$ and $r=\infty$. Equation (7.1) and the boundary condition are used to obtain the necessary terms in $p_r(r,E,\lambda)$ at $r=0$ and ∞, and these are used with the residue theorem to obtain J_r. The result is

$$J_r=-l\hbar-\hbar+g/2\sqrt{-E}\ , \tag{7.4}$$

where the values of J_r are $n_r\hbar$ with $n_r=0,1,2,\ldots$, which correspond, respectively, to $0,1,2,\ldots$, poles of $p_r(r,E,\lambda)$ in the radial effective potential well. To obtain (7.4) we have rewritten λ using $\lambda=l(l+1)\hbar^2$, $l\equiv n_\theta+n'_\phi=0,1,2,\ldots$; see the earlier θ-motion discussion. Inverting (7.4) gives the usual Coulomb energy levels.

The last illustration is the radial oscillator system described by (7.1) with $V(r)=r^2$. The analysis of this system proceeds like that of the "barrier oscillator" system given in Sec. VI; the only difference is the $-i\hbar(2/r)p_r(r,E,\lambda)$ on the left-hand side of (7.1). The result for the radial action variable is

$$J_r=\tfrac{1}{2}[E/2-l\hbar-3\hbar/2]\ , \tag{7.5}$$

where $J_r=n_r\hbar$ with $n_r=0,1,2,\ldots$, which correspond to $0,1,2,\ldots$, poles of $p_r(r,E,\lambda)$ in the physical potential well, respectively. As in the radial Coulomb case, we use $\lambda=l(l+1)\hbar^2$ to obtain (7.5). The energies are given by inverting (7.5).

VIII. HAMILTON-JACOBI DYNAMICS

In this section we return to the general quantum Hamilton-Jacobi theory outlined in Sec. II, and show how dynamical information is contained in the formalism. We examine (1) the equivalence of the Hamilton-Jacobi and Schrödinger theories. (2) How the Hamilton-Jacobi equation can be considered as a dynamical equation. (3) The connection between Hamilton-Jacobi theory and experiment. (4) The connection between classical and quantum mechanics in the context of Hamilton-Jacobi theory. We continue to consider the system governed by Hamiltonian (2.1).

In order to show the equivalence of the Hamilton-Jacobi and Schrödinger theories we generalize Hamilton's original program of associating a wave with the classical motion of a particle.[7,10] Hamilton's wave has as its phase the classical Hamilton's principal function. However, because the classical principal function is real, the classical wave theory of particle motion is incomplete. On the other hand, the discussion of Secs. II—VII shows that the quantum Hamilton's principal and characteristic functions, S and W, are complex. Thus, one can, using the quantum S and W, carry out Hamilton's original observation.

Following Hamilton, we define the waves associated with the quantum system (2.1) by[27]

$$\psi(x,E)\equiv\exp(iW(x,E)/\hbar)\ , \tag{8.1}$$

$$\Psi(x,t)\equiv\exp(iS(x,t)/\hbar)\ , \tag{8.2}$$

where $W(x,E)$ and $S(x,t)$ are the quantum Hamilton's characteristic and principal functions of Sec. II, respectively. The quantum waves $\psi(x,E)$ and $\Psi(x,t)$ are the Schrödinger time-independent and time-dependent wave functions, respectively, as we now show.

The waves $\psi(x,E)$ and $\Psi(x,t)$ satisfy the respective wave equations and the appropriate physical boundary conditions. Direct substitution of (8.1) [(8.2)] into the Hamilton-Jacobi equation (2.3) [(2.5)] leads immediately to the time-independent [dependent] Schrödinger equation for system (2.1). This shows that the quantum Hamilton-Jacobi equations (2.3) and (2.5) imply the respective Schrödinger equations.

To compare the boundary conditions in the Hamilton-Jacobi and Schrödinger theories we continue to consider system (2.1). We assume the potential $V(x)$ contains a well capable of having quantum-bound states, and that $V(x)\rightarrow0$ rapidly and smoothly as $x\rightarrow\pm\infty$ along the Rex axis. For negative energies, the wave function for large, positive x goes as

$$\psi(x,E)\simeq\exp(\pm ikx+\text{const.})$$
$$=\exp(\mp\kappa x+\text{const.})\ ,$$

where $k=\sqrt{E}=i\kappa$, κ real, >0. The requirement of normalizability on $\psi(x,E)$ makes one select the solution with the upper sign. Correspondingly, under the same conditions, the solution of (2.3) is

$$W(x,E)/\hbar\simeq\pm kx+\text{const.}=\pm i\kappa x+\text{const.}$$

In this case the boundary condition (4.3) makes one select, again, the upper sign. Thus, via (8.1), the physical boundary condition on the x dependence of $W(x,E)$ has the same effect as the physical boundary condition on the x dependence of $\psi(x,E)$. Similar arguments obtain for positive energies and for the pair Ψ,S. This shows that the Hamilton-Jacobi boundary condition implies the Schrödinger boundary condition, and, also, completes the proof that $\psi(x,E)$ [$(\Psi(x,t)$] of (8.1) [(8.2)] is the time-independent [dependent] wave function.

Another requirement placed on $\psi(x,E)$ is normalization, as distinct from normalizability. $W(x,E)$, as given, e.g., by (4.2), is determined only up to the additive function $W_0(E)$. From (8.1) and (4.2) one sees that $\operatorname{Im}W_0(E)$ can be chosen so that $\psi(x,E)$ is normalized, while $\operatorname{Re}W_0(E)$ contributes an overall, unobservable phase to $\psi(x,E)$. Thus, determination of the additive function $W_0(E)$ in Hamilton-Jacobi theory is equivalent to normalization and determination of the overall phase in Schrödinger theory.

Given $W(x,E)$ or $S(x,t)$ one can construct $\psi(x,E)$ or $\Psi(x,t)$. For states of definite energy E one can let $S=W-Et$ [See (2.6)]. Thus, for these states, knowledge of W gives S, and $\psi(x,E)$ and $\Psi(x,t)$ are constructed via (8.1) and (8.2). States containing a superposition of energies are described by $S(x,t)$, and $\Psi(x,t)$ is constructed from $S(x,t)$ via (8.2).

What is done above is to derive Schrödinger theory from Hamilton-Jacobi theory by generalizing Hamilton's classical wave program. Since, also, Schrödinger theory implies Hamilton-Jacobi theory, the two theories are equivalent.

We turn now to the dynamical content of the characteristic and principal functions, $W(x,E)$ and $S(x,t)$, and to the dynamical content of the Hamilton-Jacobi equations (2.3) and (2.5). First, the discussion of the equivalence of the Hamilton-Jacobi and Schrödinger theories shows that the dynamical content of $W(x,E)$ and

$S(x,t)$ is equivalent to the dynamical content of the wave functions $\psi(x,E)$ and $\Psi(x,t)$, respectively, i.e., $W(x,E)$ $[S(x,t)]$ and $\psi(x,E)$ $[\Psi(x,t)]$ contain the same physical information. Thus, $W(x,E)$ and $S(x,t)$ characterize the physical state of a quantum system. Second, since $W(x,E)$ and $S(x,t)$ are basic dynamical objects, and since $W(x,E)$ and $S(x,t)$ are determined by their respective Hamilton-Jacobi equations, the Hamilton-Jacobi equations are the equations of motion. That is, *a quantum Hamilton-Jacobi equation accompanied by its associated physical boundary condition, is a dynamical equation.* Finally, since the characteristic and principal functions specify the state of a quantum system, and since the Hamilton-Jacobi equations determine the characteristic and principal functions, quantum Hamilton-Jacobi theory is self-contained.

In order to connect quantum Hamilton-Jacobi theory to experiment one can proceed in one of, at least, two ways. First, one may use, e.g., the action-angle variable theory outlined in Secs. III and IV, and illustrated in Secs. VI and VII. In particular, Eqs. (3.2)—(3.5) may be used to find the energy levels. Or, second, one may build up quantum waves from the characteristic and principal functions via (8.1) and (8.2), and then invoke the usual interpretive mechanisms for the quantum waves.

We conclude with two remarks on the connection between classical and quantum mechanics which follow from the Hamilton-Jacobi formalism. First, we saw above in the discussion of the equivalence of the Hamilton-Jacobi and Schrödinger theories that the physical boundary condition on the characteristic function $W(x,E)$ is equivalent to the physical boundary condition, normalizability, on the wave function $\psi(x,E)$. But the physical boundary condition on $W(x,E)$ given in (4.3) is a classical condition. Therefore, one can write

$$\text{normalizability on } \psi \equiv \text{classical boundary condition on } W \,. \tag{8.3}$$

Expression (8.3) emphasizes that what is usually thought of as a highly quantum mechanical notion, normalizability, is simply the manifestation in quantum mechanics of a classical boundary condition. In other words, *the boundary conditions in classical and quantum mechanics are the same.*

Second, given observation (8.3), one can ask what the difference is, in the context of Hamilton-Jacobi theory, between classical and quantum mechanics. The answer is that the essential difference between the two theories is contained in the $\hbar$ terms in the Hamilton-Jacobi equations (2.3) and (2.5) and in the momentum function equation (3.2). For example, the quantum term $(\hbar/i)\partial p(x,E)/\partial x$ in (3.2) interacts with the classical term $p^2(x,E)$ to produce the poles of $p(x,E)$, and it is these poles which quantize the bound-state energies. Lastly, it may be noted that the quantum Hamilton-Jacobi and momentum function equations reduce directly to their classical counterparts when $\hbar$ is set equal to zero; this direct reduction is a property of Hamilton-Jacobi theory, and not of the other forms of mechanics.

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APPENDIX A: OPERATORS

We investigate first the operator form of the transformation equations (4.1).[4] The Hamiltonian of the system is given by (2.1), and the Schrödinger representation is assumed. Addressing the transformation equation $p=\partial W(x,E)/\partial x$ where $E=E(J)$, one begins by noting that, using the Schrödinger representation, $\langle x \mid \hat{p} \mid E \rangle = (\hbar/i)(\partial/\partial x)\langle x \mid E \rangle$. As discussed in Sec. VIII, the basic relation between the wave function $\psi(x,E)=\langle x \mid E \rangle$ and the characteristic function $W(x,E)$ is $\langle x \mid E \rangle = \exp(iW(x,E)/\hbar)$. Combining this relation with the expression for $\langle x \mid \hat{p} \mid E \rangle$, one obtains $\langle x \mid \hat{p} \mid E \rangle = [\partial W(x,E)/\partial x]\langle x \mid E \rangle$. The right-hand side of this equation can be rewritten as $\langle x \mid \partial W(\hat{x},\hat{E})/\partial \hat{x} \mid E \rangle$ provided the function of operators $\partial W(\hat{x},\hat{E})/\partial \hat{x}$ is in well-ordered form. Thus, one obtains an operator analog of (4.1)

$$\hat{p} = \partial W(\hat{x},\hat{E})/\partial \hat{x} \,. \tag{A1}$$

In order to study the operator form of the second transformation equation of (4.1), $w=\partial W(x,E(J))/\partial J$, one assumes a Schrödinger representation in which $\hat{w} = -(\hbar/i)\partial/\partial J$, $\hat{J}=J$. An argument identical to the one above that led to (A1) then yields[18]

$$\hat{w} = \partial W(\hat{x},E(\hat{J}))/\partial \hat{J} \tag{A2}$$

which is an operator analog of the second of (4.1).

Turning now to the Hamilton-Jacobi equation, one may use the operator transformation equation (A1) in Hamiltonian (2.1) to obtain the operator equation

$$(\partial W(\hat{x},\hat{E})/\partial \hat{x})^2 + V(\hat{x}) = E \,. \tag{A3}$$

This expression is an operator analog of (2.3). An operator Hamilton-Jacobi equation related to (A3) can be derived from the Schwinger action principle.[7,8] In our notation this equation is $(\partial \hat{S}/\partial \hat{x})^2 + V(\hat{x}) = -\partial \hat{S}/\partial t$ which is an operator analog of (2.5).

APPENDIX B: SEMICLASSICAL FORMS

In order to show continuity of the solution (5.2) and (5.3) one needs connection formulas for $p(x,E)$ across the turning points. To this end we exploit the relation [see (3.1) and (8.1)]

$$p(x,E) = (\hbar/i)\psi'(x,E)/\psi(x,E) \,, \tag{B1}$$

where $\psi(x,E)$ is the time-independent wave function and where prime means $\partial/\partial x$. We use the technique of Furry to find the appropriate forms for $\psi(x,E)$ in regions a, b, and c; these are[24]

$$\begin{aligned}
\psi_a &= (A/\sqrt{p_c})e^{iW_c/\hbar} , \\
\psi_b &= (2Ae^{i\pi/4}/\sqrt{p_c})\cos(W_c/\hbar-\pi/4) , \qquad \text{(B2)} \\
\psi_c &= (Ae^{i(n+1/2)\pi}/\sqrt{p_c})e^{iW_2/\hbar} ,
\end{aligned}$$

where p_c and W_c are the classical momentum and characteristic functions, respectively [see (5.1)], W_2 is the same as W_c except that the lower limit of the integral is x_2, and where n is an integer denoting the nth bound-state level. Use of (B2) in (B1) gives the semiclassical forms for $p(x,E)$: (5.2) and (5.3). In particular, the phase $-\pi/4$ is validated.

APPENDIX C: CONNECTION BETWEEN HAMILTON-JACOBI AND WKB FORMALISMS

Definition (2.3) and (4.3) might make it appear that the quantum characteristic function $W(x,E)$ is the same as the W that appears in WKB theory. That this is not the case can be seen by the following. The connection between the wave function $\psi(x,E)$ and the characteristic function $W(x,E)$ is given in (8.1), while the connection between $\psi(x,E)$ and the W's of WKB theory is

$$\psi(x,E)=Ae^{iW^{(+)}_{\mathrm{WKB}}(x,E)/\hbar}+Be^{iW^{(-)}_{\mathrm{WKB}}(x,E)/\hbar} . \qquad \text{(C1)}$$

The $W^{(\pm)}_{\mathrm{WKB}}(x,E)$ obey the same equation as the characteristic function $W(x,E)$, i.e., Eq. (2.3). In addition, the $W^{(\pm)}_{\mathrm{WKB}}(x,E)$ obey the "boundary conditions"

$$W^{(\pm)}_{\mathrm{WKB}}=\pm W_c+\hbar W_1^{(\pm)}+\hbar^2 W_2^{(\pm)}+\cdots , \qquad \text{(C2)}$$

where $W_c(x,E)$ is defined, e.g., in (5.1). The A,B in (C1) are constants which have different values in different regions of the x plane [see (B2) and Ref. 24].

Comparison of (8.1) and (C1) shows that $\psi(x,E)$ is given in terms of Hamilton's characteristic function $W(x,E)$ by a single exponential, while $\psi(x,E)$ is given in terms of the WKB functions $W^{(\pm)}_{\mathrm{WKB}}(x,E)$ by the sum of two exponentials. Further, although $W(x,E)$ and $W^{(\pm)}_{\mathrm{WKB}}(x,E)$ obey the same equation, they obey different boundary conditions: (4.3) and (C2), respectively. In particular, e.g., $W^{(-)}_{\mathrm{WKB}}(x,E)$ does not obey (4.3). Thus, $W(x,E)$ and $W^{(\pm)}_{\mathrm{WKB}}(x,E)$ are not the same functions.

The relation between the characteristic function $W(x,E)$ and the WKB functions can be illustrated by considering the WKB approximation for the wave function in region b, i.e., just below the real x axis between the turning points (see Sec. V and Appendix B). In region b, from (B2), one has

$$\begin{aligned}
\psi_b &\sim 2\cos(W_c/\hbar-\pi/4) \\
&\sim e^{iW_c/\hbar-i\pi/4}+e^{-iW_c/\hbar+i\pi/4} , \qquad \text{(C3)}
\end{aligned}$$

where we neglect the factor $Ae^{i\pi/4}/\sqrt{p_c}$ in (B2), since it does enter the present discussion. In region b one can let x be $x-i\epsilon$ with x real and ϵ real and positive. W_c is expanded: $W_c(x-i\epsilon,E)\simeq W_c(x,E)-i\epsilon p_c(x,E)$. Using this expansion in (C3) one sees that the magnitude of the second exponential relative to the first exponential is $\exp[-2\epsilon p_c(x,E)/\hbar]$. Thus, where $2\epsilon p_c(x,e)/\hbar \gg 1$ one needs only the first exponential in (C3), whereas where $2\epsilon p_c(x,E)/\hbar \ll 1$ one needs both exponentials in (C3). Thus, where $2\epsilon p_c(x,E)/\hbar \gg 1$ we see that $\psi_b \sim \exp[iW_c(x,E)/\hbar]$ (neglecting multiplicative constants), and comparing this expression to (8.1) we have $W(x,E)\simeq W_c(x,E)\simeq W^{(+)}_{\mathrm{WKB}}(x,E)$. That is, in that part of region b where $2\epsilon p_c(x,E)/\hbar \gg 1$ the characteristic function $W(x,E)$ and the WKB function $W^{(+)}_{\mathrm{WKB}}(x,E)$ are nearly the same function. In contrast however, where $2\epsilon p_c(x,E)/\hbar \ll 1$ (near the real x axis, "in" the potential well) both exponentials are required in ψ_b and one has $W(x,E)$ different than the $W^{(\pm)}_{\mathrm{WKB}}(x,E)$.

Although the above discussion is for region b, similar analyses of other regions of the x plane produce the same results. Thus, the conclusion is that the characteristic function $W(x,E)$ and the WKB function $W^{(+)}_{\mathrm{WKB}}(x,E)$ are similar in some regions of the x plane, while in other regions they are different.

APPENDIX D: MOMENTUM FUNCTION POLES

The poles of $p(x,E)$ can be located without solving for $p(x,E)$ by the use of theorems on the zeros of second-order differential equations. To employ these theorems one uses connection (B1).

Given the differential equation $d^2w/dz^2+J(z)w=0$, three theorems relevant to the present discussion are[17] A: "If throughout the interval (a,b) [on the Rez axis], either Re$J(z)\leq 0$ or Im$J(z)$ does not change sign, then there can be at most one zero of $w\cdot dw/dz$ in that interval." [w is a real function of x.] B: "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$J(z)\geq 0$ throughout T, then $w(z)$ can have no complex zero or extremum in T." 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) $w\cdot dw/dz$ has a fixed sign; let Im$J(z)$ have this sign throughout that part of the region T which lays above the real axis, then $w(z)$ can have no complex zero or extremum in T." There is a corresponding theorem for below the axis where the signs of $w\cdot dw/dz$ and Im$J(z)$ are opposite.

We illustrate how these theorems may be employed using the harmonic oscillator for which $J(z)=k^2-z^2$ is appropriate units. $J(z)$ can be decomposed into Re$J(z)=k^2-x^2+y^2$ and Im$J(z)=-2xy$ where $z=x+iy$. We define three regions: T_1: the z plane to the right of the line Re$J=0$ which passes through $x=k$; T_2: to the left of the line Re$J=0$ which passes through $x=-k$; and T_0: the region between T_1 and T_2 except for the segment $(-k,k)$ of the x axis. Theorem A, then, states that $w\cdot dw/dz$ has at most one zero on the x axis in the potential hills (i.e., in T_1 or T_2) because Re$J\leq 0$ there. At an eigenstate this zero moves to infinity. Theorem B states that there are no zeros of w in T_0 because Re$J\geq 0$ there. To use theorem C one observes that at an eigenstate $w\cdot dw/dz$ is always negative on the z axis in T_1. Further, Im$J=-2xy$ is always negative in T_1 above the x axis. Thus, w has no zeros in T_1 above the x axis by theorem C.

Similar arguments apply to T_1 below the axis, and to T_2.

In conclusion, theorems A, B, and C show that the harmonic oscillator wave function is free of zeros throughout the complex plane, except possibly on the real axis between the turning points, and at infinity. By (B1) the momentum function is free of poles in the same region.

Theorems A, B, and C are sufficient to examine the location of the poles of the momentum function of the harmonic oscillator. For the radial Coulomb problem an additional theorem, called "the zero-free star," is useful.[17] We do not give this theorem here, but merely mention that the earlier theorems plus the zero-free star are sufficient to show that the only poles of the coulomb radial momentum function are at $r=0$, between the turning points, and at $r=\infty$.

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[11] Notation: Operators are designated by a caret. Classical quantities are designated by a subscript c. The action variables differ by 2π from the usual definition. Masses m are such that $2m=1$.

[12] For the canonical set $\hat{x},\hat{p}$ we work in the Schrödinger representation, i.e., the representation where $\hat{x}\,|x\rangle = x\,|x\rangle$; x is the eigenvalue of $\hat{x}$ and $|x\rangle$ is the eigenket (see Ref. 4). For the set $\hat{Q},\hat{P}$ we work in the momentum representation where $\hat{P}\,|P\rangle = P\,|P\rangle$. E is defined as the eigenvalue of the energy: $\hat{H}\,|E\rangle = E\,|E\rangle$. p and Q are functions of eigenvalues; their interpretation is given in later sections. Use of the above representations makes the Hamilton-Jacobi formalism developed here close in spirit to the usual wave function formalism of quantum mechanics.

[13] Equation (2.3) is equivalent to the time-independent Schrödinger equation, i.e., (2.3) implies the Schrödinger equation, and the Schrödinger equation implies (2.3). We prefer to postulate (2.3), since we discuss (2.3) later as a dynamical equation. Also, (2.5) and the time-dependent Schrödinger equation are equivalent in the same sense. See Sec. VIII for further discussion of these points. Also, note that we are not doing WKB theory here. For a discussion of the connection between quantum Hamilton-Jacobi theory and the WKB formalism see Appendix C.

[14] Equations (2.4) hold unchanged in operator form: $\hat{P}=P(\hat{H})$ or $\hat{H}=E(\hat{P})$. $\hat{H}$ is the transformed Hamiltonian which is a function only of the new momentum $\hat{P}$. Also, (3.6) hold in operator form: $\hat{J}=J(\hat{H})$ or $\hat{H}=E(\hat{J})$.

[15] Note that the quantum momentum function $p(x,E)$ is distinct from the quantum momentum $\hat{p}$.

[16] The properties of $p(x,E)$ and Eq. (3.5) can be obtained also from the connection between $p(x,E)$ and the wave function $\psi(x,E)$. From (3.1) and (8.1) one has $p(x,E) = (\hbar/i)\psi'(x,E)/\psi(x,E)$ where prime means $\partial/\partial x$. Therefore, first, the zeros of the wave function in the potential well correspond to the poles of $p(x,E)$. Thus, the n in (3.5) counts also the number of zeros of the wave function. Second, from Sturm-Louiville theory (see, e.g., Ref. 17, Chaps. X and XI) the zeros of the wave function in the well are correlated with the eigenvalues: the ground state has no zeros, the first excited state has one zero, etc. Thus, the n in (3.5) labels the energy eigenvalues E in ascending order as is claimed in Sec. III on the basis of (3.2) and (3.3).

[17] E. L. Ince, *Ordinary Differential Equations* (Longmans, Green, London, 1927).

[18] There are well-known difficulties defining angle operators in quantum mechanics. However, for an angle $\hat{w}$ an exponential-type operator $\exp(i\hat{w})$ can be defined. Further, such exponential operators can be made unitary. See Ref. 19 for discussions of these points. The angle $\hat{w}$ does not play a central role in our discussion; where it does occur it is understood that the appropriate operator is the exponential of $\hat{w}$. See Appendix A.

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[20] $W(x,E)$ and $E(J)$ are defined for discrete E and J, respectively. Therefore, to take the derivative in (4.4), continuations of $W(x,E)$ and $E(J)$ are necessary. For the purposes of discussing $w(x,J)$ we assume such continuations are possible. See, also, Appendix A.

[21] While this discussion has shown that (5.3) satisfies (3.2) and (3.3), it has not shown that the phase $-\pi/4$ in (5.3) is correct; see Appendix B.

[22] See also R. A. Leacock and M. J. Padgett, Phys. Rev. Lett. 50, 3 (1983).

[23] For a discussion of the connection between the moving poles of $p(x,E)$ and the cuts of $p_c(x,E)$ see Sec. V.

[24] R. A. Leacock and T. L. Zimmerman (unpublished); W. H. Furry, Phys. Rev. 71, 360 (1947).

[25] In an actual calculation one works to a finite order N_r in α.

To solve for the $a(n,r)$ one uses the property $a(n,r)=b(n,r)=0$ for $r<0$ or $r+n<0$. For order N_r, the $a(n,r)$ are found in the sequence: $r=0$ with $n=0$ to $N_r+1, r=1$ with $n=-1$ to $N_r, \ldots, r=N_r$ with $n=-N_r$ to 1. For example, for order $N_r=0$ the sequence is $(n,r)=(00,),(1,0)$, while for order $N_r=1$ the sequence is $(n,r)=(0,0),(1,0),(2,0),(-1,1), (0,1),(1,1)$. The boundary condition (3.3) is used to solve $a^2(0,0)=b^2(0,0)$; (3.3) gives $a(0,0)=b(0,0)$. For order $N_r=0, J=ia(1,0)$, while for order $N_r=1, J=i[a(1,0)+a(1,1)\alpha]$.

[26] J. J. Loeffel, A. Martin, B. Simon, and A. S. Wightman, Phys. Lett. 30B, 656 (1969).

[27] For a different, but related, interpretation of expressions like (8.1) and (8.2) see, e.g., Sec. 32 of Ref. 4. See, also, Appendix C.