## Hamilton-Jacobi Theory and the Quantum Action Variable

Robert A. Leacock and Michael J. Padgett[a]

Department of Physics and Ames Laboratory, Iowa State University, Ames, Iowa 50011

A quantum action variable is defined in the context of a quantum Hamilton-Jacobi theory. The action variable can be used to find the exact bound-state energy levels of a quantum system without solving an equation of motion for the system wave functions.

The quantum-mechanical energy levels of a particle oscillating in a potential well are found, e.g., by solving the Schrödinger equation for, simultaneously, the energy eigenvalues and eigenfunctions. In this note we show how the bound-state energies of a quantum system can be obtained without simultaneously finding the system wave functions.

Our approach to the bound-state problem is based upon the fact that, in classical mechanics, a short cut to the system frequencies is provided by the action variable.[1] This powerful property of the classical action variable suggests defining its quantum analog. Such a definition occurs in the context of a quantum canonical transformation theory.[2,3]

We set up a quantum Hamilton-Jacobi formalism appropriate as a framework for defining quantum action-angle variables. The system considered first is a particle moving on a straight line under a force given by a potential $V$. The potential is assumed to be a well capable of containing bound states, and the energy eigenvalues considered are those of the bound states. The Hamiltonian is

$$\hat{H} = \hat{p}^2 + V(\hat{x}), \tag{1}$$

where, in the Schrödinger representation, the linear coordinate and momentum are $\hat{x} = x$, $\hat{p} = (\hbar/i)\partial/\partial x$, respectively.[4]

The theory is cast in terms of eigenvalues instead of operators. The eigenvalues for the linear coordinate, linear momentum, angle variable, action variable, and energy are $x$, $p$, $w$, $J$, and $E$, respectively.

The canonical transformation equations connecting the linear and action-angle variables have the form $p = \partial W(x,E)/\partial x$, $w = \partial W(x,E)/\partial J$, where $E = E(J)$ and where $W(x,E)$ is the *quantum Hamilton's characteristic function*.[5] Given these transformation equations, the *quantum Hamilton-Jacobi equation* for system (1) is[6]

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

$W(x,E)$ is subject to physical boundary conditions which complete its definition.

To define the action-variable eigenvalue we generalize the classical definition.[1] We define the classical action variable as $J_c = (1/2\pi) \times \int_C dx \, p_c(x,E)$, where the integral is counterclockwise around a closed contour $C$ which encloses the two turning points and the section of the real $x$ axis between them. The classical momentum function $p_c(x,E)$ is defined as $p_c(x,E) = [E - V(x)]^{1/2}$. The two turning points $x_{1,2}$ are de-

fined by $p_c(x_1,E) = p_c(x_2,E) = 0$, and the $x$ plane on which $p_c(x,E)$ is defined is given a cut from $x_1$ to $x_2$. $p_c(x,E)$ is that branch of the square root which is positive just below the cut.

Following the classical discussion, the *quantum action-variable eigenvalue* $J$ is defined as

$$J = J(E) \equiv (1/2\pi) \int_C dx\, p(x,E), \qquad (3)$$

where the contour $C$ is the same as in the classical case. The first of the transformation equations suggests defining a $p(x,E) \equiv \partial W(x,E)/\partial x$ via $W(x,E)$. Thus, using this definition and Eq. (2), we define the *quantum momentum function* $p(x, E)$, for use in (3), by

$$\frac{\hbar}{i} \frac{\partial p(x,E)}{\partial x} + p^2(x,E) = p_c^2(x,E) = E - V(x). \qquad (4)$$

The definition of $p(x,E)$ is completed by the *correspondence-principle boundary condition*,

$$p(x,E) \to p_c(x,E), \quad \hbar \to 0, \quad E \text{ fixed}. \qquad (5)$$

Before we apply (3), it is useful to find the eigenvalues $J$. By studying (4) and (5) one finds that inside the potential well, i.e., on the real $x$ axis between $x_1$ and $x_2$, $p(x,E)$ has poles of residue $\hbar/i$; note, e.g., that such a pole term satisfies (4) with the right-hand side set equal to zero. Further, (4) and (5) imply that for the ground state $p(x,E)$ has no poles in the potential well, for the first excited state $p(x,E)$ has one pole in the well, and so on; i.e., the number of poles $p(x,E)$ has in the potential well gives directly the excitation level of the system. Since these poles are enclosed by the contour $C$, one has from (3)

$$J = n\hbar = J(E), \qquad (6)$$

where $n = 0, 1, 2, \ldots$ counts the number of poles of $p(x,E)$ in the well. Note that (6), like (2)–(5), is an exact quantum mechanical expression.

The properties of $p(x,E)$ and Eq. (6) can be obtained also from the connection between $p(x,E)$ and the Schrödinger wave function. First, as shown in Ref. 7, the zeros of the wave function in the potential well correspond to the poles of $p(x,E)$. Thus, the $n$ in (6) counts also the number of zeros of the wave function. Second, from Sturm-Liouville theory (see, e.g., Ince,[8] Chaps. 10 and 11) 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 (6) labels the energy eigenvalues $E$ in ascending order as was claimed above on the basis of (4) and (5).

The power of (3)–(6) is based upon the fact that

integral (3) for $J(E)$ can be evaluated with the residue theorem without obtaining a complete solution for $p(x,E)$ from (4) and (5). In order to use the residue theorem to do the $J(E)$ integral it is necessary to know the location of the singularities of the integrand. Three methods exist for locating these singularities with only $p_c(x,E)$. First, because of (4) and (5) we see that 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 $p_c(x,E)$. [An example of a "fixed" pole is the pole at $x = \infty$ in the oscillator problem (see below), while examples of "moving" poles are the poles in the potential well which move when $E$ is changed.] Second, the moving poles of $p(x,E)$ (which correspond to the zeros of the wave function; see Ref. 7) can occur only on or near a line defined by the equation $\int_a^x dx'\, p_c(x',E) = \text{real}$, where $a$ is a turning point (see Furry[9]). Third, there exist theorems on the location of the zeros of solutions of differential equations which provide a general method for finding the poles of $p(x,E)$ without solving for $p(x,E)$ (see, e.g., Ref. 8, Chap. 21).

We illustrate (3)–(6) with four examples. The first example is the harmonic oscillator with potential $V(x) = x^2$. The only pole of the integrand of (3), outside of those in the potential well, is at $x = \infty$. Expanding $p(x,E)$ for large $x$ one has $p(x, E) = a_1 x + a_{-1}/x + \ldots$, and use of this expansion in (4) gives $a_1^2 = -1$ and $-i\hbar a_1 + 2a_1 a_{-1} = E$. Application of boundary condition (5) yields $a_1 = +i$, and so $a_{-1} = (E - \hbar)/2i$. Thus, by the residue theorem, the integral (3) for $J(E)$ is evaluated with the result $J = E/2 - \hbar/2$. Since $J = n\hbar$, $n = 0, 1, 2, \ldots$ [see (6)], the usual oscillator energy levels are obtained.

As a second illustration of (3)–(6) we consider the anharmonic oscillator. The action variable is given by (3) with the momentum function $p(x, E)$ given by (4) and (5) with $V(x) = x^2 + \lambda x^4$. The exact energy levels are given then by (6).

The task is to evaluate the integral (3) for $J(E)$. The system has four classical turning points:

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

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

where $x_3$ and $x_4$ are unphysical. In addition to the poles between $x_1$ and $x_2$, $p(x,E)$ has poles on the imaginary $x$ axis above $x_4$ and below $x_3$. Thus, when the contour $C$ is distorted it encloses these poles. One way of computing the $J(E)$ integral is as follows. One writes the classical momentum

function as

$$p_c(x,E) = (E - x^2 - \lambda x^4)^{1/2}$$
$$= \lambda^{1/2}x_4 x(1 - x_2^2/x^2)^{1/2}(1 - x^2/x_4^2)^{1/2}.$$

The two square roots in $p_c(x,E)$ are expanded; the result is $p_c(x,E) = \sum b(n,r)\alpha^r x^{1-2n}$, where the double sum is over $r = 0$ to $\infty$ and over $n = -r$ to $\infty$, and where $\alpha \equiv x_2^2/x_4^2$. ($\alpha$ is a parameter of smallness.) The quantum momentum function has the form $p(x,E) = \sum a(n,r)\alpha^r x^{1-2n}$, where the sum is over $r$ and $n$ as before. The expansions of $p(x,E)$ and $p_c(x,E)$ effectively eliminate the poles on the imaginary $x$ axis, and store their effect in the $a(n,r)$. Next, the $p_c(x,E)$ and $p(x,E)$ expansions are substituted into the right-hand and left-hand sides of (4), respectively. By collecting powers of $\alpha$ and $x$ one obtains an equation giving the unknown $a(n,r)$ in terms of the known $b(n,r)$.[10] The action variable then follows from (3) and the $p(x,E)$ expansion; the result is an asymptotic expansion of $J(E)$ in powers of $\alpha$: $J(E) = i\sum a(1,r)\alpha^r$, where the sum is over $r = 0$ to $\infty$.[10]

We have compared our results for the ground state for $\lambda = 0.1, 0.2, \ldots, 1.0$ with those found by other methods.[11] For example, for $\lambda = 0.1$, 0.4, and 1.0 we find $E = 1.065\,285$, $E = 1.2048$, and $E = 1.392$, respectively, which agree with the values in Ref. 11 to the significant figures quoted.

To consider motion in three dimensions under, e.g., a spherically symmetric potential $V(r)$ one needs the three-dimensional form of (2); this is just (2) with the replacement $\partial/\partial x \rightarrow \nabla$, where $\nabla$ is the gradient operator. The resulting equation is written in terms of spherical polar coordinates $r, \theta, \varphi$, and this equation is separated by letting

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

where $E$, $\lambda$, and $c$ are the eigenvalues of the $W_r$, $W_\theta$, and $W_\varphi$ equations, respectively. By defining $p_r(r,E,\lambda) \equiv \partial W_r(r,E,\lambda)/\partial r$ and $p_\theta(\theta,\lambda,c) \equiv \partial W_\theta(\theta,\lambda,c)/\partial\theta$ one obtains the $r$ and $\theta$ *quantum momentum function equations*[4]:

$$-i\hbar r^{-2}\partial(r^2 p_r)/\partial r + p_r^2 = E - V(r) - \lambda^2/r^2, \quad (7)$$

$$-i\hbar(\sin\theta)^{-1}\partial(\sin\theta p_\theta)/\partial\theta + p_\theta^2 = \lambda - c/\sin^2\theta, \quad (8)$$

where $p_r = p_r(r,E,\lambda)$, $p_\theta = p_\theta(\theta,\lambda,c)$, and where $J_\varphi \equiv \sqrt{c} = n_\varphi\hbar$, $n_\varphi = 0, \pm 1, \pm 2, \ldots$. The $r$ and $\theta$ momentum functions obey boundary conditions analogous to (5).

We consider first the angular motion using (8). The $\theta$ action-variable eigenvalue is $J_\theta = (1/2\pi) \times \int d\theta p_\theta(\theta,\lambda,c)$. The contour $C$ for this integral encloses the two turning points, defined by the

vanishing of the right-hand side of (8), and the section of the real $\theta$ axis between them. The integral is evaluated by letting $y = -\cot\theta$ and working in the $y$ plane. In terms of $y$ the integrand has first-order poles, apart from those in the potential well, at $y = \pm i, \infty$. By transforming Eq. (8) to the $y$ plane and using the boundary condition at the points $y = \pm i, \infty$, the necessary residues to evaluate $J_\theta$ are found. The result is $J_\theta = [\lambda + (\hbar/2)^2]^{1/2} - \hbar/2 - J_\varphi'$ where the square root is positive and where $J_\varphi'$ is the positive square root of $J_\varphi^2$. Inverting to obtain $\lambda$ yields $\lambda = (J_\theta + J_\varphi')(J_\theta + J_\varphi' + \hbar) = l(l+1)\hbar^2$, where $l = n_\theta + n_\varphi' = 0, 1, 2, \ldots$, since $J_\theta = n_\theta\hbar$, $n_\theta = 0, 1, 2, \ldots$, and since we define $n_\varphi'$ as the positive square root of $n_\varphi^2$. Thus, the angular momentum eigenvalues are obtained.

The next and last illustration is the Coulomb radial motion. The momentum function equation is (7) with $V(r) = -g/r$; $g$ is a positive, real constant. The radial action-variable eigenvalue is $J_r = (1/2\pi)\int dr p_r(r,E,\lambda)$, with $\lambda$ given previously and with the integral contour $C$ enclosing the two turning points, given by the vanishing of the right-hand side of (7) with $V = -g/r$, and the section of the real $r$ axis between them. The only first-order poles, aside from those in the potential well, are at $r = 0, \infty$. With use of (7) and the boundary condition, the necessary terms in $p_r(r, E, \lambda)$ at $r = 0, \infty$ are found, and the integral evaluated by the residue theorem. The result is $J_r = -l\hbar - \hbar + g/2\sqrt{-E}$. Since $J_r = n_r\hbar$, $n_r = 0, 1, 2, \ldots$, one obtains the Coulomb energy levels.

The above four examples show that quantum energy levels are controlled by the singularities of the quantum momentum function just as classical frequencies are controlled by the singularities of the classical momentum function.

[a] Present address: Getty Oil Company, P. O. Box 1404, Houston, Tex. 77001.

[1] H. Goldstein, *Classical Mechanics* (Addison-Wesley, New York, 1950); our notation follows this book.

[2] Quantum canonical transformation theory begins with

P. Jordan, Z. Phys. 38, 513 (1926), and 40, 809 (1927), and 44, (1927); and with P. A. M. Dirac, Proc. Roy. Soc. London, Ser. A 113, 621 (1927), and Phys. Z. Sowjetunion 3, 64 (1933), and Rev. Mod. Phys. 17, 195 (1945). These authors define transformation equations, but do not define transformation-generating functions. The path-integral formulation of quantum mechanics [R. P. Feynman, Rev. Mod. Phys. 20, 367 (1948)] can be viewed as a transformation theory. The most complete development of quantum transformation theory is given by J. Schwinger, in *Quantum Kinematics and Dynamics* (Benjamin, New York, 1970), see also references therein [e.g., Phys. Rev. 82, 914 (1951), and 91, 713 (1953)].

[3]R. J. Finkelstein, *Nonrelativistic Mechanics* (Benjamin, Reading, Mass., 1973).

[4]Operators are designated by a caret. Masses $m$ are such that $2m = 1$.

[5]Transformation equations are discussed by Jordan and Dirac, Ref. 2, and in P. A. M. Dirac, *The Principles of Quantum Mechanics* (Oxford Univ. Press, London, 1958), 4th ed., especially Sec. 32. We do not discuss $w$ further here.

[6]Equation (2) can be stated as a postulate or can be derived from Schrödinger's equation. The connection between the two equations is $\psi(x,E) \equiv \exp[iW(x,E)/\hbar]$, where $\psi(x,E)$ is the time-independent wave function. Note that we are not doing the WKB approximation here; e.g., the $W(x,E)$ of (2) is not the $W$ used in WKB theory.

[7]From $\psi(x,E) \equiv \exp[iW(x,E)/\hbar]$ (see Ref. 6) and $p(x,E) \equiv W'(x,E)$ one has $p(x,E) = -i\hbar\psi'(x,E)/\psi(x,E)$, where prime means $\partial/\partial x$. Therefore, the zeros of $\psi(x,E)$ inside the potential well correspond to the poles of $p(x,E)$. Near a zero of $\psi(x,E)$ at point $x_p$, $\psi(x,E) \simeq A(x-x_p)$ and $\psi'(x,E) \simeq A$, with $A$ constant. Thus, $p(x,E) \simeq -i\hbar/(x-x_p)$, i.e., $p(x,E)$ has a pole at $x_p$ with residue $\hbar/i$.

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

[9]W. H. Furry, Phys. Rev. 71, 360 (1947).

[10]In order to solve for the $a(n,r)$ one makes use of the property $a(n,r) = b(n,r) = 0$ when $r < 0$ or $n + r < 0$ (which restricts the $n$ values to $n = -r$ to $\infty$, for fixed $r$). For a solution to order $N_r$ in $\alpha$, the $a(n,r)$ are found in the following order: $r = 0$ with $n = 0$ to $N_r + 1$, $r = 1$ with $n = -1$ to $N_r$, ..., $r = N_r$ with $n = -N_r$ to 1. For example, for order $N_r = 1$, the $a(n,r)$ are found in the order $(n,r) = (0,0)$, $(1,0)$, $(2,0)$, $(-1,1)$, $(0,1)$, $(1,1)$; the action variable is then $J(E) = i[a(1,0) + a(1,1)\alpha]$.

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