Quantization of the classical action and eigenvalue problem

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Abstract

The eigenvalue problem in quantum mechanics is reduced to quantization of the classical action of the physical system. State function of the system, $\psi_0(\phi)$, is written in the form of superposition of two plane waves in the phase space. Quantization condition is derived from the basic requirements of continuity and finiteness for $\psi_0(\phi)$ in the whole region.

Quantization of the physical observables is a principal problem of quantum theory. In three equivalent formulations of quantum mechanics, the eigenvalue problem is solved differently and based on three independent mathematical disciplines. Heisenberg-Dirac method is based on “algebra”, Schrödinger’s approach is based on differential equations or “analysis”, and Feynman’s path integral formulation of quantum mechanics is based on geometry. To make some practical calculations using any of these approaches, a deep knowledge of the corresponding mathematical methods is required.

The quantum theory may be developed starting with classic theory and with specific experiments that led to the replacement of classical theory by the quantum theory. In this way, we need to introduce two nonclassical ideas. First, energy levels of harmonic oscillators are restricted to the values of $E = nh\nu$, with the result that energy transfers to and from such oscillators take place in quanta with $\Delta E = h\nu$. Second, only the probability of the transfer of a quantum is determined by the physical state of the system.

Modern interest to the relationship between the classical quantities and the observed behavior of quantum systems can be attributed to the continuing desire to attain a more thorough understanding of quantum-classical correspondence and develop new semiclassical approximations. Much of the attention has been focused on the classical aspects of the Coulomb problem, namely, the recent observation of wave packet recurrences in high-n Rydberg atoms that strongly suggests motion of the electron in classical Kepler orbits. These experiments have stimulated several theoretical attempts to identify Coulombic coherent states that evolve in a manner most closely resembling the classical dynamics. In particular, it was shown that the quantum dynamical evolution of the electron in a Coulomb field can be completely described by classical mechanics.

In this work we associate the eigenvalue problem with quantization of the classical action. We introduce the state function (s.f.) $\psi_0(\phi)$ of the physical system in the phase space. Using requirements of continuity and finiteness for $\psi_0(\phi)$ in the whole region, we obtain the quantization condition which results in the discrete action variables, i.e. quantization of the classical integrals of motion.

The most distinguished feature of particle motion in microscopic scale is its wave properties known as the particle-wave duality. All wave motions are periodic. Very often we are interested not so much in the details of the orbits as in the frequencies (or eigenvalues) of the motion. A very powerful method of handling such systems is provided by a variation of the Hamilton-Jacobi procedure known as the action-angle variables technique.

Value of these variables has long been demonstrated in celestial mechanics. Recent years have seen something of a renaissance elsewhere in the use and application of action-angle variables in problems involving the motions of charged particles in electromagnetic fields. The adiabatic invariance property of

\[ E = \frac{1}{2} m \omega^2 \pi^2 R^2 \]

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the action variables has led to many fruitful applications of action-angle variables in plasma physics and in the design of particle accelerators.

After the advent of Bohr’s quantum theory of the atom, it was realized that the quantum conditions could be stated most simply in terms of the action-angle variables. The quantum conditions of Sommerfeld and Wilson required that the motion be limited to such orbits for which the action variables \( J \) had discrete values that were integral multiples of \( h \), the quantum of action. As Sommerfeld stated, the method of action-angle variables then provided “a royal road to quantization”. One had only to solve the problem in classical mechanics using action-angle variables, and motion could be immediately quantized by replacing the \( J \)'s with integral multiples of Planck’s constant \( h \).

The mathematical justification for quantum mechanics evolve from a number of fundamental assumptions. First important assumption is that the state of a particle at time \( t \) completely describable by some normalized function \( \psi \) that is called the state function of the particle or system. Only those s.f. that are physically admissible correspond to realizable physical states.

The s.f. itself is not experimentally observable. Another physically necessary assumption is the probability of finding the particle at time \( t \) within a volume \( dq \) centered about \( q \), i.e. \( P(q,t) = |\psi(q,t)|^2 \).

Consider the classical motion of a particle in Hamilton-Jacobi theory, for which the Hamiltonian is a constant of motion and is identical with the total energy \( E \). Hamilton’s principal and characteristic functions are then related according to the equation

\[
S(q,p,t) = W(q,p) - Et,
\]

where \( W \) is solution of the Hamilton-Jacobi equation,

\[
\frac{1}{2m} \left( \frac{dW}{dq} \right)^2 + V(q) = E,
\]

and \( p(q) = dW/dq \) is the generalized momentum.

Since the characteristic function is independent of time, the surfaces of constant \( W \) in configuration space have fixed locations. The motion of the surface in time is similar to the propagation of a wave front. The surfaces of constant \( S \) may thus be considered as wave fronts propagating in configuration space.

The wave amplitude to be associated with the motion of the mechanical particle can be taken in the form \[ \psi = Ae^{iS/h} \] or \[ \psi = Be^{-iS/h} \], where \( h = h/2\pi \). Let us analyze the spatial part of the wave amplitude. For the conservative system, we can consider the following s.f. in configuration space, \[
\psi_0 = Ae^{i\phi} + Be^{-i\phi},
\]

where \( A \) and \( B \) are constants and

\[
\phi = \frac{1}{h} \int q \frac{dW}{dq} dq.
\]

Expression (3) can be treated as the general s.f. of the physical system. To build the physical s.f. in the whole region we need to choose the boundary conditions for the problem.

In quantum mechanics, the s.f. must be continuous and finite in the whole region \((-\infty, \infty)\). In case of free motion we have \( W = pq + const. \). For interacting particles (the potential \( V \neq 0 \)), the interval \((-\infty, \infty)\) is divided by turning points (TP) given by \( E - V = 0 \) on classically allowed regions and classically inaccessible regions.
In the classically allowed region (where \( E \geq V \)) near the turning point \( q_k \) the s.f. (3) is

\[
\psi_0^I(\phi) = A_ke^{i(\phi - \phi_k)} + B_ke^{-i(\phi - \phi_k)},
\]

and in the classically inaccessible region (where \( E < V \)) the function is

\[
\psi_0^{II}(\phi) = C_ke^{-\phi + \phi_k} + D_ke^{\phi - \phi_k}.
\]

Functions (3) and (5) must satisfy the continuity conditions, i.e. \( \psi_0^I(\phi_k) = \psi_0^{II}(\phi_k) \) and \( d[\psi_0^I(\phi_k)]/dq = d[\psi_0^{II}(\phi_k)]/dq \), at \( \phi = \phi_k \). Matching the functions (5) and (6) and their first derivatives at the TP \( q_k \) gives

\[
\begin{cases}
A_k + B_k = C_k + D_k, \\
iAk - iB_k = -C_k + D_k,
\end{cases}
\]

that yields

\[
\begin{cases}
A_k = \frac{1}{\sqrt{2}} (C_ke^{i\pi/4} + D_ke^{-i\pi/4}), \\
B_k = \frac{1}{\sqrt{2}} (C_ke^{-i\pi/4} + D_ke^{i\pi/4}).
\end{cases}
\]

The connection formulas (8) supply the continuous transition of the function (5) into (6) at the TP \( q_k \).

Consider first the two-turning-point (2TP) problem. For this problem, the whole interval \((-\infty, \infty)\) is divided by the TP \( q_1 \) and \( q_2 \) into three regions, \(-\infty < q < q_1 \) (I), \( q_1 \leq q \leq q_2 \) (II), and \( q_2 < q < \infty \) (III). The classically allowed region is given by the interval II.

In the classically inaccessible regions I and III we choose the exponentially decaying functions, i.e., \( \psi_0^I(\phi) = D_1 e^{\phi - \phi_1} \) left from the TP \( q_1 \) (we put \( C_k = 0 \) in Eq. (8)), and \( \psi_0^{III}(\phi) = C_2 e^{-\phi + \phi_2} \) right from the TP \( q_2 \) (here we put \( D_k = 0 \)).

Then, in the classically allowed region II, right from the TP \( q_1 \) we have, from (8), \( A_1 = (D_1/\sqrt{2})e^{-i\pi/4} \) and \( B_1 = (D_1/\sqrt{2})e^{i\pi/4} \), and the s.f. takes the form,

\[
\psi_0^{II}(\phi) = \sqrt{2}D_1 \cos \left( \phi - \phi_1 - \frac{\pi}{4} \right).
\]

Left from the TP \( q_2 \) [here \( A_2 = (C_2/\sqrt{2})e^{i\pi/4} \) and \( B_2 = (C_2/\sqrt{2})e^{-i\pi/4} \)] the s.f. is

\[
\psi_0^{II}(\phi) = \sqrt{2}C_2 \cos \left( \phi - \phi_2 + \frac{\pi}{4} \right).
\]

Here \( \phi_1 = \phi(q_1) \) and \( \phi_2 = \phi(q_2) \). We see that the superposition of two plane waves (3) in the phase space results in the standing wave given by Eqs. (3) and (10).

Functions (3) and (10) should coincide at each point of the interval \([q_1, q_2]\). Putting \( \phi = \phi_2 \) we have, from Eq. Eqs. (3) and (10),

\[
D_1 \cos \left( \phi_2 - \phi_1 - \frac{\pi}{4} \right) = C_2 \cos \frac{\pi}{4}.
\]

This equation is valid if

\[
\phi_2 - \phi_1 - \frac{\pi}{4} = \frac{\pi}{4} + \pi n, \quad n = 0, 1, 2, \ldots
\]

\[
\phi_2 - \phi_1 = \frac{\pi}{2} + \pi n.
\]
\[D_1 = (-1)^n C_2.\] Equation (12) is condition of the existence of continuous finite s.f. in the whole region. This condition being, at the same time, quantization condition. Taking into account (4), we have, from Eq. (12),

\[
\int_{q_1}^{q_2} dq \frac{dW}{dq} = \pi \hbar \left( n + \frac{1}{2} \right).
\]  

(13)

The action variables are defined as a set of independent functions of constants of motion [6],

\[
J_i = \oint dq_i \frac{dW}{dq_i},
\]

(14)

where the integration is to be carried over a complete period of libration or rotation, as the case may be for coordinate \( i \). Equation (13) gives quantization of the classical action for the 2TP problem (libration). The corresponding quantized action variable is

\[
J_i = \oint dq_i \frac{dW}{dq_i} = 2\pi \hbar \left( n + \frac{1}{2} \right).
\]

(15)

For rotation [in this case \( p(q) = P_q = \text{const} \) and \( q \) is cyclic coordinate], the action variable is

\[
J_q = 2\pi \hbar n.
\]

(16)

It is known, if the Hamiltonian is conserved then the Hamilton’s principal function, \( S(q_i, P_i, t) \), is the generating function to new canonical coordinates that are all cyclic and all the momenta are constants of integration (motion). The Hamilton-Jacobi equation constitutes the a partial differential equation for the generating function.

In new canonical coordinates the Hamilton’s characteristic function, \( W_i \), for coordinate \( i \) takes the form \( W_i = P_i q_i + \text{const} \). The constants of integration \( P_i \) can be evaluated in terms of specific initial conditions of the problem; in our case these are requirements of continuity and finiteness for the s.f. \( \psi_0(\phi) \) that results in quantization of the action variables \( J_i \) and, therefore, constants of motion \( P_i \).

Combining the above results we can write the physical s.f. in the whole region as

\[
\psi_0(\phi(q)) = C_n \begin{cases} 
\frac{1}{\sqrt{2}} e^{\phi(q) - \phi_1}, & q < q_1, \\
\cos(\phi(q) - \phi_1 + \frac{\pi}{4}), & q_1 \leq q \leq q_2, \\
\left(\frac{-1}{\sqrt{2}}\right)^n e^{-\phi(q) + \phi_2}, & q > q_2.
\end{cases}
\]

(17)

where \( \phi(q) = P_n q / \hbar \). The normalization coefficient, \( C_n = \{2P_n / [\pi(n + 1/2) + 1]h\}^{1/2} \), is calculated from the normalization condition \( \int_{-\infty}^{\infty} |\psi_0(q)|^2 dq = 1 \).

The s.f. (3) is general for all types of problems and allows to solve multi-turning-point problems (MTP, \( M > 2 \)), i.e. a class of the “insoluble” problems, which cannot be solved by standard methods. In the complex plane, the 2TP problem has one cut between turning points \( q_1 \) and \( q_2 \), and the phase-space integral (13) can be written as the contour integral about the cut. The MTP problems contain (in general case) bound state regions and the potential barriers, i.e. several cuts. The corresponding contour should enclose all cuts. The physical s.f. in the whole region can be built similarly to the 2TP problem with the help of the same connection formulas (4).

Consider the MTP problem with \( \nu \) cuts \([E - V(q) > 0 \text{ on each cut}]\), where all cuts are finite intervals and the effective potential \( V(q) \) (with non-communicating potential wells) is infinite between the intervals.
(In case if the potential is finite in the whole region, we need to take into account the effect of tunneling and the quantization condition will be more complicate [3]). Then the integral around the contour \( C \) can be written as sum of contour integrals around each of the cut. Hence the \( \mu = 2\nu \) TP quantization condition (and quantized action variable) can be written as [3, 4]

\[
J_i = \oint \frac{dW}{dq_i} dq_i = 2\pi \hbar \left( N + \frac{\mu}{4} \right),
\]

where \( N = \sum_{k=1}^{\nu} n_k \) is the total number of zeroes of the s.f. on the \( \nu \) cuts and \( \mu = 2\nu \) is the number of turning points (or Maslov’s index [8], i.e., number of reflections of the s.f. on the walls of the potential).

To exhibit the properties of the method, let us consider the Coulomb problem \( [V(r) = -\alpha/r] \) and confine our discussion to the bound case. In spherical polar coordinates, the Hamilton-Jacobi equation,

\[
\left( \frac{\partial W}{\partial r} \right)^2 + \frac{1}{r^2} \left( \frac{\partial W}{\partial \theta} \right)^2 + \frac{1}{r^2 \sin^2 \theta} \left( \frac{\partial W}{\partial \varphi} \right)^2 = 2m[E - V(r)],
\]

has been demonstrated to be completely separable. The motion in each of the coordinates will be periodic - libration in \( r \) and \( \theta \), and rotation in \( \varphi \). The action variables are

\[
J_\varphi = \oint \frac{\partial W}{\partial \varphi} d\varphi = \oint P_\varphi d\varphi,
\]

\[
J_\theta = \oint \frac{\partial W}{\partial \theta} d\theta = \oint \sqrt{P_\theta^2 - \frac{P_\varphi^2}{\sin^2 \theta}} d\theta,
\]

\[
J_r = \oint \frac{\partial W}{\partial r} dr = \oint \sqrt{2m[E - V(r)] - \frac{P_\varphi^2}{r^2}} dr,
\]

where \( P_\varphi^2, P_\varphi \) are the constants of separation and, at the same time, integrals of motion.

The first integral is \( J_\varphi = 2\pi P_\varphi \). To calculate the integral (21) we use the method of stereographic projection. This means that, instead of integration about a contour \( C \) enclosing the classical turning points, we exclude the singularities outside the contour \( C \), i.e., at \( \theta = 0 \) and \( \infty \). Excluding these infinities we have, for the integral (21), \( J_\theta = I_0 + I_\infty \). Integral \( I_0 = -2\pi P_\varphi \), and \( I_\infty \) is calculated with the help of the replacement \( z = e^{i\theta} \) that gives \( I_\infty = 2\pi P_\theta \). Therefore, \( J_\theta = 2\pi(P_\theta - P_\varphi) \).

For the Coulomb potential, the integral (22) can be calculated analogously. Using the method of stereographic projection, we should exclude the singularities outside the contour enclosing the classical turning points \( r_1 \) and \( r_2 \), i.e. at \( r = 0 \) and \( \infty \). Excluding these infinities we have, for the integral (22), \( J_r = I_0 + I_\infty \), where \( I_0 = -2\pi P_\theta \) and \( I_\infty = 2\pi \alpha m/\sqrt{2mE} \). The total integral is \( J_r = -(J_\theta + J_\varphi) + \pi\alpha \sqrt{-2m/E} \) that supplies the functional dependence of \( E \) upon the action variables,

\[
E = -\frac{2\pi^2 \alpha^2 m}{(J_r + J_\theta + J_\varphi)^2},
\]

Discrete values of the action variables are given by Eq. (17) that results in the exact energy spectrum for the Coulomb problem,

\[
E_n = -\frac{\alpha^2 m}{2(n_r + l + 1)^2 \hbar^2},
\]
where \( l = n_\theta + n_\varphi \). The exact eigenvalues for other central potential can be reproduced analogously.

In conclusion, we have reduced the eigenvalue problem in quantum mechanics to quantization of the classical action. We have considered the classical problem in Hamilton-Jacobi theory using action-angle variables. We have introduced the s.f. of the system, \( \psi_0(\phi) \), in the form of superposition of two plane waves in the phase space. Using general requirements of continuity and finiteness for \( \psi_0(\phi) \) in the whole region, we have obtained the quantization condition for the action variables and the physical s.f. for the problem.

The method has allowed us to reproduce the exact eigenvalues for known solvable potentials and multi-turning-point problems, i.e. a class of “insoluble” problems, which cannot be solved by standard methods \( ^4 \). It is applicable not only to separable, but non-separable potentials, as well. For the non-separable potentials, the quantization condition is multidimensional integral with a single quantum number for non-separable variables.

The physical s.f. \( \psi \) corresponds to the main term of the asymptotic series in the theory of the second-order differential equations. For the conservative systems, we have used canonical coordinates that are all cyclic and all the momenta are constants of motion. This means that particles in stationary states move like free particles-waves in enclosures. This has allowed us to write the oscillating part of the s.f. in the form of a standing wave, which describes free finite motion of particles-waves in enclosures.

There is a simple connection of the method considered here with the Feynman path integrals \( ^5 \): this approach corresponds to the path of “minimum” action. The physical s.f. obtained above corresponds to the classical path.

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