Hamilton Jacobi Formalism in Quantum Mechanics

Sambit Bikas Pal

06MS03
Physics
IISER Kolkata

This article deals with the Hamilton Jacobi formalism in quantum mechanics. A procedure for solving the energy eigenvalues for bound state problems utilizing the action variable has been discussed. Finally as an example, the one-dimensional harmonic oscillator problem has been solved using this formalism.

I. INTRODUCTION

Various mechanical problems in classical mechanics can be elegantly solved by following the Hamilton Jacobi formalism. Hamilton Jacobi theory allows one to arrive at the frequencies of periodic systems, without delving into the full solution of the dynamical problem. Following the classical theory, the formalism of canonical transformations and Hamilton-Jacobi formulation can be extended(2) to quantum mechanics. In quantum mechanics energy eigenstates of a particle in a potential well are usually found out by solving the Schrödinger equation for the eigenfunctions and eigenvalues. However, as in the case of classical periodic problems, quantum Hamilton Jacobi formalism allows calculation of the bound state energies of the system without requiring the determination of the wavefunctions.
The basis of this formalism is the quantum Hamilton-Jacobi equation, which along with the physical boundary conditions, is equivalent to the Schrödinger equation or Heisenberg's equation of motion.

II. CLASSICAL HAMILTON JACOBI THEORY

A. Canonical Transformations in Classical Mechanics

Before going into quantum Hamilton Jacobi formalism and quantum canonical transformations, let us briefly have a review of canonical transformations and Hamilton Jacobi theory in classical mechanics.
In classical mechanics, we have the Variational Principle as,

$$\delta \int_1^2 (L)\, dt = 0 \tag{1}$$

$$\Rightarrow \delta \int_1^2 (p_i \dot{q}_i - H)\, dt = 0 \tag{2}$$

where L and H as usual denotes the Lagrangian and Hamiltonian of the system, respectively.
A total time derivative can be added to the integrand without altering the action integral.

$$\delta \int_1^2 \left(p_i \dot{q}_i - H - \frac{dF}{dt} \right) dt = 0 \tag{3}$$

Such a transformation which preserves the canonical relations

$$\dot{P}_i = -\frac{\partial H'}{\partial Q_i}$$
$$\dot{Q}_i = \frac{\partial H'}{\partial P_i}$$

between the new canonically conjugate coordinates (P_i, Q_i), is called a canonical transformation.

B. Hamilton-Jacobi Theory in Classical Mechanics

Hamilton Jacobi method is a well developed formalism in classical mechanics, which provides a powerful method of solving dynamical equations. This method essentially tries to effect a canonical transformation from the old coordinates and momenta (p_i, q_i) at a time t to a new set of constant quantities, such that the new canonically conjugate positions and momenta (Q_i, P_i) of the transformed Hamiltonian H' are constants in time. From the Hamilton's equations of motion, it is evident that the new positions and momenta will be constants if the new Hamiltonian vanishes. Hence one needs to find a generator F, such that

$$H' = H(p_i, q_i, t) + \frac{\partial F}{\partial t} = 0 \tag{4}$$

The generator F is taken to be a function of the old coordinates q_i and new constant momenta P_i. Hence,

$$p_i = \frac{\partial F(q_i, P_i, t)}{\partial q_i} \tag{5}$$

$$Q_i = \frac{\partial F(q_i, P_i, t)}{\partial P_i} \tag{6}$$

$$\tag{7}$$

The relation $p_i = \dfrac{\partial F}{\partial q_i}$ leads to

$$H\left(\frac{\partial F}{\partial q_i}, q_i, t\right) + \frac{\partial F}{\partial t} = 0 \tag{8}$$

So what we have is a 1^{st} order PDE in $n+1$ variables, whose solution involves $n+1$ constants of integration, taken to be the new constant momenta P_i.

1. Hamilton's Principal Function

$F(q_i, P_i, t)$ is customarily denoted by S and known as Hamilton's Principal Function. Taking the total time derivative of S

$$\frac{dS}{dt} = \frac{\partial S}{\partial q_i}\dot{q}_i + \frac{\partial S}{\partial t} \tag{9}$$
$$= p_i\dot{q}_i - H \tag{10}$$
$$= L \tag{11}$$

one finds, S differs from the indefinite time integral of L only by a constant

$$S = \int L dt + const. \tag{12}$$

2. Hamilton's Characteristic Function

If the system is conservative, i.e. if H does not involve time explicitly, Hamilton's Principal Function can be written in the form,

$$S(q, \alpha, t) = W(q, \alpha) - Et$$

and this quantity, $W(q, \alpha)$ is called Hamilton's Characteristic function

III. QUANTUM HAMILTON JACOBI FORMALISM

The Hamilton-Jacobi formalism in quantum mechanics, is built on similar lines as that of the classical theory. In analogy to classical systems, the quantum action variable can be exploited to arrive at the energy eigenvalues for bound state potential problems without going into the complications of solving for the corresponding wavefunctions. Thus the standard procedure of solving the Schrödinger equation for the eigenvalues and eigenfunctions can be bypassed.
In order to get acquainted with the formalism let us have a look at a system having a potential well $V(x)$ capable of containing bound states.
The Hamiltonian for the system can be written as

$$\hat{H} = \hat{p}^2 + V(\hat{x}) \tag{13}$$

Where, $\hat{x}$ and $\hat{p}$ in Schrödinger representation are,

$$\hat{x} = x \tag{14}$$
$$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x} \tag{15}$$

A. Quantum Canonical Transformations

As before we seek a *quantum* canonical transformation to a new set of coordinates, Q and P, such that the new Hamiltonian is independent of Q. Written in terms of eigenvalues, the quantum canonical transformations are

$$p = \frac{\partial W(x, E(P))}{\partial x} \tag{16}$$
$$Q = \frac{\partial W(x, E(P))}{\partial P} \tag{17}$$

where $W(x, E)$ is the quantum Hamilton's characteristic function. Here one is free to choose the new momentum, however it has to be defined only in terms of E

$$P = P(E)$$

An equivalent description in terms of operator formalism is also possible(4). However in such a formalism, it is necessary to define operator ordering properly in order to avoid complications arising out of non-commutativity of operators.

B. Quantum Hamilton Jacobi Equation and Hamilton's Characteristic Function

Given the above transformation relations, the Quantum Hamilton Jacobi Equation for the characteristic function is written as,

$$\frac{\hbar}{i}\frac{\partial^2 W(x,E)}{\partial x^2} + \left[\frac{\partial W(x,E)}{\partial x}\right] = E - V(x) \tag{18}$$

$W(x, E)$, has to satisfy certain boundary conditions, which will be dealt with later. One thing should be noted here, we can either take the above equation as a postulate or can derive it from the Schrödinger equation, if one perceives the Schrödinger equation to be more physical and fundamental. Connection between the two is

$$\psi(x, E) \equiv e^{[iW(x,E)]/\hbar} \tag{19}$$

where $\psi(x, E)$ is the time-independent wave function. Substituting $\psi(x, E) = e^{[iW(x,E)]/\hbar}$ in the Schrödinger equation,

$$\begin{aligned}
&\left[-\hbar^2\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) &&= E\psi(x)\\
\Rightarrow\ &\left[-\hbar^2\frac{\partial^2}{\partial x^2} + V(x)\right]e^{iW/\hbar} &&= Ee^{iW/\hbar}\\
\Rightarrow\ &\left[i\hbar W" - W'^2\right]e^{iW/\hbar} &&= (E-V)e^{iW/\hbar}\\
\Rightarrow\ &\frac{\hbar}{i}W" + W'^2 &&= E - V
\end{aligned} \tag{20}$$

we get back eqn(18).

C. Hamilton's Principal Function

If time-dependence is considered, the quantum Hamilton Jacobi equation for the principal function S can be

written as

$$\frac{\hbar}{i}\frac{\partial^2 S}{\partial x^2} + \left[\frac{\partial S}{\partial x}\right] = -\frac{\partial S}{\partial t} - V(x) \tag{21}$$

The only difference between eqn.(18) and eqn.(21) is that E in eqn.(18) has been replaced by $-\frac{\partial S}{\partial t}$ in eqn.(21). For time independent case, the time part can be separated as

$$S = W - Et \tag{22}$$

where W does not depend on t. This leads to the previous QHJE for the Hamilton's Characteristic Function. The time independent Hamilton Jacobi theory using the Hamilton's characteristic function W can be applied for stationary states, since the stationary states are the ones which don't time evolve provided the Hamiltonian has no explicit time dependence.

D. Quantum Action variable/Momentum function

Following classical mechanics as a guide, one can define the quantum action variable and the quantum momentum function, provided the system under consideration obeys certain assumptions, which are respectively

- Potential $V(x)$ should be such that it allows periodic motion.
- Energy eigenvalues considered are those of bound states.

One can define the quantum momentum function as

$$p(x,E) \equiv \frac{\partial W(x,E)}{\partial x} \tag{23}$$

which when substituted in the Quantum Hamilton Jacobi, leads to

$$\begin{aligned}\frac{\hbar}{i}\frac{\partial p(x,E)}{\partial x} + p^2(x,E) &= E - V(x) \\ &= {p_c}^2(x,E)\end{aligned} \tag{24}$$

where, $p_c^2(x,E)$ is the classical momentum function. In the limit $\hbar \to 0$, $p(x,E) \to p_c(x,E)$. This can be considered as a form of the correspondence principle.
As stated earlier,

$$\psi(x,E) = e^{\frac{iW(x,E)}{\hbar}} \tag{25}$$

from which it follows that,

$$p(x,E) = \frac{\partial W(x,E)}{\partial x} = \frac{\hbar}{i}\frac{1}{\psi}\frac{\partial \psi(x,E)}{\partial x} \tag{26}$$

The great importance of the above result is that the zeroes of $\psi(x,E)$ are poles of $p(x,E)$.

Having obtained the momentum function, one can define the quantum action variable as

$$J(E) \equiv \frac{1}{2\pi}\int_C dx\ p(x,E)$$

where, the contour C, is a counterclockwise contour enclosing the real x-axis between the two classical turning points.
The zeroes of $\psi(x,E)$ change their position with energy as a consequence of which the poles of $p(x,E)$ will also change their position. These poles are named *moving poles*. Apart from these, $p(x,E)$ will have *fixed poles* corresponding to the singularities of the potential $V(x)$ itself.

1. Quantization condition for the action variable

The definition of the action variable in terms of the contour integral of the momentum function, in itself leads to an exact quantization condition.
Suppose $\psi(x,E)$ has a zero at x_0, $\psi(x,E) = (x-x_0)\phi(x)$. The momentum function,

$$\begin{aligned} p(x,E) &= \frac{\hbar}{i}\frac{1}{\psi}\frac{\partial \psi(x,E)}{\partial x} \\ &= \frac{\hbar}{i}\frac{1}{(x-x_0)\phi(x)}\left[\phi(x) + (x-x_0)\phi'(x)\right] \\ &= \frac{\hbar}{i}\left[\frac{1}{x-x_0} + \frac{\phi'(x)}{\phi(x)}\right] \end{aligned} \tag{27}$$

Hence there is a simple pole at $x = x_0$ with residue $= \frac{\hbar}{i}$. From Sturm-Liouville theory, the zeroes of wavefunction are well correlated with eigenvalues. Ground state has no zeroes, first excited state has one zero and so on. Hence for the n^{th} eigenstate, there are n nodes in the wavefunction, corresponding to n poles in $p(x,E)$. Consequently by Cauchy's residue theorem, the integral for the Action variable leads to the quantization condition described before.

$$\begin{aligned} J(E) &\equiv \frac{1}{2\pi}\int_C dx\ p(x,E) \\ &= i\sum(\text{Residues}) \\ &= n\hbar \end{aligned} \tag{28}$$

E. Characteristic Function/Angle variable

In terms of the Hamilton's characteristics function, the canonical transformation equations are,

$$p = \frac{\partial W(x,E(J))}{\partial x} \tag{29}$$

$$w = \frac{\partial W(x,E(J))}{\partial J} \tag{30}$$

Here, w, J are a special case of the conjugate set Q, P considered earlier. Once $W(x, E)$ and the action variable J is defined, the angle variable gets defined by,

$$w(x, J) \equiv \frac{\partial W(x, E(J))}{\partial J} \tag{31}$$

However the angle variable will not be required in the process of calculating the energy eigenvalue and they have been included just for the sake of completeness of the formalism.

F. Obtaining Energy Eigenvalues

There is one hurdle in evaluating the contour integral for $J(E)$. The locations of moving poles are not known *a-priori*, however the location of fixed poles are known. By exploiting this fact and by suitable deformation of the contour and change of variables, $J(E)$ can be computed for many potentials. Having done that, application of the quantization condition and inversion of $J(E)$, will provide the energy eigenvalues.
In the following section, we shall take up the example of a one dimensional harmonic oscillator in order to see the quantum Hamilton-Jacobi formalism in action.

IV. ONE DIMENSIONAL HARMONIC OSCILLATOR

Let us take the case of a one dimensional harmonic oscillator with potential,

$$V(x) = \frac{1}{2} m\omega^2 x^2 \tag{32}$$

The Action variable integral along with the quantization condition as derived earlier is,

$$J(E) \equiv \frac{1}{2\pi} \int_C dx\ p(x, E) = n\hbar \tag{33}$$

In this case, the classical turning points are $\pm\sqrt{2E/(m\omega^2)}$. The contour C encloses, in anti-clockwise direction, the two classical turning points and the part of the real x axis between them. The only fixed pole of the integrand, outside those in the well, is at $x = \infty$, hence C may be distorted to enclose the pole at ∞. Substituting $x = \frac{1}{s}$, leads to

$$J = \frac{1}{2\pi} \int_C \frac{ds}{s^2}\ p(s, E) \tag{34}$$

where C in the complex s plane encloses $s = 0$
The momentum equation becomes

$$\frac{\hbar}{i} \frac{\partial p(s, E)}{\partial s} - \frac{p^2(s, E)}{s^2} = -\frac{2mE}{s^2} + \frac{m\omega^2}{2s^4} \tag{35}$$

The momentum function, when expanded in power series gives,

$$p(s, E) = \sum_{n=0}^{\infty} a_n s^n + \sum_{q=1}^{\infty} \frac{b_q}{s^q} \tag{36}$$

Substituting the expansion and comparing coefficients,

$$b_1^2 = -m^2\omega^2 \tag{37}$$
$$2a_0 b_1 = 0 \tag{38}$$
$$-i\hbar b_1 + 2a_1 b_1 + a_0^2 = 2mE \tag{39}$$

b_1 comes out to be $\pm im\omega$. The ambiguity in sign can be removed using the correspondence principle / boundary condition stated earlier, it is the $+ve$ sign that is acceptable. The other coefficients,

$$a_0 = 0 \tag{40}$$
$$a_1 = \frac{2E - \hbar\omega}{2i\omega} \tag{41}$$

The action variable is therefore,

$$J(E) = \frac{2E - \hbar\omega}{2\omega} = n\hbar \tag{42}$$

So finally

$$E = \left(n + \frac{1}{2}\right) \hbar\omega \tag{43}$$

which is the well known result for a harmonic oscillator.

V. SUMMARY

In the discussion above we have seen that, analogous to classical mechanics, one can define quantum canonical transformation and can arrive at the quantum Hamilton Jacobi equation, which in physical content, is equivalent to the Schrödinger equation. Having arrived at the quantum Hamilton Jacobi equation, one can define the quantum momentum function and quantum action variable. Thereby utilizing the nature of the complex momentum function one can impose certain quantization condition on the action variable. We have also seen that by evaluation of the contour integral of the action variable by suitable deformation of the contour and taking into account the quantization condition one arrives at the energy eigenvalues for the bound state problems. Finally the discussion ends with explicit example of the problem of a 1D quantum harmonic oscillator solved using this formalism.

References

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