Chapter 2

The Hamilton-Jacobi Formalism

This thesis would be dealing with the time independent Hamiltonian. In what follows, we briefly discuss the Hamilton Jacobi formalism in context of classical mechanics in section 2.1. In section 2.2 we develop this formalism in context of quantum mechanics. This formalism is applied to the harmonic oscillator, in both the classical (section 2.1) and to quantum (in section 2.3) approach for comparison and to elucidate the working of this method.

2.1 The classical Hamilton-Jacobi Formalism

In classical mechanics, the Hamilton Jacobi theory is well developed and provides an independent and often a powerful method of solving the dynamical equations [1]. We first consider the general approach wherein, the Hamiltonian \( H(q, p, t) \) is any general function of \( q \), \( p \) and \( t \). A canonical transformation from the coordinate and momenta \((q, p)\) at time \( t \), to a new set of constant quantities, (such as the \( 2n \) initial values \((q_0, p_0)\), at \( t = 0 \)) is sought such that the new coordinate system, of the transformed Hamiltonian, \( K \); \( Q_i \) and \( P_i \) are constants in time. This is automatically ensured by requiring that the transformed Hamiltonian \( K \) is identically zero. We then have,

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The equations of transformation relating the old and the new canonical variables,

\[ \frac{\partial K}{\partial P_i} \equiv \dot{Q}_i = \{Q_i, K\} = 0, \quad (2.1) \]
\[ -\frac{\partial K}{\partial Q_i} \equiv \dot{P}_i = \{P_i, K\} = 0. \quad (2.2) \]

are then exactly the solution of the problem, as they give the coordinates and momenta as a function of their initial values and time.

\[ K \text{ is related to the old Hamiltonian, using canonical transformation; given by} \]
\[ K = H(q, p, t) + \frac{\partial F}{\partial t}. \quad (2.4) \]

\( K \) is required to be zero and \( F \), the generating function, is then taken as a function of the old coordinates \( q_i \), the new constant momenta \( P_i \) and time \( t \). i.e., \( F_2(q_i, P_i, t) \), which is one of the possible forms for the generating functions involving canonical transformations. Therefore,

\[ p_i = \frac{\partial F_2}{\partial q_i}, \quad (2.5) \]
\[ Q_i = \frac{\partial F_2}{\partial P_i}. \quad (2.6) \]

We then have (2.4) as
This is the Hamilton-Jacobi equation, and constitutes a partial differential equation, in $(n + 1)$ variables, $q_1, \cdot \cdot \cdot , q_n, t$, for the generating function $F_2$. A complete solution for this first order partial differential equation involves $n + 1$ variables involving $n + 1$ constants of integration. The momenta $P_i$ which have not been specified, are required to be constants. We therefore take these $n$ independent constants of integration $\alpha_i$ to be the new (constant) momenta. This generating function $F_2 = S$, is called the Hamilton's principal function, and is denoted by, $S(q_1, q_2, \cdot \cdot \cdot , q_n, \alpha_1, \cdot \cdot \cdot , \alpha_n t)$. Therefore (2.5) and (2.6) can now be written as,

\[
\begin{align*}
\dot{q}_i &= \frac{\partial S(q, \alpha, t)}{\partial q_i} , \\
\dot{\alpha}_i &= \frac{\partial S(q, \alpha, t)}{\partial \alpha_i} .
\end{align*}
\] (2.9) (2.10)

At $t = t_0$, from (2.9) we have ‘$n$’ equations involving ‘$n$’ $\alpha$’s, with the initial values of $q_i$ and $p_i$ which are known; and one is able to calculate these constants in terms of the initial values of the problem. Similarly the constant $\beta_i$ can be obtained from the initial conditions. Therefore,

\[
q = q(\alpha_i, \beta_i, t) ,
\] (2.11)

which solves the problem, by giving the coordinates as function of time and initial conditions.

It is seen that the above approach is applicable only when $S$ could be separated into two parts, one involving $q$ and the other time. Such a separation is always
possible whenever the Hamiltonian does not involve time explicitly. We then have the Hamilton-Jacobi equations for $S$ as,

$$\frac{\partial S}{\partial t} + H(q_i, \frac{\partial S}{\partial q_i}) = 0 . \tag{2.12}$$

From the above equation we see that the first term involves only dependence on $t$, while the second one depends only on $q_i$. The time variation can therefore be separated by assuming a trial solution

$$S(q_i, \alpha_i, t) = W(q_i, \alpha_i) - \alpha_1 t . \tag{2.13}$$

We thus have

$$H \left( q_i, \frac{\partial W}{\partial q_i} \right) = \alpha_1 \tag{2.14}$$

which no longer involves time. One of the constants of integration, appearing in $S$, namely $\alpha_1$, is thus equal to this constant value of $H$. This time independent function $W$ appears merely as a part of the original generating function (the characteristic function) when $H$ is constant, and becomes the new generating function, denoted by $W(q, P)$ and is termed as the Hamilton's characteristic function in literature; We then have the equations of transformation as in (2.5) and (2.6) given by,

$$p_i = \frac{\partial W}{\partial q_i}, \quad Q_i = \frac{\partial W}{\partial P_i} = \frac{\partial W}{\partial \alpha_i} .$$

and the condition that determines $W$ is that $H$ is equal to the new momentum $\alpha_1$. Therefore,
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Since $W$ does not involve time, the new and the old Hamiltonians are equal, it follows that

$$K = a_1,$$

and $W$ generates a canonical transformation in which, all the new coordinates are cyclic. The canonical equations for $P$ give,

\begin{align*}
    \dot{P}_i &= -\frac{\partial K}{\partial Q_i} = 0, P_i = \alpha_i, \\
    \dot{Q}_i &= \frac{\partial K}{\partial P_i} = 1, i = 1, \\
    &= 0, \quad i \neq 1,
\end{align*}

as the new Hamiltonian depends only on one of the momenta $\alpha_i$. For (2.18) we have the following solutions;

\begin{align*}
    Q_1 &= l + \beta_1 \equiv \frac{\partial W}{\partial \alpha_1}, \\
    Q_i &= \beta_i \equiv \frac{\partial W}{\partial \alpha_i}, \quad i \neq 1.
\end{align*}

So the only coordinate that is not simply a constant of motion is $Q_l$. It is not necessary for one to choose $\alpha_1$ and the constants of integration in $W$, as the new constant momenta. In general one can make use of a particular set of $n$ independent functions of the $\alpha_i$’s as the transformed momenta. Given 7,’s are these constants, we have

$$\dot{Q}_i = \frac{\partial K}{\partial \gamma_i} = \nu_i.$$
where $\nu_i$'s are functions of $\gamma_i$'s. Therefore,

$$Q_i = \nu_i t + \beta_i . \quad (2.21)$$

When the Hamiltonian does not involve time explicitly, both these methods are suitable, and the generating functions are then related to each other according to the formula

$$S(q, P, t) = W(q, P) - \alpha t . \quad (2.22)$$

The Hamilton-Jacobi theory is applicable to periodic systems where one defines the action variable $J_i$, given by

$$J_i = \int p_i dq_i , \quad (2.23)$$
as the transformed (constant) momentum $P$, where the integration is carried over a complete period. So one has $H = H(J)$ and the characteristic function $W = W(q, \cdots, q_n, J_1 \cdots J_n)$. The corresponding generalized coordinate $Q_i$ conjugate to $J_i$ is defined as the angle variable $w_i = \frac{\partial}{\partial J_i}$ and the equation of motion for this is given by

$$\dot{w}_i = \frac{\partial H(J_1 \cdots J_n)}{\partial J_i} = \mu_i(J_1 \cdots J_n) ,$$

where $\mu_i$'s are a set of constant functions, which implies,

$$w_i = \mu_i t + \beta_i , \quad (2.24)$$
as arrived at earlier in (2.21). Now the change in $w$ for a complete cycle of $q_j$ is,
where $r$ is period for a complete cycle of $q$ and $v$ is the reciprocal of the period $r$ and is therefore the frequency associated with the periodic motion of $q$. Thus, one is able to arrive at the frequencies of a periodic system without having to completely solve the equations of motion. Let us apply the above technique to the classical harmonic oscillator for elucidating the power of this method, for which the action variable is given by,

\begin{equation}
E = \frac{1}{2} \omega^2 q^2.
\end{equation}

The substitution,
in (2.27) along with some further simplification gives

\begin{equation}
J = \oint p dq = \oint \sqrt{2mE - m^2 \omega^2 q^2} dq.
\end{equation}

where $E$ is the total energy and $\omega^2 = k/m$. The substitution,

\begin{equation}
q = \sqrt{\frac{2\alpha}{m\omega}} \sin \theta,
\end{equation}

in (2.27) along with some further simplification gives

\begin{align}
J &= \frac{2\pi E}{\omega}, \\
\Rightarrow E \equiv H &= \frac{J \omega}{2\pi}.
\end{align}

(2.29)
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Therefore.

\[
\frac{\partial H}{\partial J} \equiv \nu = \frac{w}{2\pi} = \frac{1}{2\pi} \sqrt{\frac{k}{m}},
\]  

(2.30)

which is the standard formula for the frequency of the harmonic oscillator problem. Applying the Hamilton-Jacobi formalism, one is thus able to directly arrive at the frequencies of periodic systems, without having to solve the equations of motion.

2.2 The quantum Hamilton-Jacobi Formalism

The quantum Hamilton-Jacobi (QHJ) formalism is built on lines of the classical Hamilton-Jacobi theory and has been studied since the inception of quantum mechanics [2]. In fact, this approach was christened as the “Royal road to quantization” in the early days of quantum mechanics [3]. It has recently been shown that, in analogy to the classical periodic systems, the quantum action variable can be profitably employed to arrive at the energy eigenvalues for potential problems, without the necessity of obtaining the corresponding wave functions [4]. This is to be contrasted with the standard procedure for tackling bound state problems, where the Schrodinger equation is solved both for the eigenvalues and eigenfunctions [6].

The quantum equivalent of the Hamiltonian is the Schrodinger (representation of the Hamiltonian) equation wherein \( x \) and \( p \) are operators rather than mere observables and this is given as

\[
\hat{H} = \frac{\hat{p}^2}{2m} + V(x)
\]

(2.31)
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A quantum canonical transformation to a new set of coordinates $Q$ and $P$ is done such that the new Hamiltonian is independent of $Q$; Although, a complete operator formalism can be given an equivalent formulation in terms of the eigenvalues $(x, p, Q, P$ and $E)$ of $\dot{x}, \dot{p}, P, Q$ and $H$ respectively, is pursued here to avoid the complication arising from operator ordering. Parallel to the classical case, the corresponding “quantum” characteristic function $W(x, E)$ yields:

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

and

$$Q = \frac{\partial W(x, E)}{\partial P} ,$$

where $W(x, E)$ is the corresponding “quantum” characteristic function and the “quantum” Hamilton-Jacobi equation for the characteristic function is given as

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

$W(x, E)$ is required to satisfy certain boundary conditions associated with its definition and will be discussed a little later in this section. The new momentum $P$, is defined only in terms of only $E$, $P = P(E)$ and the QHJ equation for Hamilton's principal function is postulated as in the classical case as
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Here \( p(x, E) = (E - V(x))^{1/2} \) is the classical momentum function and this is used to calculate the physical turning points, between which, the classical motion takes...
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place, are defined as the points where \( p_c(x,E) \) vanishes. \( p_c(x,E) \) has a branch cut enclosing these physical turning points, in the complex \( x \) plane in which \( p_c(x,E) \) is defined by taking that branch of the square root as positive at a point just below the cut. This helps in determining the sign of \( p_c(x,E) \) throughout the complex plane by analytical continuation. Also note that

\[
p(x, E) \xrightarrow{\hbar \to 0} p_c(x, E) .
\]

This can be thought of as a manifestation of the correspondence principle or as a boundary condition on the QMF. As will be seen explicitly later, the above condition helps in determining \( p(x, E) \) unambiguously. The quantum characteristic function \( W(x,E) \) is related to the energy eigenvectors in the coordinate representation as,

\[
\psi(x, E) = \langle x | E > = e^{iW(x,E)/\hbar} ,
\]

and in the same representation,

\[
\langle x | \hat{p} | E > = -i\hbar \frac{\partial}{\partial x} \langle x | E > = \frac{\partial W}{\partial x} \langle x | E > = p(x, E) \langle x | E >
\]

Thus, one gets

\[
p(x, E) = \frac{\hbar}{i \psi} \frac{1}{\partial x} \psi(x, E).
\]

It is straightforward to check that the Schrodinger equation goes over to the corresponding quantum H-J equation under the above substitution and vice versa.

The quantum analog of the classical action variable is defined as
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It is thus seen that, \( p(x, E) \) has a first order pole at \( x_0 \) with residue \(-i\hbar\). One can also verify the correctness of Eq. (2.41) directly from the quantum H-J equation. Substituting Eq. (2.41) in the QHJ equation, one sees that the contributions of these poles from \( p^2(x, E) \) and \(-i\hbar \frac{\partial p(x, E)}{\partial x}\) cancel each other only if they are of first order, each having the residue \(-i\hbar\). The first order poles are of quantum mechanical origin and their positions are energy dependent, being the same as the zeros of the energy eigenfunction. Just as the zeros of the wave function change their positions with energy, so do the location of the corresponding poles in the QMF. These poles will be referred to as the moving poles.

The quantum H-J equation shows that, \( p(x, E) \) can have singularities in the complex \( x \)-plane, other than the moving poles on the real axis. These singular points correspond to the singular points of the potential term \( V(x) \). The locations of these

\[
J(E) \equiv \frac{1}{2\pi} \oint_C dx \, p(x, E).
\] (2.39)

Here, \( C \) is a counterclockwise contour in the complex \( x \)-plane, enclosing the real line between the classical turning points. The wave function is known to have nodes between the classical turning points. These nodes correspond to poles of the quantum momentum function. To see this clearly, near a zero of the wave function, located at \( x_0 \), we write,

\[
\psi = (x - x_0) \phi(x).
\] (2.40)

This implies,

\[
p \approx \frac{\hbar}{i} \frac{1}{x - x_0} + \cdots.
\] (2.41)

It is thus seen that, \( p(x, E) \) has a first order pole at \( x_0 \) with residue \(-i\hbar\). One can also verify the correctness of Eq. (2.41) directly from the quantum H-J equation.
singularities are, quite obviously, independent of energy; these poles will be called fixed poles.

For a given energy level, the quantum number \( n \) equals the number of nodes of the wave function and hence it counts the number of moving poles of \( p(x, E) \) inside the contour \( C \) appearing in the definition of the quantum action variable given by Eq. (2.39). The residue of each of these poles is \(-i\hbar\). Hence, we have

\[
J(E) = n\hbar
\]

as an exact quantization condition.

Even though this approach appears similar to that of the familiar WKB scheme, it is worth pointing out that Eq. (2.42), when inverted for \( E \), reproduces the exact quantized energy eigenvalues.

Although, the location and the number of the moving poles are not known \( a \ pri\( r i \), a suitable deformation of the contour in the complex plane and change of variables allows one to compute \( J(E) \) for many potentials, in terms of the fixed poles whose locations and residues are \( k\) n\( o\)\( w\)n. In what follows, the QHJ formalism is applied to the harmonic oscillator problem in quantum mechanics both for comparison with the classical harmonic oscillator problem as well as to show the working of the formalism.
2.3 Harmonic oscillator

The QHJ equation for the harmonic oscillator problem with \( V(x) = m\omega^2 x^2 / \hbar \),

\[
p^2 + \frac{i}{\hbar} \frac{\partial p(x, E)}{\partial x} = 2m(E - \frac{m\omega^2 x^2}{2}) \equiv p_c^2 .
\]

The turning points, determined from \( p_c^2(x, E) = 0 \), are \( -x_1 = x_2 = +\sqrt{2E/(m\omega^2)} \).

The quantization condition is given by

\[
J(E) = (1/2\pi) \oint_C p(x, E) dx = n\hbar .
\]

Figure 2.1: Contours for the harmonic oscillator problem.

Here \( C \) is the contour enclosing the moving poles between the two turning points \( x_1 \) and \( x_2 \) (see Fig. 2.1). Noticing that, there is only one fixed pole of \( p(x, E) \) at
\( x \to \infty \), to evaluate \( J(E) \), one considers an integral \( I_{\Gamma_R} \) over a circular contour \( \Gamma_R \) having radius \( R \) and oriented in the anti-clockwise direction. The QMF has no other singular points. Hence, for this case, \( J(E) \) coincides with \( I_{\Gamma_R} \):

\[
I_{\Gamma_R} = J(E) .
\]

For the evaluation of the contour integral \( I_{\Gamma_R} \), one makes a change of variable \( x = 1/y \) to get,

\[
I_{\Gamma_R} = (1/2\pi) \oint_{\Gamma_R} dx p(x, E) = (1/2\pi) \oint_{\gamma_0} dy \tilde{p}(y, E)/y^2 .
\]

Here, \( \tilde{p}(y, E) = p(1/y, E) \) and the counter clockwise contour \( \gamma_0 \) encloses only one singular point in the \( y \) plane, i.e., the pole at \( y = 0 \). The corresponding contour integral can be straightforwardly calculated. Note that there is no negative sign before the integral; the direction of the contour changes sense under this mapping, which is compensated by the negative sign coming from the integration measure. In this example \( J(E) \) and \( I_{\Gamma_R} \) are equal, though the relation between \( J(E) \) and \( I_{\Gamma_R} \) will change from one example to another as will be discussed in the following chapter; the method of computing \( I_{\Gamma_R} \) however remains the same for all the examples.

The QHJ equation written in the \( y \) variable becomes

\[
\tilde{p}^2(y, E) + i\hbar y^2 \frac{\partial \tilde{p}(y, E)}{\partial y} = 2m(E - \frac{m\omega^2}{2y^2}) = \tilde{p}_c^2 .
\]

To calculate the contribution of the pole at \( y = 0 \), \( \tilde{p}(y, E) \) is expanded in a Laurent series as,
Thus the quantization condition $J(E) = n\hbar$ when inverted for $E$, gives
\[ E = \left( n + \frac{1}{2} \right) h\omega. \]
References


