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Quantization of Holonomic Systems Using WKB Approximation

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Abstract The Lagrange multipliers for holonomic systems are introduced as generalized coordinates, then, the system is enlarged to be singular system. The Hamilton-Jacobi function is obtained. This function is used to determine the solution of the equations of motion for holonomic systems and to quantize these systems using the WKB approximation. Two examples are considered to demonstrate the application of our formalism. The solution of the two examples are found to be in exact agreement with the Euler-Lagrange equations.

Keywords Hamilton-Jacobi formulation · Constrained systems · WKB appraximation · Holonomic systems

1 Introduction

The investigation of constrained dynamic systems may be discussed under two basic headings: the investigation of regular Lagrangian with given constraints and the investigation of systems with singular Lagrangians. The study of regular Lagrangians with holonomic constraint equations, $f_\alpha\ (q_i, t)\ = 0, i = 1, 2, \ldots, n$ and $\alpha = n+1, n+2, \ldots, n+m$ is discussed in standard texts [1, 7]. On the other hand, the study of singular Lagrangians was initiated by Dirac [3]. He showed that, in the presence of constraints, the number of degrees of freedom of the dynamic system can be reduced. His approach was extended to continuous systems [2]. Other researchers [4–6, 11, 12] followed Dirac and showed interest in singular theories.

A powerful approach, the canonical method, has been developed for investigating singular systems [8, 9, 13]. In this approach the equations of motion are written as total differential equations and the formulation leads to a set of Hamilton-Jacobi partial differential

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equations which are familiar in regular systems. In addition, Rabei [14] treated the Lagrange multipliers as generalized coordinates. Thus, the regular Lagrangian with given holonomic constraints are treated as singular Lagrangian. The Hamilton's equations of motion for this singular system are constructed. Besides, the general theory for solving the Hamilton-Jacobi partial differential equations of singular systems is given by Rabei et al. [15]. The action function for these systems is obtained in the configuration space. Thus, the singular system is quantized using the WKB approximation [10, 15–17].

The purpose of the present work is to construct the Hamilton-Jacobi partial differential equations for regular Lagrangians with given holonomic constraints which is the so-called holonomic systems. The Hamilton-Jacobi function is obtained and the solutions of the equations of motion are found using this function. Then the holonomic systems is quantized using the WKB approximation.

2 Hamilton-Jacobi Formulation and WKB Approximation

The standard method for incorporating the constraint functions to the equations of motion is the use of the so-called Lagrange multipliers. The motion of a holonomic system could in principle be determined by making use of the n Euler-Lagrange Equations,

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = \lambda_\alpha \frac{\partial f_\alpha}{\partial q_i}, \quad i = 1, 2, \ldots, n \tag{2.1}$$

and the m constraints

$$f_\alpha\,(q_i, t) = 0, \quad \alpha = n+1, n+2, \ldots, n+m \tag{2.2}$$

where L is regular which is a function of n generalized coordinates q_i and n generalized velocities $\dot{q}_i$ as well as the time t. Now, let us construct the new Lagrangian by adding the holonomic constraints (2.2) multiplied by the Lagrange multipliers to the regular Lagrangian i.e.

$$\acute{L}(q_i, \lambda_\alpha, \dot{q}_i, t) = L(q_i, \dot{q}_i, t) + \lambda_\alpha f_\alpha \tag{2.3}$$

where a repeated suffix assumes a summation over values of that suffix. We introduce the Lagrange multipliers as generalized coordinates. Thus, the new Lagrangian is singular. The Hesse determinant of $\acute{L}$ is $(n+m) \times (n+m)$ determinant formed by the partial derivatives of this extended Lagrangian with respect to $\dot{q}_i$ and $\dot{\lambda}_\alpha$. In other words, the following determinant vanishes

$$\begin{vmatrix} \frac{\partial^2 \acute{L}}{\partial \dot{q}_i \partial \dot{q}_j} & \frac{\partial^2 \acute{L}}{\partial \dot{q}_i \partial \dot{\lambda}_\alpha} \\ \frac{\partial^2 \acute{L}}{\partial \dot{\lambda}_\beta \partial \dot{q}_j} & \frac{\partial^2 \acute{L}}{\partial \dot{\lambda}_\beta \partial \dot{\lambda}_\alpha} \end{vmatrix} \tag{2.4}$$

The Euler-Lagrange equations for the extended Lagrangian will be increased by m equations

$$\frac{d}{dt}\left(\frac{\partial \acute{L}}{\partial \dot{q}_i}\right) - \frac{\partial \acute{L}}{\partial q_i} = 0 \tag{2.5}$$

$$\frac{d}{dt}\left(\frac{\partial \acute{L}}{\partial \dot{\lambda}_\alpha}\right) - \frac{\partial \acute{L}}{\partial \dot{\lambda}_\alpha} = 0 \tag{2.6}$$

Equations (2.5) leads to (2.1) while (2.6) gives the holonomic constraints (2.2). The canonical Hamiltonian

$$H_0 = \dot{q}_i p_i + \dot{\lambda}_\alpha p_\alpha - \acute{L} \tag{2.7}$$

can be calculated using the definition of the canonical momenta

$$p_i = \frac{\partial \acute{L}}{\partial \dot{q}_i} \tag{2.8}$$

$$p_\alpha = \frac{\partial \acute{L}}{\partial \dot{\lambda}_\alpha} \tag{2.9}$$

Making use of (2.8) the generalized velocities can be obtained in terms of generalized coordinates q_i and generalized momenta p_i, i.e. $\dot{q}_i = W(p_i, q_i, t)$. Thus, the canonical Hamiltonian H_0 can be written as

$$H_0 = W(p_i, q_i, t)p_i - L(q_i, W(p_i, q_i, t), t) - \lambda_\alpha f_\alpha(q_i, t) \tag{2.10}$$

Following to the canonical method [13] the set of the Hamilton-Jacobi partial differential equations read as

$$\grave{H}_0 = p_0 + H_0 \tag{2.11}$$

$$\acute{H}_\alpha = p_\alpha \tag{2.12}$$

which can be written in compact form as

$$\frac{\partial S}{\partial t} + H_0 = 0 \tag{2.13}$$

$$\frac{\partial S}{\partial \lambda_\alpha} = 0 \tag{2.14}$$

where S is the Hamilton-Jacobi function. Following to Rabei et al. [15], the solution of the above Hamilton-Jacobi partial differential equations can be constructed as

$$S(q_i, \lambda_\alpha, t) = f(t) + W(E_{i,} q_i) + f_\alpha(\lambda_\alpha) + A \tag{2.15}$$

where E_i are the n constants of integration and A is some other constant. Here, λ_α are the Lagrange multipliers, and are treated as independent variables, just as the time t. Thus the equations of motion can be obtained using the canonical transformation as follows

$$\beta_i = \frac{\partial S}{\partial E_i} \tag{2.16}$$

$$p_i = \frac{\partial S}{\partial q_i} \tag{2.17}$$

$$p_\alpha = \frac{\partial S}{\partial \lambda_\alpha} \tag{2.18}$$

where β_i are constants and can be determined from the initial conditions. The above equations can be solved to furnish the coordinates q_i and the momenta p_i as $q_i = q_i(\beta_i, E_{i,} \lambda_\alpha, t)$, $p_i = p_i(\beta_i, E_{i,} \lambda_\alpha, t)$.

The semiclassical expansion (WKB approximation) of Hamilton-Jacobi function of constrained systems has been investigated by Rabei et al. [15]. Following this reference the wavefunction for the holonomic system can be constructed as

$$\Psi(q_i, \lambda_\alpha, t) = \prod_{i=1}^{n} \Psi_{0i}(q_i) \exp\left[\frac{i}{\hbar} S(q_i, \lambda_\alpha, t)\right] \tag{2.19}$$

where $\Psi_{0i}(q_i) = \frac{1}{\sqrt{P_i}}$. The above wave function (2.19) satisfies the conditions

$$\acute{H}_0 \Psi = 0$$

$$\acute{H}_\alpha \Psi = 0$$

in the semiclassical limit $\hbar \longrightarrow 0$.

3 Examples

Our formalism will be made clear by discussing the following simple examples:

3.1 Adisc Rolling Down an Inclined Plane

As a first example let us discuss the motion of a disk of mass M and radius R that is rolling down an inclined plane without slipping. The extended Lagrangian which includes the constraints is given by:

$$\acute{L} = \frac{1}{2} M \dot{y}^2 + \frac{1}{4} M R^2 \dot{\theta}^2 + M g y \sin\phi + \lambda(y - R\theta) \tag{3.1}$$

where g is the acceleration of gravity and ϕ is the angle of inclination. The Hamiltonian of this system reads

$$H_0 = \frac{p_y^2}{2M} + \frac{p_\theta^2}{MR^2} - M g y \sin\phi - \lambda(y - R\theta) \tag{3.2}$$

where the canonical momenta are

$$p_y = \frac{\partial S}{\partial y}, \qquad p_\theta = \frac{\partial S}{\partial \theta} \tag{3.3}$$

Thus (2.13) becomes

$$\frac{\partial S}{\partial t} + \frac{(\partial S/\partial y)^2}{2M} + \frac{(\partial S/\partial \theta)^2}{MR^2} - M g y \sin\phi - \lambda(y - R\theta) = 0 \tag{3.4}$$

Making use of (2.15), the action function takes the following form:

$$S(y, \theta, \lambda, t) = f(t) + W(y, \theta, E_y, E_\theta) + f(\lambda) + A \tag{3.5}$$

where A is a constant, $f(t) = -Et$ and $f(\lambda) = E_\lambda$ which is a constant. Inserting (3.5) in to (3.4) we obtain

$$-E + \frac{(\partial W/\partial y)^2}{2M} + \frac{(\partial W/\partial \theta)^2}{MR^2} - M g y \sin\phi - \lambda(y - R\theta) = 0 \tag{3.6}$$

Using the separation of variables

$$W(y,\theta) = W_y(y) + W_\theta(\theta) \tag{3.7}$$

we arrive at

$$\frac{(\partial W_y/\partial y)^2}{2M} - Mgy\sin\phi - \lambda y = E_y \tag{3.8}$$

$$\frac{(\partial W_\theta/\partial\theta)^2}{MR^2} + \lambda R\theta = E - E_y \equiv E_\theta \tag{3.9}$$

where E_y and E_θ are constants.

Solving these equations we obtain

$$W_y = \frac{\{2M[E_y + (\lambda + Mg\sin\phi)y]\}^{\frac{3}{2}}}{3M(\lambda + Mg\sin\phi)} \tag{3.10}$$

$$W_\theta = \frac{-2[M(E_\theta - \lambda R\theta)]^{\frac{3}{2}}}{3M\lambda} \tag{3.11}$$

Thus, the action function takes the form

$$S = -(E_y + E_\theta)t + \frac{\{2M[E_y + (\lambda + Mg\sin\phi)y]\}^{\frac{3}{2}}}{3M(\lambda + Mg\sin\phi)} - \frac{2}{3M\lambda}[M(E_\theta - \lambda R\theta)]^{\frac{3}{2}} + E_\lambda + A \tag{3.12}$$

Using (2.16) we get

$$\beta_y = \frac{\partial S}{\partial E_y} = -t + \frac{\{2M[E_y + (\lambda + Mg\sin\phi)y]\}^{\frac{1}{2}}}{\lambda + Mg\sin\phi} \tag{3.13}$$

This equation can be solved for y to give

$$y = \left(\frac{\lambda}{2M} + \frac{1}{2}g\sin\phi\right)t^2 + \frac{\beta_y}{M}(\lambda + Mg\sin\phi)t + \left(\frac{\lambda + Mg\sin\phi}{2M}\right)\beta_y^2 - \frac{E_y}{\lambda + Mg\sin\phi} \tag{3.14}$$

Similarly,

$$\beta_\theta = \frac{\partial S}{\partial E_\theta} = -t - \frac{1}{\lambda}[M\ \ (E_\theta - \lambda R\theta)]^{\frac{1}{2}} \tag{3.15}$$

which can be solved for θ to give

$$\theta(t) = \frac{-\lambda}{MR}t^2 - \frac{2\beta_\theta\lambda}{MR}t + \frac{1}{R}\left(\frac{E_\theta}{\lambda} - \frac{\lambda\beta_\theta^2}{M}\right) \tag{3.16}$$

Thus, taking the second time derivative of (3.14) and (3.16) and making use of the constraint

$$y = R\theta \tag{3.17}$$

we get the Lagrange multipliers as

$$\lambda = -\frac{1}{3} Mg\sin\phi \tag{3.18}$$

and the accelerations

$$\ddot{y} = \frac{2}{3} g\sin\phi \tag{3.19}$$

$$\ddot{\theta} = \frac{2}{3R} g\sin\phi \tag{3.20}$$

which are in agreement with that obtained by conventional methods.

We are now in a position to quantize our system. The wavefunction of this example is given by:

$$\begin{aligned}\Psi(y,\theta,t) &= \frac{1}{\sqrt{p_y p_\theta}} \exp\left(\frac{i}{\hbar}\right) S \\ &= \{2M[E_y + (\lambda + Mg\sin\phi)y]\}^{\frac{-1}{4}} \\ &\quad \times [MR^2(E_\theta - \lambda R\theta)]^{\frac{-1}{4}} \times \exp\left\{\frac{i}{\hbar}\left[-(E_y + E_\theta)t\right.\right. \\ &\quad \left.\left. + \frac{\{2M[E_y + (\lambda + Mg\sin\phi)y]\}^{\frac{3}{2}}}{3M(\lambda + Mg\sin\phi)} - \frac{2}{3M\lambda}[M(E_\theta - \lambda R\theta)]^{\frac{3}{2}}\right]\right\}\end{aligned} \tag{3.21}$$

The Schrödinger equation takes the form

$$\acute{H}_0\Psi = \left\{\frac{\hbar}{i}\frac{\partial}{\partial t} - \frac{\hbar^2}{2M}\frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{MR^2}\frac{\partial^2}{\partial\theta^2} - Mgy\sin\phi - \lambda(y - R\theta)\right\}\Psi = 0 \tag{3.22}$$

After some algebra, it is easy to show that in the semiclassical limit $\hbar \longrightarrow 0$, $H_0\Psi = E\Psi$.

3.2 Atwood's Machine

As a second example, we consider the simple Atwood's machine, where the Hamiltonian of the system can be written in the form

$$H_0 = \frac{p_{x_1}^2}{2m_1} + \frac{p_{x_2}^2}{2m_2} - m_1 g x_1 - m_2 g x_2 - \lambda(\ell - x_1 - x_2) \tag{3.23}$$

The momenta are

$$p_{x_1} = \frac{\partial S}{\partial x_1}, \qquad p_{x_2} = \frac{\partial S}{\partial x_2} \tag{3.24}$$

Thus, the Hamilton-Jacobi equation reads:

$$\frac{\partial S}{\partial t} + \frac{(\partial S/\partial x_1)^2}{2m_1} + \frac{(\partial S/\partial x_2)^2}{2m_2} - m_1 g x_1 - m_2 g x_2 - \lambda(\ell - x_1 - x_2) = 0 \tag{3.25}$$

We see that the function S takes the general form

$$S = f(t) + W(x_1, x_2, E_{x_1}, E_{x2}) + f(\lambda) + A \tag{3.26}$$

and as before

$$f(\lambda) = E_\lambda \quad \text{and} \quad f(t) = -Et \tag{3.27}$$

Then, the Hamilton-Jacobi equation becomes

$$\frac{\partial S}{\partial t} + \frac{(\partial W/\partial x_1)^2}{2m_1} + \frac{(\partial W/\partial x_2)^2}{2m_2} - m_1 g x_1 - m_2 g x_2 - \lambda(\ell - x_1 - x_2) = 0 \tag{3.28}$$

If we make the separation

$$W(x_1, x_2) = W_{x_1}(x_1) + W_{x_2}(x_2) \tag{3.29}$$

we obtain

$$\frac{(\partial W_{x_1}/\partial x_1)^2}{2m_1} - m_1 g x_1 + \lambda x_1 = E_{x_1} \tag{3.30}$$

$$\frac{(\partial W_{x_2}/\partial x_2)^2}{2m_2} - m_2 g x_2 + \lambda x_2 = -\lambda\ell + E - E_{x_1} \equiv E_{x_2} \tag{3.31}$$

Integration of these two equations gives

$$W_{x_1} = \frac{[2m_1(E_{x_1} + (m_1 g - \lambda)x_1)]^{\frac{3}{2}}}{3m_1(m_1 g - \lambda)} \tag{3.32}$$

and

$$W_{x_2} = \frac{[2m_2(E_{x_2} + (m_2 g - \lambda)x_2)]^{\frac{3}{2}}}{3m_2(m_2 g - \lambda)} \tag{3.33}$$

So we get for the function S

$$\begin{aligned} S = -(E_{x_1} + E_{x_2} + \lambda\ell)t + \frac{[2m_1(E_{x_1} + (m_1 g - \lambda)x_1)]^{\frac{3}{2}}}{3m_1(m_1 g - \lambda)} \\ + \frac{[2m_2(E_{x_2} + (m_2 g - \lambda)x_2)]^{\frac{3}{2}}}{3m_2(m_2 g - \lambda)} + E_\lambda + A \end{aligned} \tag{3.34}$$

Using (2.16) we get

$$\beta_{x_1} = \frac{\partial S}{\partial E_{x_1}} = -t + \frac{[2m_1(E_{x_1} + (m_1 g - \lambda)x_1)]^{\frac{1}{2}}}{m_1 g - \lambda} \tag{3.35}$$

and

$$\beta_{x_2} = \frac{\partial S}{\partial E_{x_2}} = -t + \frac{[2m_2(E_{x_2} + (m_2 g - \lambda)x_2)]^{\frac{1}{2}}}{m_2 g - \lambda} \tag{3.36}$$

which can be solved for x_1 and x_2 to give

$$x_1(t) = \left(\frac{m_1 g - \lambda}{2m_1}\right) t^2 + \left(\frac{m_1 g - \lambda}{m_1}\right) \beta_{x_1} t + \left(\frac{m_1 g - \lambda}{2m_1}\right) \beta_{x_1}^2 - \frac{E_{x_1}}{m_1 g - \lambda} \tag{3.37}$$

and

$$x_2(t) = \left(\frac{m_2 g - \lambda}{2m_2}\right) t^2 + \left(\frac{m_2 g - \lambda}{m_2}\right) \beta_{x_2} t + \left(\frac{m_2 g - \lambda}{2m_2}\right) \beta_{x_2}^2 - \frac{E_{x_2}}{m_2 g - \lambda} \tag{3.38}$$

Taking the second time derivative of these two equations and making use of the equation of constraint, we obtain the accelerations as:

$$\ddot{x}_1 = \frac{(m_1 - m_2) g}{m_1 + m_2} = -\ddot{x}_2 \tag{3.39}$$

and for the force of constraint we get $\lambda = \frac{2m_1 m_2}{m_1 + m_2} g$.

Now we come to the quantization of our system. The wavefunction takes the form

$$\begin{aligned} \Psi(x_1, x_2, t) &= \frac{1}{\sqrt{P_{x_1} P_{x_2}}} \exp\left(\frac{i}{\hbar}\right) S \\ &= [2m_1(E_{x_1} + (m_1 g - \lambda) x_1)]^{\frac{-1}{4}} [2m_2(E_{x_2} + (m_2 g - \lambda) x_2)]^{\frac{-1}{4}} \\ &\quad \times \exp\left\{ \frac{i}{\hbar} [-(E_{x_1} + E_{x_2} + \lambda \ell) t] + \frac{[2m_1(E_{x_1} + (m_1 g - \lambda) x_1)]^{\frac{3}{2}}}{3m_1(m_1 g - \lambda)} \right. \\ &\quad \left. + \frac{[2m_2(E_{x_2} + (m_2 g - \lambda) x_2)]^{\frac{3}{2}}}{3m_2(m_2 g - \lambda)} + E_\lambda \right\} \end{aligned} \tag{3.40}$$

and the Schrödinger equation reads

$$\acute{H}_0 \Psi = \left\{ \frac{\hbar}{i} \frac{\partial}{\partial t} - \frac{\hbar^2}{2m_1} \frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_2} \frac{\partial^2}{\partial x_2^2} - m_1 g x_1 - m_2 g x_2 - \lambda(\ell - x_1 - x_2) \right\} \Psi \tag{3.41}$$

Calculation of the required terms and substitution above give

$$\begin{aligned} \acute{H}_0 \Psi = \Bigg\{ &-(E_{x_1} + E_{x_2} + \lambda \ell) - \frac{5\hbar^2}{8m_1} [m_1(m_1 g - \lambda)]^2 [2m_1(E_{x_1} + (m_1 g - \lambda) x_1)]^{-2} \\ &+ E_{x_1} + (m_1 g - \lambda) x_1 - \frac{5\hbar^2}{8m_2} [m_2(m_2 g - \lambda)]^2 [2m_2(E_{x_2} + (m_2 g - \lambda) x_2)]^{-2} \\ &+ E_{x_2} + (m_2 g - \lambda) x_2 - m_1 g x_1 - m_2 g x_2 - \lambda(\ell - x_1 - x_2) \Bigg\} \Psi \end{aligned} \tag{3.42}$$

So after cancellation and taking the semiclassical limit $\hbar \longrightarrow 0$, we get $H_0 \Psi = E \Psi$.

4 Conclusion

In this work the regular Lagrangian with holonomic constraints is treated as a singular Lagrangian. We observed that the holonomic system is enlarged to be a singular system.

The Lagrange multipliers are incorporated to the Hamilton's equations as well as to the Hamilton-Jacobi function for this system. The solutions of the equations of motion obtained using this function are found to be in exact agreement with those obtained using the Euler-Lagrange equations. In this formalism we have shown that the quantum wave function for holonomic system is obtained using the theory of WKB approximation given by Rabei et al. [15]. The quantum results are found to be in exact agreement with the classical results.

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