Quantization of constrained systems using the WKB approximation

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A general theory for solving the Hamilton-Jacobi partial differential equations for constrained Hamiltonian systems is proposed. The quantization of constrained systems is then applied using the WKB approximation. The constraints become conditions on the wave function to be satisfied in the semiclassical limit.

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I. INTRODUCTION

For a physical system whose phase space consists of $2N$ degrees of freedom, $q=(q_1,\ldots,q_N)$; $p=(p_1,\ldots,p_N)$, constraints appear when some relations exist between a subset of the coordinates and momenta. This means that some of the momenta are not independent. When this happens, the Lagrangian of the system is called singular; otherwise it is called regular [1,2].

It was Dirac [3,4] who first set up a formalism for treating singular systems and the constraints involved for the purpose of quantizing his field, with special emphasis on the gravitational field.

Another powerful approach—the canonical—has been developed for investigating singular systems [5–7]. This hinges on defining an equivalent Lagrangian in phase space which is constructed by introducing generalized momenta. For singular systems, however, these momenta are not independent, because of the presence of constraints. The formulation then leads to a set of Hamilton-Jacobi partial differential equations (HJPDEs), and the equations of motion are written as total differential equations of many variables.

The construction of HJPDEs for constrained Hamiltonian systems is of prime importance. The Hamilton-Jacobi theory provides a bridge between classical and quantum mechanics. The principal interest in this theory is based on the hope that it might provide some guidance concerning fields. In this Brief Report we wish to extend the Hamilton-Jacobi formulation to constrained dynamical systems and to quantize these systems using the WKB approximation.

II. THE HAMILTON-JACOBI FORMULATION

We shall first review briefly the formulation of the Hamilton-Jacobi partial differential equations for constrained systems. The starting point is a singular Lagrangian $L=L(q_i,\dot{q}_i)$, $i=1,2,\ldots,N$, such that the rank of the Hessian matrix is $N-R$, $R<N$. Hence the generalized momenta p_i, corresponding to the generalized coordinates q_i, are defined as

$$p_a=\frac{\partial L}{\partial \dot{q}_a}, \quad a=1,2,\ldots,N-R, \tag{1}$$

$$p_\mu=\frac{\partial L}{\partial \dot{q}_\mu}, \quad \mu=N-R+1,\ldots,N. \tag{2}$$

One can solve Eq. (1) for the velocities $\dot{q}_a$ as

$$\dot{q}_a=w_a(q_i,\dot{q}_\mu,p_a). \tag{3}$$

Substituting Eq. (3) in Eq. (2), we get

$$H'_\mu(q_i,p_i)=p_\mu+H_\mu=0, \quad \nu=N-R+1,\ldots,N, \tag{4}$$

which are called primary constraints [3,4]. Here and throughout the Brief Report, Einstein's summation rule for repeated indices is used.

Following [6,7], the corresponding set of the HJPDEs can be written as

$$H'_\alpha\left(q_\beta,q_a,p_\mu=\frac{\partial S}{\partial q_\mu},p_a=\frac{\partial S}{\partial q_a}\right)=0,$$

$$\alpha,\beta=0,N-R+1,\ldots,N, \tag{5}$$

$S(t,q_a,q_\mu)$ being the Hamilton-Jacobi function.

III. THEORY FOR DETERMINING THE HAMILTON-JACOBI FUNCTION

Under certain conditions it is possible to separate the variables in the Hamilton-Jacobi equations; the solution can then always be reduced to quadratures [8,9]. In practice, the Hamilton-Jacobi technique becomes a useful computational tool only when such a separation can be effected. In general, a coordinate q_i is said to be separable in the Hamilton-Jaobi equations when Hamilton's principal function can be split into two additive parts, one of which depends only on the coordinate, whereas the second is entirely independent of q_i. Thus, we can guess a general solution for Eq. (5) in the form

$$S(q_a,q_\mu,t)=f(t)+W_a(E_a,q_a)+f_\mu(q_\mu)+A, \tag{6}$$

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where E_a are the $(N-R)$ constants of integration and A is some other constant. Here q_μ are treated as independent variables, just like the time t.

Once we have found the Hamilton-Jacobi function S, the equations of motion can be obtained in the manner of regular systems, using the so-called canonical transformations [10], as follows:

$$\lambda_a = \frac{\partial S}{\partial E_a}, \tag{7}$$

$$p_i = \frac{\partial S}{\partial q_i}, \tag{8}$$

where λ_a are constants that can be determined from the initial conditions.

Equation (7) can be solved to furnish q_a in terms of λ_a, E_a, q_μ, and t: $q_a = q_a(\lambda_a, E_a, q_\mu, t)$, and the momenta can be determined using Eq. (8): $p_i = p_i(\lambda_a, E_a, q_\mu, t)$.

Two remarks are in order here. The first is that, if the Hamiltonian H_μ does not depend on p_a, the separation of variables will be straightforward. The second is that if H_μ depends on p_a and H_0 depends on q_μ, the separation of variables will not be achieved directly. In this case a suitable change of variables that combine q_a and q_μ should be introduced. Then one can redefine the Lagrangian in terms of the new variables and restart the problem.

IV. THE WKB APPROXIMATION

It is well known that the Hamilton-Jacobi equation for unconstrained systems leads naturally to a semiclassical approximation, namely the WKB approximation, that is very successful in integrable problems and, since the early days of quantum mechanics, in determining the approximate spectra of bound-state problems for certain potentials [11,12]. We shall see that this is applicable for constrained systems as well.

The Schrödinger equation in one dimension for a single particle in a potential $V(q)$ reads

$$i\hbar \frac{\partial \psi(q,t)}{\partial t} = \left[-\frac{\hbar^2}{2}\frac{\partial^2}{\partial q^2} + V(q) \right] \psi(q,t). \tag{9}$$

We can rewrite this equation by using $\psi(q,t) = \exp[iS(q,t)/\hbar]$ [12]:

$$-\frac{\partial S}{\partial t}\psi = \left[\frac{1}{2}\left(\frac{\partial S}{\partial q}\right)^2 - \frac{i\hbar}{2}\frac{\partial^2 S}{\partial q^2} + V \right]\psi.$$

Assuming $\psi \neq 0$, this leads to

$$-\frac{\partial S}{\partial t} = \frac{1}{2}\left(\frac{\partial S}{\partial q}\right)^2 - \frac{i\hbar}{2}\frac{\partial^2 S}{\partial q^2} + V. \tag{10}$$

Taking the formal limit $\hbar \to 0$, we obtain the classical Hamilton-Jacobi equation

$$-\frac{\partial S}{\partial t} = \frac{1}{2}\left(\frac{\partial S}{\partial q}\right)^2 + V. \tag{11}$$

Thus, in this limit, quantum mechanics reduces to classical mechanics.

Next, consider the expansion $S(q,t) = S_0 + \hbar S_1 + \hbar^2 S_2 + \cdots$. This is the so-called $\hbar$ expansion or semiclassical expansion. Substituting it into Eq. (10), we find

$$-\frac{\partial S_0}{\partial t} = \frac{1}{2}\left(\frac{\partial S_0}{\partial q}\right)^2 + V,$$

$$-\frac{\partial S_1}{\partial t} = \frac{1}{2}\left[-i\frac{\partial^2 S_0}{\partial q^2} + 2\left(\frac{\partial S_0}{\partial q}\right)\left(\frac{\partial S_1}{\partial q}\right) \right], \tag{12}$$

and similarly for higher terms in $\hbar$. The leading equation has only S_0, and it is exactly the same as the Hamilton-Jacobi equation. Once one has solved these equations starting from $S_0, S_1, \ldots$, one has solved, in effect, for the wave function ψ in terms of a systematic expansion in $\hbar$.

The WKB approximation is used mostly for the time-independent case; in other words, for an eigenstate of energy E. Then the wave function has the ordinary time dependence $e^{-iEt/\hbar}$. For one-dimensional problems, the Hamilton-Jacobi function S takes the form $S(q,t) = S(q) - Et$. Therefore only S_0 has the time dependence $S_0(q,t) = S_0(q) - Et$, while higher-order terms do not depend on time.

The lowest term S_0 in Eq. (12) satisfies the Hamilton-Jacobi equation

$$E = \frac{1}{2}\left(\frac{\partial S_0}{\partial q}\right)^2 + V. \tag{13}$$

This differential equation can be solved immediately to yield

$$S_0(q) = \pm \int \sqrt{2[E - v(q')]}\,dq' = \int p(q')\,dq'. \tag{14}$$

Once we know S_0, we can solve for S_1. Starting from Eq. (12) and using $\partial S_1/\partial t = 0$, we find $S_1(q) = (i/2)\ln p(q) + \text{const}$.

Therefore the general solution of the Schrödinger equation up to this order is

$$\psi(q,t) = \frac{c}{\sqrt{p(q)}} \exp\left[\pm \frac{i}{\hbar}\int \sqrt{2[E - V(q')]}\,dq' \right] e^{-iEt/\hbar};$$

the overall constant c is, of course, undetermined from this analysis.

We have so far considered the one-dimensional problem. The transformation from the one-dimensional to the N-dimensional case is achieved by expanding the wave function ψ as

$$\psi(q_i,t) = \left[\prod_{i=1}^{N} \psi_{0i}(q_i) \right] e^{iS(q_i,t)/\hbar}, \qquad \psi_{0i}(q_i) \equiv \frac{1}{\sqrt{p(q_i)}}.$$

For constrained systems, the rank of the Hessian matrix is $N-R$. Thus, the wave function ψ reduces to

$$\psi(q_a,q_\mu,t)=\left[\prod_{a=1}^{N-R}\psi_{0a}(q_a)\right]e^{iS(q_a,q_\mu,t)/\hbar}. \quad (15)$$

This wave function represents our main result. It satisfies the following conditions: $\hat{H}'_0\psi=0$, $\hat{H}'_\mu\psi=0$.

In passing, it is interesting to use the representation

$$\psi=A(\vec{q},t)\exp\left(\frac{iS(\vec{q},t)}{\hbar}\right),$$

which is simply the so-called Madelung transformation [13]. Substituting back into the Schrödinger equation (9), one can split up the resulting equation into two real equations by separating the real and imaginary parts.

The real part leads to the equation

$$\frac{\partial S}{\partial t}+\frac{1}{2m}(\vec{\nabla}S)^2+V-\frac{\hbar^2}{2m}\frac{\nabla^2 A}{A}=0.$$

This is the quantum Hamilton-Jacobi equation. In addition to the kinetic energy and the classical potential V, the Hamiltonian contains another term, the well-known quantum potential Q:

$$Q(\vec{q},t)\equiv-\frac{\hbar^2}{2m}\frac{\nabla^2 A}{A}.$$

For constrained systems, the quantum potential can be treated in the same manner as for regular systems. Clearly, setting $Q=0$, one gets back the classical Hamilton-Jacobi equation. This means that the classical limit can be defined as the case in which the quantum potential may be suppressed.

On the other hand, the imaginary part gives the continuity equation

$$\frac{\partial A^2}{\partial t}+\vec{\nabla}\cdot\left(A^2\frac{\vec{\nabla}S}{m}\right)=0.$$

Here $A^2(\vec{q},t)$ is the probability density, and the expression inside the parentheses represents the standard definition of the current density.

V. AN ILLUSTRATIVE EXAMPLE

Consider the following singular Lagrangian:

$$L=\frac{1}{2}(\dot{q}_1^2+\dot{q}_2^2)+\dot{q}_3^2+(\dot{q}_1-\dot{q}_2-q_3)\dot{q}_3+2q_1+q_2+q_3. \quad (16)$$

The corresponding generalized momenta are

$$p_1=\dot{q}_1+\dot{q}_3,\quad p_2=\dot{q}_2-\dot{q}_3,$$
$$p_3=p_1-p_2-q_3=-H_3. \quad (17)$$

Here the primary constraint is represented by the third equation of (17).

The Hamiltonian H_0 is calculated as $H_0=\frac{1}{2}(p_1^2+p_2^2)-2q_1-q_2-q_3$. The corresponding set of HJPDEs (5) reads

$$H'_0=\frac{\partial S}{\partial t}+\frac{1}{2}\left[\left(\frac{\partial S}{\partial q_1}\right)^2+\left(\frac{\partial S}{\partial q_2}\right)^2\right]-2q_1-q_2-q_3=0,$$

$$H'_3=\left(\frac{\partial S}{\partial q_3}\right)-\left(\frac{\partial S}{\partial q_1}\right)+\left(\frac{\partial S}{\partial q_2}\right)+q_3=0. \quad (18)$$

These are two coupled partial differential equations.

To simplify the problem, let us change the variables according to $u=q_1+q_3$, $v=q_2-q_3$. Rewriting the Hamiltonian and the HJPDEs in terms of these new variables we have

$$H_0=\frac{1}{2}(p_u^2+p_v^2)-2u-v;$$

$$H'_0=p_0+H_0=\frac{\partial S}{\partial t}+\frac{1}{2}\left[\left(\frac{\partial S}{\partial u}\right)^2+\left(\frac{\partial S}{\partial v}\right)^2\right]-2u-v$$
$$=0, \quad (19)$$

$$H'_3=p_3+H_3=\left(\frac{\partial S}{\partial q_3}\right)+q_3=0.$$

The Hamilton-Jacobi function S [Eq. (6)] can then be determined by

$$S(u,v,q_3,t)=f(t)+W_1(u,E_1)+W_2(v,E_2)+f_3(q_3)+A. \quad (20)$$

Since the Hamiltonian H_0 is time independent, one can write $f(t)=-(E_1+E_2)t$.

The first equation of (19) can now be written as

$$-E_1-E_2+\left[\frac{1}{2}\left(\frac{\partial W_1}{\partial u}\right)^2-2u\right]+\left[\frac{1}{2}\left(\frac{\partial W_2}{\partial v}\right)^2-v\right]=0.$$

Separation of variables in this equation leads to

$$W_1(u,E_1)=\int\sqrt{2(E_1+2u)}\,du,$$

$$W_2(v,E_2)=\int\sqrt{2(E_2+v)}\,dv.$$

From the second equation of (19), one finds $f_3=-\frac{1}{2}q_3^2$.

With these results, the Hamilton-Jacobi function becomes

$$S=-(E_1+E_2)t+\int\sqrt{2(E_1+2u)}\,du$$
$$+\int\sqrt{2(E_2+v)}\,dv-\frac{1}{2}q_3^2+A. \quad (21)$$

The solution for the generalized coordinates can be obtained from the transformation [Eq. (7)]

$$\lambda_1=\frac{\partial S}{\partial E_1}=-t+\int\frac{du}{\sqrt{2(E_1+2u)}},$$

$$\lambda_2=\frac{\partial S}{\partial E_2}=-t+\int\frac{dv}{\sqrt{2(E_2+v)}}.$$

These two equations can readily be solved to give

$$q_1=-q_3-\frac{E_1}{2}+t^2+2\lambda_1 t+\lambda_1^2,$$

$$q_2=q_3-E_2+\frac{1}{2}t^2+\lambda_2 t+\frac{1}{2}\lambda_2^2. \tag{22}$$

The other half of the equations of motion—the momenta p_i—can be determined using Eq. (8), after substituting the results for q_1 and q_2. We then have

$$p_1=\frac{\partial S}{\partial q_1}=\sqrt{2(E_1+2u)}=2t+2\lambda_1,$$

$$p_2=\frac{\partial S}{\partial q_2}=\sqrt{2(E_2+v)}=t+\lambda_2, \tag{23}$$

$$p_3=\frac{\partial S}{\partial q_3}=t-q_3+2\lambda_1-\lambda_2.$$

One gets the same results using the canonical method. These results can also be obtained using Dirac's approach.

The wave function (15) for this example can be determined as

$$\psi(u,v,q_3,t)=\psi_{0u}(u)\psi_{0v}(v)e^{iS/\hbar}, \tag{24}$$

where

$$\psi_{0u}(u)=\frac{1}{\sqrt{p_u}}=[2(E_1+2u)]^{-1/4},$$

$$\psi_{0v}(v)=\frac{1}{\sqrt{p_v}}=[2(E_2+v)]^{-1/4}.$$

Now let us apply the HJPDEs (19) to the wave function ψ, after representing them as operators:

$$H_0'\psi=\left[\frac{\hbar}{i}\frac{\partial}{\partial t}-\frac{\hbar^2}{2}\left(\frac{\partial^2}{\partial u^2}+\frac{\partial^2}{\partial v^2}\right)-2u-v\right]\psi,$$

$$H_3'\psi=\left[\frac{\hbar}{i}\frac{\partial}{\partial q_3}+q_3\right]\psi. \tag{25}$$

After some algebra, we have

$$\begin{aligned}H_0'\psi=\Big[&-(E_1+E_2)-\frac{5\hbar^2}{2}[2(E_1+2u)]^{-2}\\&+\frac{1}{2}[2(E_1+2u)]-\frac{5\hbar^2}{8}[2(E_2+v)]^{-2}\\&+\frac{1}{2}[2(E_2+v)]-2u-v\Big]\psi,\end{aligned} \tag{26}$$

$$H_3'\psi=[-q_3+q_3]\psi.$$

Taking the limit $\hbar\to 0$ in Eq. (26), we get $H_0'\psi\equiv 0$, $H_3'\psi\equiv 0$.

VI. CONCLUSION

This work has aimed at, first, shedding further light on constrained systems, especially on determining the Hamilton-Jacobi function S; and, second, quantizing these systems using the WKB approximation.

The HJPDEs for constrained systems are obtained using the canonical method [6,7]. In this work the Hamilton-Jacobi function S in configuration space is determined in the same manner as for regular systems. Finding S enables us to get the solutions of the equations of motion. These solutions are obtained in terms of the time and the coordinates that correspond to dependent momenta; these are treated as independent variables, just like the time t.

This is followed by determining a suitable wave function for constrained systems. The constraints become conditions on the wave function to be satisfied in the semiclassical limit, in addition to the Schrödinger equation.

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