Hamilton's principle and Schrodinger's equation derived from Gauss' principle of least squares

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HAMILTON'S PRINCIPLE AND SCHRÖDINGER'S EQUATION DERIVED FROM GAUSS' PRINCIPLE OF LEAST SQUARES

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It is shown that the Hamilton's principle in classical mechanics and the Schrödinger equation in quantum mechanics can both be derived from an application of Gauss' principle of least squares.

Key words: Gauss' principle of least squares, Hamilton's principle, Schrödinger equation, non-linear equations, linearization.

1. INTRODUCTION

The essence of Gauss' principle of least squares seems to be the following: Natural laws are many faceted that allow the same law to be manifested in different ways. When there are deviations between the two different manifestations of the same law, nature will tolerate the differences but will perform a global moderation by minimizing the total, accumulated, properly weighted, squared deviations to smooth out the differences, thereby achieving the most harmonious order. Thus, in the application of statistical treatment of observational data, one assumes the existence of a hidden yet to be discovered analytical law and treats the observational data as a manifestation of that law.

It is said that Gauss himself seemed to have favored this principle to make it his preferred topic in lecture [1]. Gauss not only applied this principle in his calculation of the orbit of the planet Ceres but also used it to formulate mechanical systems with constraints [1]. For this formulation the basic concept that Gauss explored was the concept of force. On the one hand there is the inertial force

carried by the moving particle and represented by acceleration. On the other hand there is the external force acting on the particle and represented by a force field. In a space without constraint these two forces are but two different representations of the same thing and should be in perfect accord without any deviation. However, with constraints limiting some of the liberties of the possible motions, deviations can occur. It is by the application of the principle of least squares, taking into account the constraints, that one will find the equations of motion of such constrained system. This formulation of Gauss is known as the principle of least constraint. It does produce the same results that can be obtained from other formulations based on different principles. However this formulation of Gauss based on his principle of least squares does not seem to have received wide acceptance. The reason for not being widely accepted may be due to the fact that it is acceleration rather than velocity that entered its formulation.

The fundamental formulation of mechanics that is currently widely used, especially after the birth of quantum mechanics, is the Hamiltonian formulation [1,2]. The basis of the Hamiltonian formulation is the Hamilton's principle. The essence of the Hamilton's principle is the existence of a function, not containing acceleration, called Lagrangian that holds all the essential information of the whole system. In a conservative mechanical system a Lagrangian is the difference of the total kinetic and the total potential energies which do not involve accelerations. The equations of motion of individual components are obtained by making the time integral of the Lagrangian stationary, resulting in the Euler-Lagrange equations. Thus it appears that the Hamilton's principle is different from and unrelated to the Gauss principle of least squares. It is the purpose of this article to show that the Hamilton's principle can be derived from an application of the Gauss' principle of least squares.

Now, in the era of quantum physics the Schrödinger equation takes the place of classical equations of motions. The Schrödinger equation is now so well established that most of the textbooks on quantum mechanics are more concerned about its applications than about its discovery or interpretations. To obtain the Schrödinger equation one simply adopts the rule to replace classical dynamic variables by their appropriate operators in the well prescribed Hamiltonian. Nevertheless, there are some discussions of alternative means to reach the Schrödinger equation such as by ways of Feynmann path integral [3,4], stochastic or diffusion theories [5-10], etc. What Schrödinger himself did was by means of variational principle based on the Hamilton-Jacobi equation. In this way he established the time independent equation as eigenvalue problem. However, he soon commented in the following paper that such a variational procedure he followed is not comprehensible hence not to be further followed

[11]. It is the purpose of this article to try to understand from the view point of Gauss' principle of least squares the Schrödinger's variational procedure. We find that a judicious application of the Gauss principle of least squares can lead to the Schrödinger equation.

In order to carry out such an application we shall formulate the Gauss' principle of least squares in such a way that the acceleration does not enter the formulation so that the objection to the original Gauss' formulation may be removed. We shall here explore the idea of velocity. The essence of our idea is to represent velocity in two different ways: One in terms of particle's trajectory and the other in terms of field. The particle's trajectory is described by the set of Newtonian ordinary differential equations while the field aspect is described by the Hamilton-Jacobi partial differential equation. These two types of descriptions are equivalent. One should note here that there is no need to know the Hamiltonian formulation of mechanics to establish the Hamilton-Jacobi equation [12]. What we shall do is to keep one of the representations fixed and allow the other representaion to deviate from this reference. It turns out that if the field aspect is fixed the Hamilton's principle will follow as a consequence. If, on the other hand, the average of trajectory aspect is fixed we then obtain a set of coupled non-linear partial differntial equations which are equivalent to the Schrödinger equation.

2. FORMULATION OF GAUSS' PRINCIPLE OF LEAST SQUARES

For simplicity we shall consider the motion of a single paricle in a force field of the type of Lorentz force. Generalization to a system of many particles in a similar type of force field is straightforward. The equatioin of motion is

$$m\frac{d}{dt}\mathbf{v} = -\left(\nabla\Phi - \frac{\partial}{\partial t}\mathbf{A}\right) - \mathbf{v}\times(\nabla\times\mathbf{A}). \tag{2.1}$$

When this set of ordinary differential equations are solved, we will get

$$\mathbf{x} = \mathbf{x}(t, \mathbf{a}, \mathbf{b}), \tag{2.2}$$

where the **a** and **b** are two independent set of integration constants. If we calculate the velocities along these trajectories, we find

$$\frac{d}{dt}\mathbf{x}(t, \mathbf{a}, \mathbf{b}) = \mathbf{v}_t(t, \mathbf{a}, \mathbf{b}). \tag{2.3}$$

We shall call the velocity calculated in this way the trajetory aspect. However, we may consider the velocity as a vector field. If we

introduce a scalar function S to be determined and set

$$\mathbf{v}_f = \frac{1}{m}(\nabla S + \mathbf{A}), \tag{2.4}$$

we can transform (2.1) into the following Hamilton-Jacobi equation [12]:

$$\frac{\partial}{\partial t}S + \frac{1}{2m}(\nabla S + \mathbf{A})^2 + \Phi = 0. \tag{2.5}$$

The undetermined S is to be found as the real solutions of the above Hamilton-Jacobi equation. We shall call the volcity calculated from (2.4) based on the solutions of (2.5) the field aspect. If the same initial conditions are imposed to and satisfied by both descriptions, the results are exactly the same. However, the two kinds of descriptions may not always be exactly the same. This may happen when the two descriptions do not satisfy exactly the same set of initial conditions or when the solutions to the Hamilton-Jacobi equation become complex etc.. Thus deviations between the two descriptions are expected and shall be allowed.

Now, we introduce the sum of squared deviations occurring at each spacetime point between the two kinds of descriptions

$$Z = m\left(\mathbf{v}_t - \frac{1}{m}(\nabla S + \mathbf{A})\right) \cdot \left(\mathbf{v}_t - \frac{1}{m}(\nabla S^* + \mathbf{A})\right), \tag{2.6}$$

The asterisk indicates complex conjugate. Then, the squared deviations defined in (2.6) accumulated in the allowed spacetime and weighted by a yet to be determined weight function ρ is

$$J = \int \rho Z dt d^3x. \tag{2.7}$$

We now state that, according to Gauss' principle of least squares, the possible motions of this system are obtained from minimizing the accumulated squared deviations given by (2.7). That is,

$$\delta J = 0 \tag{2.8}$$

is the way to obtain possible motions.

3. DERIVATION OF HAMILTON'S PRINCIPLE

We shall now apply the Gauss principle formulated in the last section to derive Hamilton's principle. For this application we shall keep the field aspect fixed to serve as a reference. Thus S is taken to be real that always satisfies the Hamilton-Jacobi equation (2.5) no matter what virtual trajectory the particle undergoes. Now we set

$$\rho = \delta(\mathbf{x} - \mathbf{x}'(t)), \tag{3.1}$$

where $\mathbf{x}'(t)$ is the virtual trajectory the particle takes. Then (2.8) becomes

$$\delta J = \delta \int_{t_0}^{t_1} Z dt = 0. \tag{3.2}$$

Expanding (2.4), we find

$$Z = 2\left[-\frac{d}{dt}S - \Phi + \frac{1}{2}mv_t^2 - \mathbf{v}_t \cdot \mathbf{A}\right] + 2\left[\frac{\partial}{\partial t}S + \frac{1}{2m}(\nabla S + \mathbf{A})^2 + \Phi\right]. \tag{3.3}$$

Since we are assuming the S to always satisfy the Hamilton-Jacobi equation and that a total time derivative of a function does not contribute to the result of a variational principle, (3.2) becomes

$$\delta \int_{t_0}^{t_1} \left[\frac{1}{2}mv_t^2 - \mathbf{v}_t \cdot \mathbf{A} - \Phi\right] dt = 0. \tag{3.4}$$

This is exactly the Hamilton principle to obtain possible motions. The Lagrangian appears naturally in this process as the integrand.

4. DERIVATION OF SCHRÖDINGER EQUATION

For this application we shall keep the trajectory aspect fixed to serve as the reference. This time the S can become complex. Thus, writing out (2.7) explicitly, we get

$$J = 2\int \rho \left[\frac{1}{2}mv_t^2 - \mathbf{v}_t \cdot \mathbf{A} - \Phi - \frac{1}{2}\frac{d}{dt}(S + S^*)\right] dt d^3x$$
$$+ 2\int \rho \left[\frac{1}{2m}(\nabla S + \mathbf{A}) \cdot (\nabla S^* + \mathbf{A}) + \frac{1}{2}\frac{\partial}{\partial t}(S + S^*) + \Phi\right] dt d^3x. \tag{4.1}$$

What we are going to keep as a constant to serve as the refernece is the first integral. Therefore, the condition to find possible equations of motion for the S and S^* is

$$\delta \int \rho \left[\frac{1}{2m}(\nabla S + \mathbf{A}) \cdot (\nabla S^* + \mathbf{A}) + \frac{1}{2}\frac{\partial}{\partial t}(S + S^*) + \Phi \right] dt d^3x = 0. \tag{4.2}$$

Here the Φ and $\mathbf{A}$ are the scalar and vector fields which define the system and are fixed. The ρ is yet to be specified, and the S, and S^* are the unknown functions to be varied and determined. Now in a variational calculation it is very important to distinguish what can or can not vary independently. We regard the S and the S^* as independent and can vary independently. However there are two possibilities for the ρ. (a) ρ can be considered as an independent function so that it can also vary independently. (b) ρ can be considered as a dependent function of S and S^* so that its variation is related to the variations of S and S^*.

Case (a): ρ is an independent function.

In this case we obtain from (4.2) the following result:

$$\begin{aligned}
&\int \delta\rho \left\{ \frac{1}{2m}(\nabla S + \mathbf{A}) \cdot (\nabla S^* + \mathbf{A}) + \frac{1}{2}\frac{\partial}{\partial t}(S + S^*) + \Phi \right\} dt d^3x \\
&- \int \delta S^* \left\{ \frac{1}{2m}\nabla \cdot [\rho(\nabla S + \mathbf{A})] + \frac{1}{2}\frac{\partial}{\partial t}\rho \right\} dt d^3x \\
&- \int \delta S \left\{ \frac{1}{2m}\nabla \cdot [\rho(\nabla S^* + \mathbf{A})] + \frac{1}{2}\frac{\partial}{\partial t}\rho \right\} dt d^3x \\
&= 0,
\end{aligned} \tag{4.3}$$

where integrations by parts have been performed. Therefore we obtain

$$\frac{1}{2m}(\nabla S + \mathbf{A}) \cdot (\nabla S^* + \mathbf{A}) + \frac{1}{2}\frac{\partial}{\partial t}(S + S^*) + \Phi = 0, \tag{4.4}$$

$$\frac{1}{m}\nabla \cdot [\rho(\nabla S + \mathbf{A})] + \frac{\partial}{\partial t}\rho = 0, \tag{4.5}$$

$$\frac{1}{m}\nabla \cdot [\rho(\nabla S^* + \mathbf{A})] + \frac{\partial}{\partial t}\rho = 0. \tag{4.6}$$

Writing $S = S_r + iS_i$, we obtain, from (4.4)-(4.6),

$$\frac{1}{2m}[(\nabla S_r + \mathbf{A})^2 + (\nabla S_i) \cdot (\nabla S_i)] + \frac{\partial}{\partial t}S_r + \Phi = 0, \tag{4.7}$$

$$\frac{\partial}{\partial t}\rho + \frac{1}{m}\nabla \cdot [\rho(\nabla S_r + \mathbf{A})] = 0, \tag{4.8}$$

$$\frac{1}{m}\nabla \cdot [\rho \nabla S_i] = 0. \tag{4.9}$$

This set of coupled non-linear partial differential equations (4.7)-(4.9) is a possible generalization of the Hamilton-Jacobi equation that follows from Gauss' principle of least squares. $S_i = 0$ is a special case that satisfies (4.9) and makes (4.7) and (4.8) become the ordinary Hamilton-Jacobi equation and the equation of conservation law for ρ.

Case (b): $\rho = \rho(S, S^*) = \rho(S_r, S_i)$.

In this case we obtain, from (4.2),

$$\begin{aligned} &\left(\frac{\partial}{\partial S_r}\rho\right)\left\{\frac{1}{2m}[(\nabla S_r + \mathbf{A})^2 + (\nabla S_i)^2] + \frac{\partial}{\partial t}S_r + \Phi\right\} \\ &- \frac{\partial}{\partial t}\rho - \frac{1}{m}\nabla \cdot [\rho(\nabla S_r + \mathbf{A})] = 0 \end{aligned} \tag{4.10}$$

$$\begin{aligned} &\left(\frac{\partial}{\partial S_i}\rho\right)\left\{\frac{1}{2m}[(\nabla S_r + \mathbf{A})^2 + (\nabla S_i)^2] + \frac{\partial}{\partial t}S_r + \Phi\right\} \\ &- \frac{1}{m}\nabla \cdot [\rho(\nabla S_i)] = 0; \end{aligned} \tag{4.11}$$

(4.10) and (4.11) include (4.7)-(4.9) as special solutions. We shall now demonstrate that (4.10) and (4.11) are equivalent to the Schrödinger equations. For this purpose we introduce

$$\Psi = \exp(iS/\hbar), \tag{4.12}$$

$$\Psi^* = \exp(-iS^*/\hbar), \tag{4.13}$$

$$\rho = \Psi\Psi^* = \exp(-2S_i/\hbar); \tag{4.14}$$

we then obtain, from (4.10) and (4.11),

$$\frac{\partial}{\partial t}\rho + \frac{1}{m}\nabla \cdot \left[\frac{\hbar}{2i}(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*) + \mathbf{A}\Psi\Psi^*\right] = 0, \tag{4.15}$$

$$\begin{aligned} &\Psi^*\left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla + \mathbf{A}\right)\cdot\left(\frac{\hbar}{i}\nabla + \mathbf{A}\right)\Psi + \frac{\hbar}{i}\frac{\partial}{\partial t}\Psi + \Phi\Psi\right] \\ &+ \Psi\left[\frac{1}{2m}\left(\frac{-\hbar}{i}\nabla + \mathbf{A}\right)\cdot\left(\frac{-\hbar}{i}\nabla + \mathbf{A}\right)\Psi^* - \frac{\hbar}{i}\frac{\partial}{\partial t}\Psi^* + \Phi\Psi^*\right] = 0. \end{aligned} \tag{4.16}$$

Now, it can be seen that (4.15) and (4.16) are equivalent to the pair of Schrödinger equations

$$\frac{\hbar}{i}\frac{\partial}{\partial t}\Psi + \frac{1}{2m}\left(\frac{\hbar}{i}\nabla + \mathbf{A}\right)\cdot\left(\frac{\hbar}{i}\nabla + \mathbf{A}\right)\Psi + \Phi\Psi = 0, \qquad (4.17)$$

$$\frac{-\hbar}{i}\frac{\partial}{\partial t}\Psi^* + \frac{1}{2m}\left(\frac{-\hbar}{i}\nabla + \mathbf{A}\right)\cdot\left(\frac{-\hbar}{i}\nabla + \mathbf{A}\right)\Psi^* + \Phi\Psi^* = 0. \qquad (4.18)$$

Therefore the Schrödinger equations are seen to be the linearized version of the more general set of non-linear equations (4.10) and (4.11) which are derived from the application of Gauss' principle of least squares.

5. REMARK AND DISCUSION

The Gauss principle of least squares that we used here is based on the idea that the same motion can be described by two different means: one by the particle's trajectory and the other by a field satisfying the Hamilton-Jacobi equation. By allowing these two descriptions to have deviations and then minimizing the accumulated squared deviations we find Hamilton's principle on the one hand and the Schrödinger equation on the other hand. The question of whether to describe a certain phenomenon more appropriately by means of particle and its trajectories or by means of field and the prpagation as waves is an old one ever since the time of Newton and Huygens. This question became an important issue around the turn of this century. It is thought that the birth of quantum physics harmonizes and resolves this conflict. However, to harmonize apparent conflicts is precisely the spirit of the Gauss principle of least squares. Thus it should not be a surprise that Schrödinger equation can be derived from Gauss' principle. However, to reach the Schrödinger equation we allowed the S to become complex quantity. The imaginary part S_i looks somewhat like a diffusion or osmotic motion. Moreover, the weight function ρ is assumed to be given by the relations (4.12)-(4.14). If we were to assume different relations for ρ, equations different from the Schrödinger equation might be obtained. Therefore, Gauss' principle contains more possibilities yet to be explored. What would be the meaning or the use of such possible equations derivable from Gauss' principle of least squares is a matter that remains to be seen.

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