On Schrödinger's variation principle

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On Schrödinger's variation principle [1]

Shoju Kudaka and Shuichi Matsumoto

Almost a century has passed since the birth of quantum theory. Yet even now it is hard to say that we have a sufficiently established concept of the quantization procedure for a given dynamical system. However, the fact that we have had much success in theoretical and applied areas proves that the theory is indeed effective in describing the quantum world. We feel that the opportunity for a further evolution of the theory lies in reexamining this unbalanced situation and searching for a more universal concept of quantization.

We can find in one of Schrödinger's historic articles[1)] an interesting variation principle from which he derived his wave equation for a quantized system. Although he did not emphasize the principle itself, the authors feel that Schrödinger's variation principle touches on the essence of the quantization procedure. Our objective in this article is to review this principle, and to show that it has some remarkable characteristics.

It is in this article that Schrödinger first proposed the quantization of classical dynamical systems: First, he considers the Hamilton-Jacobi equation

$$H\left(q, \frac{\partial S}{\partial q}\right) = E$$

and substitutes $K \log \psi$ for S, where $\psi(q)$ is an unknown function. (The background to this substitution is given in another paper[2)].) The equation then becomes a quadratic form of the function ψ and its first derivatives. Second, he integrates over q space, and considers the variation of the integral due to the change of ψ. He then arrives at the correct wave equation for the quantized system.

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For example, let H be the Hamiltonian for a particle moving in a potential V. Then from the Hamilton-Jacobi equation, substituting $K \log \psi$ for the Hamilton-Jacobi function S, we get

$$\left(\frac{\partial\psi}{\partial x}\right)^2 + \left(\frac{\partial\psi}{\partial y}\right)^2 + \left(\frac{\partial\psi}{\partial z}\right)^2 - \frac{2m}{K^2}(E-V)\psi^2 = 0. \quad (1)$$

The variation defined by

$$\delta \int \left[\left(\frac{\partial\psi}{\partial x}\right)^2 + \left(\frac{\partial\psi}{\partial y}\right)^2 + \left(\frac{\partial\psi}{\partial z}\right)^2 - \frac{2m}{K^2}(E-V)\psi^2\right] dxdydz = 0 \quad (2)$$

leads us to

$$\Delta\psi + \frac{2m}{K^2}(E-V)\psi = 0, \quad (3)$$

which is, of course, the quantum theoretical wave equation for such a particle.

Schrödinger proceeds, in his paper, to analyze equation (3), and does not return to any discussion of the general relation between such a variation principle and quantization procedures. Such an argument seems not to be in his subsequent papers either.

This intriguing variation principle turns out to have some unexpected universalities. We will consider these through some simple calculations in the following.

When Schrödinger considered the above variation problem, he used Cartesian coordinates to describe the motion of the particle. Let us here go through an equal procedure in terms of polar coordinates. The Hamiltonian has the form

$$H = \frac{1}{2m}\left(p_r^2 + \frac{1}{r^2}p_\theta^2 + \frac{1}{r^2\sin^2\theta}p_\phi^2\right) + V(r),$$

and therefore, assuming the expression

$$S = K \log \psi,$$

we have the equality

$$\left(\frac{\partial\psi}{\partial r}\right)^2 + \frac{1}{r^2}\left(\frac{\partial\psi}{\partial \theta}\right)^2 + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial\psi}{\partial \phi}\right)^2 - \frac{2m}{K^2}(E-V)\psi^2 = 0$$

from the Hamilton-Jacobi equation. The postulate that the variation of the left hand side of the equality should be zero:

$$\delta \int \left[\left(\frac{\partial \psi}{\partial r} \right)^2 + \frac{1}{r^2} \left(\frac{\partial \psi}{\partial \theta} \right)^2 + \frac{1}{r^2 \sin^2 \theta} \left(\frac{\partial \psi}{\partial \phi} \right)^2 - \frac{2m}{K^2}(E - V)\psi^2 \right] r^2 \sin \theta dr d\theta d\phi = 0$$

leads us to

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{2m}{K^2}(E - V)\psi = 0, \quad (4)$$

which is exactly equivalent to (3).

Dirac's quantization method[3)] assumes some commutation relations between canonical variables q_i, p_i and interprets the equation

$$H\psi = E\psi$$

as a fundamental equation for the quantized dynamical system. His method gives the correct wave equation (3) if we use Cartesian coordinates for the variables q_i; however, as is well known, treatment of the polar coordinate representation does not proceed so smoothly. This suggests that Schrödinger's variation principle is more universal than Dirac's method.

Next let us consider Schrödinger's variation principle for a dynamical system with a constraint. As a simple example, we consider the case of a particle with mass m on a slope inclined at θ perpendicular to a uniform gravitational field with the acceleration g. The Lagrangian for this particle is given by

$$L = \frac{m}{2}(\dot{q}_1^2 + \dot{q}_2^2) - mgq_2 - \lambda(aq_1 + bq_2),$$

where q_1, q_2 are the coordinates of the particle, λ is an additional variable, and we have set

$$a = -\sin\theta, \qquad b = \cos\theta.$$

The conjugate momenta are given by

$$p_1 = \frac{\partial L}{\partial \dot{q}_1} = m\dot{q}_1, \quad p_2 = \frac{\partial L}{\partial \dot{q}_2} = m\dot{q}_2$$

and

$$p_\lambda = \frac{\partial L}{\partial \dot{\lambda}} = 0.$$

Therefore we should consider

$$H = \frac{1}{2m}(p_1^2 + p_2^2) + mgq_2 + \lambda(aq_1 + bq_2) + u\phi_1 \tag{5}$$

as the total Hamiltonian, with the constraint

$$\phi_1 \equiv p_\lambda = 0$$

and where u is a Lagrange's undetermined multiplier.

Since we have

$$[\phi_1, H_T] = -(aq_1 + bq_2) \equiv -\phi_2, \quad [\phi_2, H_T] = \frac{1}{m}(ap_1 + bp_2) \equiv \frac{1}{m}\phi_3$$

and

$$[\phi_3, H_T] = -(\lambda + bmg) \equiv -\phi_4, \quad [\phi_4, H_T] = u,$$

the motion of the particle is restricted within the submanifold M defined by $\phi_1 = \phi_2 = \phi_3 = \phi_4 = 0$ in the phase space.

Introducing new variables Q and P by equations

$$q_1 = Q\cos\theta, \quad q_2 = Q\sin\theta \tag{6}$$

and

$$p_1 = P\cos\theta, \quad p_2 = P\sin\theta, \tag{7}$$

we can easily show that

$$(Q, \phi_2, \phi_4; P, \phi_3, \phi_1)$$

are new canonical variables, and that Q, P can be interpreted as canonical variables on the submanifold M. Hence the motion of the particle can be described with the variables Q, P, in which case the Hamiltonian has the form

$$K(Q, P) = \frac{P^2}{2m} - mgaQ.$$

Therefore it seems to be very natural that we adopt the equation

$$\frac{\hbar^2}{2m}\frac{d^2\psi}{dQ^2} + mgaQ\psi = -E\psi \tag{8}$$

as the wave equation for the quantized dynamical system.

Now our concern is whether Schrödinger's variational method leads us to the same equation (8). If we follow his method, we have to substitute $K\log\psi$ for the function S in the Hamilton-Jacobi equation

$$H(q, \partial S/\partial q) = E,$$

where ψ is a function of variables q_1, q_2 and $q_3 \equiv \lambda$, and the Hamiltonian is given by (5). Then we have

$$\frac{1}{2m}\left[\left(\frac{K}{\psi}\frac{\partial\psi}{\partial q_1}\right)^2 + \left(\frac{K}{\psi}\frac{\partial\psi}{\partial q_2}\right)^2\right] + mgq_2 + q_3(aq_1 + bq_2) = E,$$

and hence

$$\left(\frac{\partial\psi}{\partial q_1}\right)^2 + \left(\frac{\partial\psi}{\partial q_2}\right)^2 - \frac{2m}{K^2}\left[E - mgq_2 - q_3(aq_1 + bq_2)\right]\psi^2 = 0.$$

We have to take the integral of the left hand side of the above equality over q space, and consider its variation due to the change in the function ψ. Here, because of the existence of the constraints $\phi_1 = \phi_2 = \phi_3 = \phi_4 = 0$, the integral should not be taken over the whole (q_1, q_2, q_3) space but rather over a subspace defined by

$$\phi_2 = aq_1 + bq_2 = 0, \quad \phi_4 = q_3 + bmg = 0.$$

A coordinate in this subspace is given by Q introduced in equation (6) above. Moreover it is easily shown that

$$\left(\frac{\partial\psi}{\partial q_1}\right)^2 + \left(\frac{\partial\psi}{\partial q_2}\right)^2 = \left(\frac{\partial\psi}{\partial Q}\right)^2 + \left(\frac{\partial\psi}{\partial\phi_2}\right)^2.$$

Therefore, the variation of the integral turns out to be

$$\delta\int\left[\left(\frac{\partial\psi}{\partial Q}\right)^2 - \frac{2m}{K^2}\left[E + mgaQ\right]\psi^2\right]dQ = 0,$$

which leads us to the equation

$$\frac{d^2\psi}{dQ^2} + \frac{2m}{K^2}(E + mgaQ)\psi = 0,$$

which is indeed identical to equation (8).

We have shown some interesting facts concerning Schrödinger's variation principle. We do not yet know whether they are accidental results for restricted examples, or whether they suggest that his variation principle touches on a fundamental essence of the quantum theory. A more systematic study will be given in subsequent papers.

References

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Department of Mathematics
College of Education
University of the Ryukyus
Nishihara-cho, Okinawa 903-0129
Japan