LEAST ACTION PRINCIPLES FROM WAVE MECHANICS

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Abstract: Maupertuis' principle of least action is derived from Schrödinger's variational principle of wave mechanics. The path from Schrödinger to Maupertuis goes through two new variational principles, more user friendly than the traditional Maupertuis principle.

The classical limit of quantum mechanics remains a subject of interest even after 70 years of research. Here we discuss a new derivation of classical least action principles. It is well known that Dirac and Feynman [1] derived Hamilton's Principle from a path integral formulation of Quantum Mechanics. But there is a much older and more obscure least action principle bearing the name of Maupertuis [2]. We review the very intimate connection of Maupertuis' Principle (MP) to Schrödinger's variational principle of wave mechanics [3]. The path from Schrödinger to Maupertuis passes through two new variational principles, the Reciprocal Maupertuis Principle and the General Maupertuis Principle. Our discussion will clarify why the traditional formulation is so inconvenient to use. The new principles, though physically equivalent, do not suffer from these drawbacks. We start by reviewing the traditional formulation, to establish the notation we will use.

The principle of least action owes its name to Maupertuis [2]. But the precise formulation, for a single particle moving in a plane is due to Euler (1744), and the generalization to a system

of particles is due to Lagrange (1760). Their formulation is very awkward, as we shall elaborate later in the context of an example. We quote a typical complaint:

> "In almost all textbooks, even the best, this principle is presented so that it is impossible to understand."
>
> K. Jacobi, Lectures on Dynamics, 1842-43 (see ref. [4]).

These difficulties, motivated Hamilton to formulate a new action and a new action principle. Jacobi also reformulated Maupertuis' Principle, but we shall need here the traditional Euler-Lagrange formulation. Our discussion is limited to the periodic motion of one particle in a potential well, in one dimension. A more general discussion is given elsewhere [3].

The Maupertuis Principle (MP) asserts that the actual motion of a particle is such as to render stationary a definite integral, the action W (also called the "restricted" action). The action W is the integral of pdq along a possible (trial) trajectory q(t). The integral is taken from the actual starting point to the actual end point. These points are held fixed during the search for the true path. The trial trajectory is subject to the constraint that energy E is held fixed along the trajectory. The least action principle (MP) may therefore be denoted as:

$$\text{MP:} \qquad (\delta W)_E = 0 \tag{1}$$

where the subscript E indicates that the energy E is fixed.

We turn now to wave mechanics where instead of trial trajectories we have trial wavefunctions ψ. The true wave function is also the solution of a variational principle (due to Schrödinger) $(\delta \langle \psi | H | \psi \rangle)_n = 0$, with normalized ψ. This variational principle applies to all eigenstates ψ_n. We focus on variations in the subspace of states with a large quantum number $n \gg 1$. The quantum number n is fixed by orthogonality to lower states. If n is large, the

quasiclassical approximation (WKB) is good. For these states the quantum variational principle has the form:

$$\delta\langle H\rangle_n = \delta\left(\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}\right)_n = 0 \,. \tag{2}$$

Since the wavefunctions ψ are in the quasiclassical region, the quantum expectation values $<H>_n$ may be evaluated classically as time averages of the classical Hamiltonian, $<H_{classical}>$:

$$\langle H\rangle_n = \langle H_{classical}\rangle = \frac{1}{T}\int_0^T H(q(t)\,,\,p(t))\,dt \tag{3}$$

where T is the period of the classical trajectory q(t), $p(t) = m\dot{q}(t)$ corresponding to ψ. Formula (3) may be derived using a WKB representation for ψ. The condition of fixed n for ψ in (2) corresponds for the classical trajectories to fixed action W_n, through the Bohr-Sommerfeld-Wilson quantization rule

$$W_n = \oint p\,dq = nh \tag{4}$$

Therefore, instead of varying trial wavefunctions with fixed n in the quantum principle (2), we may vary trial trajectories with the constraint of fixed action W in a classical principle:

$$(\delta\bar{E})_W = 0 \tag{5}$$

where we denote by $\bar{E}$ (mean energy) the expectation value (3) of the classical Hamiltonian. The classical principle (5) states that the actual trajectory is selected from a set of trial trajectories of the same action W, by the stationarity of the mean energy $\bar{E}$. By reciprocity - which we shall prove below - the principle (5) is equivalent to

$$(\delta W)_{\bar{E}} = 0 \tag{6}$$

The principle (6) says that the true trajectory is selected from a set of trial trajectories of fixed

mean energy by the extremum (or stationarity) of the action W. The traditional Maupertuis Principle (1) is a special case of (6), where the energy is held fixed locally, not only in the mean. Because (6) implies energy conservation one can restrict $\bar{E}$ to E. Thus we see that the MP can be simply derived from Schrödinger's variational principle of quantum mechanics. The principle (6) is a general form of Maupertuis Principle (GMP), with a weaker constraint on virtual paths, namely fixed mean energy $\bar{E}$. The principle (5) is the Reciprocal Maupertuis Principle (RMP) [5]. The classical limit of the variational principle of wave mechanics (2) is the RMP (5).

The reciprocity between (5) and (6) is best understood if one replaces the constrained variational principle (5) say, by an unconstrained formulation, using a Lagrange multiplier λ. One obtains $\delta\bar{E} = \lambda\delta W$, which shows the equivalence of (5) and (6).

The new classical variational principles (5) and (6) are more advantageous also in practice, as the weaker constraint $\bar{E}$ fixed (in (5)) is easier to enforce than the constraint of fixed E in (1). This is especially true in one dimension [3], as we shall illustrate with two simple examples.

Example 1: The simplest example is free particle motion along a straight line from $x = 0$ to $x = 2$. This example illustrates how energy conservation is a consequence of the principles (5) and (6). We take as a trial trajectory motion with velocity v_1 from $x = 0$ to $x = 1$ and velocity v_2 from $x = 1$ to $x = 2$. Then the action $W = (v_1 + v_2)$ and the mean energy, $\bar{E}$, after a short computation is found to be $\bar{E} = v_1v_2/2$. We assume the mass of the particle is unity. We can take v_1 as a variational parameter, and use either (5) or (6) to find that these principles require $v_1 = v_2$, in other words the energy is conserved locally. It is important to note that the traditional Maupertuis principle assumes local energy conservation and therefore does not permit our simple trial trajectory.

Example 2: A less trivial example is a particle in a quartic oscillator, with Hamiltonian

$$H = p^2/2 + \frac{1}{4} x^4 \tag{7}$$

where we can take as a trial trajectory a harmonic oscillator $x(t) = A \sin \omega t$, with the frequency ω as a variational parameter. One has to compute the action W and the mean energy $\bar{E}$ on the trial trajectory:

$$W = mA^2 \pi \omega \tag{8}$$

$$\bar{E} = \frac{W\omega}{4\pi} + \frac{3}{32} \frac{W^2}{m^2 \pi^2 \omega^2} \tag{9}$$

To implement the Reciprocal Maupertuis Principle (5) one sets to zero the partial derivative of $\bar{E}$ with respect to ω for fixed W. This determines the frequency ω

$$\omega = \left(\frac{3W}{4\pi m^2} \right)^{1/3} \tag{10}$$

which in turn determines the period T as a function of mean energy

$$T(\bar{E}) = \frac{2\pi}{\omega} = 2\pi \left(\frac{m^2}{2\bar{E}} \right)^{1/4} \tag{11}$$

The functional form of $T(\bar{E})$ is correct, and the numerical coefficient has an error of 0.75%, when compared to the exact result. The procedure used shows great similarity with the quantum

variational principle which is the origin of the RMP (5).

In summary, Schrödinger's variational principle becomes in the classical limit the reciprocal Maupertuis principle of mechanics, and this is equivalent to a generalized Maupertuis principle. Restriction to energy conserving virtual paths leads to the traditional form of MP. The relaxation of the constraint of fixed energy E in the traditional form (1) is the key to this bridge between classical and quantum mechanics.

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[4] cf. V.A. Arnold, "Mathematical Methods of Classical Mechanics" Second Edition, Springer-Verlag, 1989, footnote 77 p. 246. The remainder of the footnote, which we do not reproduce in the text is very amusing.

[5] G. Karl and V.A. Novikov, Phys. Rev. 51D, 5069 (1995) and J.E.T.P. 107, 1403 (1995).