NEW VARIATIONAL PRINCIPLES IN CLASSICAL AND SEMICLASSICAL MECHANICS

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We demonstrate that reciprocal Maupertuis' Principle is the classical limit of Schrödinger's Variational Principle in Quantum Mechanics

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Dedication

Misha Marinov loved analytical mechanics and understood its beauty. Canonical transformations, Poisson structures, symplectic geometry etc. were the notions that he constantly used in his original papers, and in his famous review on path integral. One of the authors (NV) had the pleasure to attend his remarkable lectures at ITEP that preceded the review paper. The subtle relation between Quantum and Classical Mechanics was one of the major subjects in these lectures.

We believe that Misha would have enjoyed to read that there exists a new formulation of Classical Mechanics (new variational principle) that follows from Quasiclassical limit of Quantum Mechanics. This paper is based on the results we published in Ref. 1 and in Ref. 2 in collaboration with Chris Gray.

1 Schrödinger's quantum Variational Principle and its classical limit

The fundamental theory is Quantum Mechanics. Classical Mechanics is only a special limit of Quantum Mechanics. In other words Quantum mechanics can be a starting point for the derivation of Classical mechanics. One expects therefore to derive the variational principles of classical mechanics from the variational principles of quantum mechanics.

It is widely known that Hamilton's Principle can be derived in the framework of Feynman path integral formulation of quantum mechanics.[3] We use the old Schrödinger version of quantum mechanics to derive new principle of classical mechanics. In some sense this principle can be considered as a reciprocal to the known Maupertuis principle.

The details of reaching the limit of classical mechanics from the quantum domain are notoriously delicate and difficult. We start by recalling that Schrödinger's variational principle of wave mechanics has the form

$$\delta\left(\frac{\langle\psi_n|\hat{H}|\psi_n\rangle}{\langle\psi_n|\psi_n\rangle}\right) = 0\,, \tag{1}$$

where the quantum system has a Hamiltonian $\hat{H}(\hat{p},\hat{q})$ which is a function of the operators of position $\hat{q}$, and conjugate momenta $\hat{p}$. Although this principle is employed most often to find the ground state $|\psi_0\rangle$ of the quantum system, the principle applies to all eigenstates $|\psi_n\rangle$ of the operator $\hat{H}$ (see, e.g., Ref. 4). This point is elaborated in detail in Ref. 1, where more references can be found.

At large quantum numbers n we step into the domain of Classical Mechanics. We want to demonstrate that at large quantum numbers n, the Schrödinger principle turns into the following classical variational principle

$$0 = \left(\delta \, \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle} \right)_n \stackrel{n \gg 1}{\longrightarrow} \delta \left(\frac{1}{T} \int_0^T H(q,p) \, dt \right)_W \equiv (\delta \bar{E})_W = 0 \,, \tag{2}$$

where mean energy is defined as

$$\bar{E} = \frac{1}{T} \int_0^T H(q,p) \, dt \,, \tag{3}$$

and action W is

$$W = \int_A^B p \, dq \,, \tag{4}$$

where T is the time of propagation of the system from initial point A to final point B in configuration space.

We start with the simplest case of periodic motion in one dimension. On the RHS of (2) the Hamiltonian $H(q,p)$ is the classical counterpart of the quantum Hamiltonian $\hat{H}(\hat{p}, \hat{q})$. On the LHS of (2) the quantum variation is made at large n, with n fixed.[1] The state $|\psi_n(q)\rangle$ corresponds to a classical (periodic) trajectory with precisely the same energy E_n. We consider the trial wavefunctions and trial trajectories such that they match each other.

When we use a WKB representation for all trial wavefunctions on the LHS of (2) we have

$$\int \psi^* \psi dq = \text{const} \int_{q_{\min}}^{q_{\max}} dq/v = \text{const} \int_0^T dt = \text{const} \; T \,, \tag{5}$$

where v is the velocity and T is the period of motion. In the same approximation the numerator of the LHS (2) becomes *const* $\int_0^T H(q,p) \, dt$, with the same constant as the denominator. Therefore the quantum expectation on the LHS becomes a classical time average on the RHS of (2), i.e.

$$\frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle} \longrightarrow \frac{1}{T} \int_0^T H(q,p) \, dt \equiv \bar{E} \,, \tag{6}$$

if we use WKB wavefunctions for $|\psi_n\rangle$. This, of course, is well known.

All that remains to be discussed is how the constraint of fixed W arises on the RHS of (2). We recall that quantization means that only certain classical energies possible on the RHS match quantum energies E_n on the LHS. For periodic motion in one dimension, the constraint on the energy for an allowed quantum state n, derived in the WKB approximation for large n, is

$$W = \oint p \, dq = 2 \int_{q_{\min}}^{q_{\max}} dq \, \sqrt{2m(E_n - V(q))} = nh \,. \tag{7}$$

This is the Bohr-Sommerfeld-Wilson quantization rule, which for n fixed means precisely that the action W is to be kept fixed on the RHS of (2), if n is fixed on the left.

Thus, for one-dimensional system we have completed the derivation of the Classical Variational Principle from Quantum Mechanics. It says that variation of mean energy $\bar{E}$ at fixed short action W is zero for true path. It looks like the new variational Principle different from the Hamilton and Maupertuis Principles.

Next step is to consider systems with N degrees of freedom. Unfortunately, in this general case Quantum Mechanics does not help much. For integrable systems we can prove that quantum average can be replaced by time average over classical quasi-periodic motions when all quantum numbers $n_i \gg 1$. For chaotic non-integrable motions this is rather plausible statement for very large time T. As for the reliable proof, it is absent yet. But the main trouble is with the classical analog of quantum numbers n. We guess that for general systems it is classical action W that has to replace quantum numbers n in quasiclassical limit (exactly like in the case of dimension one).

Thus, Quantum Mechanics gives no rigorous proof. But it gives a certain hint that

$$(\delta \bar{E})_W = 0 \tag{8}$$

in classical limit. We are going to find rigorous proof of this Variational Principle in the framework of Classical Mechanics without any reference to Quantum Mechanics.

2 The four variational principles of mechanics

The starting point is the relation between the Lagrangian $L(q, \dot{q})$ and Hamiltonian $H(q,p)$

$$L(q, \dot{q}) = p\,\dot{q} - H(q,p)\,, \tag{9}$$

which we integrate over some arbitrary time interval $(0,t)$ along some trial trajectory $q(t'), p(t')$, connecting fixed endpoints, to obtain

$$S = \int_0^t dt' L = \int_0^t dt' p\,\dot{q}\, - \int_0^t dt' H\,. \tag{10}$$

Using the definitions of S in Eq. (10), W in Eq. (4) and $\bar{E}$ in Eq. (3), we can rewrite Eq. (10) as

$$S = W - \bar{E}t\,. \tag{11}$$

For *real* trajectories, where $\bar{E} = E$, equation (11) is well known.[4] Taking an arbitrary variation of our trial trajectory $q(t') \to q(t') + \delta q(t')$, with fixed endpoints, as we assume throughout, and an arbitrary variation of our endtime $t \to t + \delta t$, we have (to the first order in $\delta q(t')$ and δt)

$$\delta S + \bar{E}\delta t = \delta W - t\,\delta\bar{E}\,. \tag{12}$$

We now show that the two sides of this general kinematic relation each vanish when we consider variations around a true trajectory, i.e.

$$\delta S = -E\delta t\,, \quad \delta W = t\delta\bar{E}\,, \tag{13}$$

where we have used $\bar{E} = E$ on a true trajectory in the first of (13).

To derive the first of the relations (13), we recall the Hamilton Principle (HP)

$$(\delta S)_t = 0\,, \tag{14}$$

which is valid for true trajectories. Here t is fixed. This relation implies also that for variations around a true trajectory where both S and t vary we must have

$$\delta S = \lambda\delta t\,, \tag{15}$$

where λ is some (Lagrange) multiplier. Indeed, if (15) were not valid, so that $\delta S = \lambda\delta t +$[terms dependent on $\delta q(t')$], we could have a situation where $\delta t = 0$ but $\delta S \neq 0$ that violates Eq. (14). (We recall that δt and $\delta q(t')$ are independent variations). In order to see that $\lambda = -E$, we specialize to the case of variations between two true trajectories with endtimes t and $t+dt$. In this case (15) reads $\partial S/\partial t = \lambda$, and hence $\lambda = -E$ in order to reproduce the well known relation $\partial S/\partial t = -E$. This completes the proof of the first, and hence of the second, of the relations (13).

We now specialize the unconstrained relations (13) by applying constraints. If, in the first of (13), we take the constraint of fixed t (i.e. $\delta t = 0$), we regain the Hamilton Principle (HP) (14). If, on the other hand, we fix S, i.e. set $\delta S = 0$, we get a Reciprocal Hamilton Principle (RHP):

$$(\delta t)_S = 0\,. \tag{16}$$

This principle was unknown in the literature in general formulation of Eq. (16). But many special cases of (RHP) were discussed earlier by many authors starting from Rayleigh (see list of references in Ref. 2).

Let us consider the second of the unconstrained relations (13). If we fix $\bar{E}$, i.e. set $\delta\bar{E} = 0$, we get reformulated Maupertuis' Principle (MP):

$$(\delta W)_{\bar{E}} = 0\,. \tag{17}$$

In our reformulation we relax the constraint of fixed energy E for virtual paths. We allow a larger class of trial trajectories (or "virtual" paths) which do not necessarily conserve energy E. Instead of fixing the energy we keep the *mean energy* $\bar{E}$ fixed. The old set of trial trajectories with fixed $E = \bar{E}$ is a subset of this larger set. Now both quantities W and $\bar{E}$ are *global* whereas in the traditional formulation of MP the constraint (E fixed) was so to say *local.* Thus we get nontrivial generalization of Maupertuis' Principle.

For fixed W (i.e. $\delta W = 0$) we get Reciprocal Maupertui's Principle (RMP):

$$(\delta \bar{E})_W = 0\,. \tag{18}$$

This is exactly the classical limit of Schrödinger's Quantum Variational Principle that we discussed in the previous section.

This constitutes an abstract proof of the MP and RMP variational principles of classical dynamics. We have an economical derivation of three other variational principles starting from the HP. The argument we are using is an adaptation of Gibbs' familiar argument in thermodynamics,[5] when discussing the Legendre transform relation of free energy, energy, temperature, and entropy. In the case of Classical Mechanics we have similar set of relations for $S, t, W, \bar{E}$:

$$(\delta \bar{E})_W = 0 \qquad \Leftarrow \text{reciprocity} \Rightarrow \qquad (\delta W)_{\bar{E}} = 0\,, \tag{19}$$

$$(\delta S)_t = 0 \qquad \Leftarrow \text{reciprocity} \Rightarrow \qquad (\delta t)_S = 0\,, \tag{20}$$

$$(\delta S)_t = 0 \qquad \Leftarrow \text{ Legendre } \Rightarrow \qquad (\delta W)_{\bar{E}} = 0\,. \tag{21}$$

$$(\delta S)_t = 0 \quad \overset{\text{reciprocity}}{\longleftrightarrow} \quad (\delta t)_S = 0 \;\;, \tag{22}$$

$$(\delta S)_t = 0 \quad \overset{\text{Legendre}}{\longleftrightarrow} \quad (\delta W)_{\bar{E}} = 0 \;\;. \tag{23}$$

It is clear that the four principles (14), (16), (17) and (18) are equivalent. However, this does not mean that they are equally useful for solving particular problems. The RMP (18) makes a smooth connection to the Quantum Mechanical Variational Principle. We also find that the RMP is well suited to solve approximately classical problems by a procedure which is very similar to that used in the variational method of solution of quantum problems (see Refs. 1 and 2).

3 Percival's Variational Principle for invariant tori

In this section we are going to consider one interesting application of RMP. For integrable systems, all bounded motions are quasi-periodic, whereas for non-integrable systems only finite fraction of bounded motions are quasi-periodic, the rest are chaotic. A quasiperiodic motion is confined to a torus in phase space. Percival[6] has derived a variational principle for these tori. We show that his principle is a special case of RMP.

We consider the initial and final points of the trajectory to be close together, and the trajectory very long (i.e. the time $T \to \infty$). For a true path, the trajectory winds around the torus with uniform density, so that time average can be replaced by phase average:

$$\bar{E} = \frac{1}{T}\int_0^T H(q,p)dt = \int \frac{d\Theta^N}{(2\pi)^N}\, H\big(q(\Theta_k), p(\Theta_k)\big)\,, \tag{24}$$

where Θ_k are the angle variables parametrizing the torus. The torus is determined by the set of actions W_k that are constants of motions and that correspond to the set of fundamental loops of the torus. The action W for a long trajectory can be written as

$$W = \sum_k N_k W_k\,. \tag{25}$$

where $N_k = \nu_k T$ is the winding number for angle Θ_k and ν_k is the frequency.

Consider now an arbitrary small deformation of a given invariant torus and a trial trajectory on the trial torus. We can choose the trial trajectory such that it covers the trial torus uniformly as well. Thus,

$$W = \sum_k N_k \overline{W}_k\,, \tag{26}$$

where $\overline{W}_k$ is the mean action on the trial torus:

$$\overline{W}_k = \int \frac{d\Theta^{N-1}}{(2\pi)^{N-1}}\, W_k = 2\pi \int \frac{d\Theta^N}{(2\pi)^N}\; \vec{p}\cdot\frac{\partial \vec{q}}{\partial \Theta_k}\,. \tag{27}$$

We are now in position to apply the unconstrained version of the Maupertuis principle

$$\delta\bar{E} - \frac{\delta W}{T} = 0 \tag{28}$$

for the considered varied paths. Since the endpoints for real and trial trajectories are the same, we have equal winding numbers N_k for the two trajectories. Thus, the equation can be rewritten as

$$0 = \delta\bar{E} - \sum_k \left(\frac{N_k}{T}\right) \delta\overline{W}_k = \delta\bar{E} - \sum_k \nu_k\, \delta\overline{W}_k \tag{29}$$

$$\text{or} \qquad \delta\left(\bar{E} - \sum_k \nu_k \overline{W}_k\right) = 0\,, \tag{30}$$

where ν_k are the frequencies for the invariant torus. This equation is Percival's variational principle[6] for invariant tori: the mean energy $\bar{E}$ is extremized with the set of mean actions $\overline{W}_k$ held fixed. The constant Lagrange multipliers ν_k are the invariant torus frequencies.

$$\left(\delta\bar{E}\right)_{\overline{W}_k} = 0\,. \tag{31}$$

In the time of Old Quantum Mechanics this relation was used as a postulate for quantization of integrable systems.[7]

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