Quantum mechanics for multivalued Hamiltonians

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When the Lagrangian is not quadratic in the velocities, the situation may arise that the expression for the velocities in terms of the momenta is multivalued. As a consequence, the classical motion is unpredictable since at any time one can jump from one branch of the Hamiltonian to another. Yet, the quantum theory turns out to be perfectly smooth, with wave functions which are regular functions of time. We show that the path integral automatically picks up a unique combination of the branch Hamiltonians, which is a natural generalization of the Brouwer degree of the Legendre map.

Although one often restricts oneself in practice to Lagrangians quadratic in the velocities which yield Hamiltonians quadratic in the momenta, there is no reason of principle that prevents one from analyzing the quantum mechanics of more complicated systems. There may be of course severe factor ordering problems in the Hamiltonian but provided those are solved, the general formalism of quantum mechanics can deal with any Hamiltonian. But these remarks, however true, presuppose that at least a unique Hamiltonian exists and this is not always the case.

Indeed, if one starts from a Lagrangian which is a polynomial in the velocities of degree higher than two, the momenta are polynomials in the velocities of degree higher than one. Consequently, to express the velocities in terms of the momenta, one needs to solve a system of nonlinear algebraic equations. For generic choices of the coefficients in the Lagrangian, those equations will have more than one real root, at least for a range of values of the momenta. This situation is found, for example, in extensions of Einstein's theory of gravitation which involve topological invariants continued to higher dimensions.[1]

If the expression for the velocities in terms of the momenta is multivalued, the Hamiltonian becomes also multivalued in the p's. This implies that one cannot predict the classical motion of the system if the initial q's and p's are given. The reason is that at any moment in time one does not know which "branch" of the Hamiltonian to use, thus one may propagate for a while with one choice of the Hamiltonian, then switch to another and so on. Since the switching may be done after arbitrarily small time intervals, one may visualize the classical motion as a succession of zigzags which happen in an unpredictable manner. It should be emphasized here that, as it will be seen in a simple example below, this difficulty is not tied to an insistence in using a Hamiltonian formalism but it also follows directly from the Lagrangian equations of motion themselves.

At first sight, the above description of the problem would seem discouraging enough as to make one believe that the systems in question are to be thought of as unphysical. However, there are instances in which the quantum mechanics of a system that seems pathological classically is quite allright. Roughly speaking, when one sums over all histories, singular properties of the extremal history have a tendency to be smoothed up.

With this perspective in mind, we have examined the quantum mechanics of a system for which $\dot{q}$ is a multivalued function of the p's, and we have found the remarkable property that the quantum-mechanical amplitude is perfectly well defined and unique. Through the path integral, a unique effective Hamiltonian emerges. For the range of momenta which made the original classical Hamiltonian single valued, the effective Hamiltonian coincides with it. When the momenta are such that the original Hamiltonian is multivalued, possessing several branches, the effective Hamiltonian is a linear combination of the various branch Hamiltonians with coefficients which differ from each other at most by their relative sign. The choice of signs is of a topological nature and is closely related to the Brouwer degree of the map from the $\dot{q}$'s to the p's.

Once the effective Hamiltonian is known it may be used, turning the analysis upside down, to define what the classical theory meant in the first place. This means that the original Lagrangian becomes only a heuristic starting point and is replaced, for the troublesome range of the $\dot{q}$'s, by another one. One may say that in the classical limit, the sum over all the zigzag extremal histories of the original Hamiltonian is replaced by the contribution of the single, smooth, extremal history of the effective Hamiltonian.

In order to make the discussion as transparent as possible, we will analyze explicitly the simplest possible example and will indicate at the end how the conclusions are generalized.

That simplest possible example is a system with a single degree of freedom described by an action which is quartic in the velocity,

$$S \equiv \int L\,dt = \int \left(\tfrac{1}{4}\dot{q}^4 - \tfrac{1}{2}\alpha\dot{q}^2\right)dt \ . \tag{1}$$

The variational equation which derives from (1) reads

$$\frac{d}{dt}p(\dot{q})=0 , \tag{2}$$

with

$$p(\dot{q})\equiv\frac{\partial L}{\partial \dot{q}}=\dot{q}^3-\alpha\dot{q} \tag{3}$$

and clearly implies $p(\dot{q})=p_0$.

In order to solve completely the equation of motion, one needs to express $\dot{q}$ as a function of the integration constant p_0 from (3). This, however, can only be done uniquely if $\alpha<0$, in which case the analysis presents no new qualitative feature compared to quadratic Lagrangians.

Novel properties arise when $\alpha>0$. In that instance, the number $\mathcal{N}f^{-1}(p)$ of inverse images $\dot{q}$ which are mapped on a given p by the Legendre map f from $\dot{q}$ to p defined by (3) is then no longer equal to one. Rather, $\mathcal{N}f^{-1}(p)$ can take the values one, two, or three, according to whether p lies outside the closed interval $[p_1,p_2]$, is equal to one of the critical values p_1 or p_2, or is within the open interval (p_1,p_2) (see Fig. 1). The three inverse images of a point $p\in(p_1,p_2)$ will be denoted in the sequel by $\dot{q}_{\rm I}$, $\dot{q}_{\rm II}$, and $\dot{q}_{\rm III}$, respectively (with $\dot{q}_{\rm I}<\dot{q}_{\rm II}<\dot{q}_{\rm III}$).

It results from the existence of many inverse images that if the initial value p_0 of the momentum lies in the range (p_1,p_2), the velocity $\dot{q}$ can take, at any instant, any of the the three values $\dot{q}_0^{\rm I}$, $\dot{q}_0^{\rm II}$, or $\dot{q}_0^{\rm III}$ which solve (3). The equations of motion allow for an arbitrary number of jumps from one of the inverse velocities to any other, since these jumps leave p unchanged and thus do not violate (2). The behavior of the system described by the Lagrangian (1) appears therefore to be unpredictable for a range of initial data of nonvanishing extent.[2]

That same problem can also be seen in the Hamiltonian formulation of the variational principle. Even though there is a single Hamiltonian function $H(\dot{q})$ in terms of the velocity,

$$H(\dot{q})=p(\dot{q})\dot{q}-L(\dot{q}) , \tag{4}$$

one finds that there are three different Hamiltonians in phase space for momenta in the range (p_1,p_2). These Hamiltonians correspond to the three roots of (3) and will be denoted $H_{\rm I}(p)$, $H_{\rm II}(p)$, and $H_{\rm III}(p)$. The time evolution can be generated by either $H_{\rm I}(p)$, $H_{\rm II}(p)$, or $H_{\rm III}(p)$ and again, one can switch at any time from one of these functions to another.

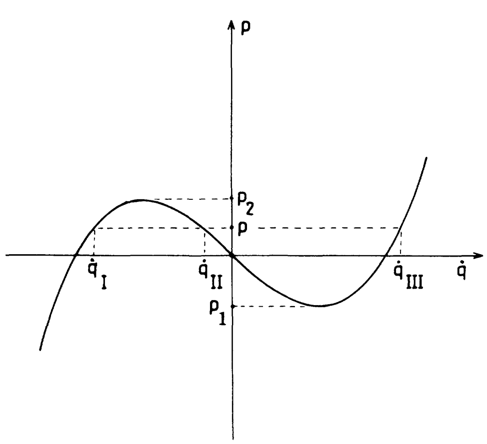

FIG. 1. The Legendre map f from $\dot{q}$ to p for the Lagrangian one, with $\alpha>0$.

The absence of a well-defined Hamiltonian formulation would seem to put the quantum theory in as bad a position as the classical one, since there is no indication at this point as to how to propagate the wave functions.

It turns out, however, that through the sum over paths, one can associate a perfectly smooth quantum theory to the action (1). This results from the single valuedness of the Hamiltonian as a function of the velocity, which can be used to postulate an expression for the transition amplitude $\langle q_2,t_2\,|\,q_1,t_1\rangle$ which possesses the following desirable properties.

(i) $\langle q_2,t_2\,|\,q_1,t_1\rangle$ can be viewed as the matrix element of a unitary evolution operator which becomes the identity as $t_2\to t_1$.

(ii) The new correspondence rules should reduce to the old ones when the Hamiltonian is single valued as a function of the momenta.

In order to arrive at the appropriate expression for the transition amplitude, one first notes that the original variational principle based on (1) can be replaced by an equivalent first-order one, in which one varies independently both the coordinate q and the velocity (which we denote from now on by u in order to emphasize that it is treated as an independent variable),[3]

$$S_H[q(t),u(t)]=\int_{t_1}^{t_2}[p(u)\dot{q}-H(u)]dt . \tag{5}$$

The extremals of (5) are in one-to-one correspondence with the extremals of (1), except at the critical values $p=p_1$ and $p=p_2$, where $\partial^2L/\partial u\,\partial u$ vanishes and where (5) possesses additional solutions. But, as it will be seen, these points are given zero weight in the path integral.

Now if the Legendre map $p=f(u)\equiv u^3-\alpha u$ was everywhere invertible, it would be straightforward to check that the sum over paths

$$\langle q_2,t_2\,|\,q_1,t_1\rangle =\int\int \mathcal{D}q(t)\mathcal{D}u(t)\prod_t\frac{\partial^2L}{\partial u\,\partial u}\exp\left[\frac{i}{\hbar}S_H[q(t),u(t)]\right] \tag{6}$$

would reproduce the standard Hamiltonian path integral, which is in direct relation with the evolution operator. This would simply follow from performing the change of integration variables $u\to p$ in (6), whose Jacobian cancels the local measure $\partial^2L/\partial u\,\partial u$.

In our case, however, the Hamiltonian sum over paths is not available. Nevertheless, the expression (6) still possesses a definite meaning since it is directly written in terms of well-defined functions of the velocity. For this reason, (6) will be adopted here as the defining expression of the transition amplitude from which the quantum theory should be derived.

By construction, the expression (6) fulfills the second condition (ii) above. It remains to be proved that (i) holds as well, i.e., that an operator interpretation of (6) can be given. This will be shown by rewriting (6) as a phase-space path integral.

To achieve this goal, one cannot blindly perform the change of variables $u \rightarrow p$ by brute force, since the Legendre map is not invertible. While a given path $q(t),u(t)$ in position-velocity space defines a single path $q(t),p(t)$ in phase space, a phase-space path corresponds in general to an infinity of paths $q(t),u(t)$, in which the velocity arbitrarily jumps from one root of (3) to another.

The idea, then, is to break the sum (6) as

$$\int\int \mathcal{D}q(t)\mathcal{D}p(t)\exp\left[\frac{i}{\hbar}S^{\text{eff}}[q(t),p(t)]\right], \tag{7}$$

where $S^{\text{eff}}[q(t),p(t)]$ is obtained by summing first the integrand of (6) over all paths in coordinate-velocity space which correspond to the same phase-space path,

$$\exp\left[\frac{i}{\hbar}S^{\text{eff}}[q(t),p(t)]\right] = \sum_{f^{-1}(p(t))}\exp\left[\frac{i}{\hbar}S_H[q(t),u(t)]\right]. \tag{8}$$

The transformation from (6) to (7) can be precisely implemented through the slicing of the time interval $[t_1,t_2]$.[4] On each slice, one can divide the u integration line in three different regions, $[-\infty,\dot{q}_1]$, $[\dot{q}_1,\dot{q}_2]$, $[\dot{q}_2,+\infty]$, on each of which the map $p=p(u)$ can be inverted, and one performs separately the change of variables from u to p on each of these regions. One finds, after some elementary transformations, that the u integral at a given time, for a time-slicing parameter ϵ, becomes

$$\int_{-\infty}^{+\infty} du\,\frac{\partial^2 L}{\partial u\,\partial u}\exp\{i[p(u)(q_{i+1}-q_i)-\epsilon H(u)]\} = \int_{-\infty}^{+\infty} dp\,\exp\{i[p(q_{i+1}-q_i)-\epsilon H^{\text{eff}}(p)]\}+O(\epsilon^2). \tag{9}$$

Here q_{i+1} and q_i are the values of q at time t_{i+1} and t_i, respectively ($t_2-t_1=N\epsilon$, $t_{i+1}-t_i=\epsilon$), while $H^{\text{eff}}(p)$ is given by

$$H^{\text{eff}}(p)=H_{\text{I}}(p)\Theta(p_2-p)-H_{\text{II}}(p)\Theta(p_2-p)\Theta(p-p_1) + H_{\text{III}}(p)\Theta(p-p_1) \tag{10}$$

in terms of the Heaviside step function Θ.

The effective Hamiltonian (10) is a single-valued function of p. It is continuous at the critical values p_1 and p_2 because $H_{\text{II}}=H_{\text{I}}$ or H_{III} there.

The rule (10) can be extended to any continuous function $g(u)$ of the velocity and gives a single-valued function $g^{\text{eff}}(p)$ of the momentum,

$$g^{\text{eff}}(p)=g_{\text{I}}(p)\Theta(p_2-p)-g_{\text{II}}(p)\Theta(p_2-p)\Theta(p-p_1) + g_{\text{III}}(p)\Theta(p-p_1). \tag{11}$$

It is actually the only prescription for yielding a continuous $g^{\text{eff}}(p)$ which is linear in the three different branches $g_{\text{I}}, g_{\text{II}}, g_{\text{III}}$, with coefficients which are independent from g (i.e., universal). These coefficients turn out to possess a topological significance, since they are equal to ± 1 according to whether the Legendre map preserves (I, III) or reverses (II) the orientation. If one takes for $g(u)$ the constant function 1, $g^{\text{eff}}(p)$ reduces to the Brouwer degree of the Legendre map,[5]

$$g^{\text{eff}}(p)=\sum_{u\in f^{-1}(p)}\text{sgn}\,df_p=\deg f, \tag{12}$$

and is, of course, equal to 1.

Because of (9), the path integral (6) can be written as in (7), with an effective action equal to

$$S^{\text{eff}}[q(t),p(t)]=\int_{t_1}^{t_2}(p\dot{q}-H^{\text{eff}})dt. \tag{13}$$

The effective action not only is a local functional of q and p, but also takes the standard canonical form. As such, it enables one to revert to more traditional formulations of the quantum theory.

The path integral can indeed be viewed now as the matrix element of the evolution operator

$$U(t_2,t_1)=\exp[-i(t_2-t_1)H^{\text{eff}}/\hbar] \tag{14}$$

between appropriate coordinate eigenstates. What plays the role of the Hamiltonian operator in the Schrödinger equation is thus the topological combination $H^{\text{eff}}(p)$ of the various branch Hamiltonians.

The fact that the path integral leads to a satisfactory quantum theory of the usual type sheds a new light on the meaning of the "classical" variational principle associated with the original action (1). Indeed, one can ask oneself what is the "classical limit" of the quantum theory just constructed, i.e., which path, if any, dominates the path integral in the limit of large actions.

Because the action functional (5) possesses an infinity of stationary points, the condition of constructive interference does not single out a unique path in coordinate-velocity space which can be thought of as the classical history of the system. It is not that the system possesses a classical limit which is unpredictable, it is simply that this classical limit is ill-defined in the sense that no single path dominates the sum as $\hbar \rightarrow 0$.

By contrast, the phase-space path integral (7), obtained by summing first $\exp iS$ over all paths $q(t),u(t)$ which correspond to the same phase-space path $q(t),p(t)$ is dominated, in the limit of large actions, by a single path. That single path replaces the infinity of extremals of the original action and solves the deterministic equations associated with the effective Hamiltonian H^{eff}.

The analysis of the simple model displayed here extends straightforwardly to more general cases with many degrees of freedom, provided that the Brouwer degree of the Legendre map from $\dot{q}^i$ to $p_i \equiv \partial L / \partial \dot{q}^i$ is everywhere finite and equal to a nonvanishing constant $D \neq 0$.[6]

The transition amplitude can again be written as

$$\langle q_2^i, t_2 | q_1^i, t_1 \rangle = \int \int \mathcal{D}q(t) \mathcal{D}u(t) \prod_t \frac{1}{D} \det \left[\frac{\partial^2 L}{\partial u^j \partial u^i} \right] \times \exp \left[\frac{i}{\hbar} S[q(t), u(t)] \right] . \tag{15}$$

A region in p space with k inverse images is covered by the integral (15) k^+ times positively and k^- times negatively, with $k = k^+ + k^-$ and $D = k^+ - k^-$. By repeating the steps which led from (6) to (7)–(13), one finds that the integral (15) can be replaced by

$$\langle q_2^i, t_2 | q_1^i, t_1 \rangle = \int \int \mathcal{D}q(t) \mathcal{D}p(t) \exp \left[\frac{i}{\hbar} \int (p\dot{q} - H^{\text{eff}}) dt \right] . \tag{16a}$$

Here H^{eff} is given by

$$H^{\text{eff}}(p,q) = \frac{1}{D} \sum_{u \in f^{-1}(p)} (\text{sgn} df_p) H(u,q) \tag{16b}$$

in agreement with (10). The effective Hamiltonian (16b) is continuous and reduces to the original Hamiltonian when this one is single valued. The quantum theory defined by the path integral (16a) possesses not only a clear operator interpretation, but also a smooth, deterministic, classical limit, whose dynamical equations are the Hamiltonian equations implied by the effective Hamiltonian (16b).

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[1] C. Teitelboim and J. Zanelli, in *Constraints Theory and Relativistic Dynamics,* edited by G. Longhi and L. Lusanna (World-Scientific, Singapore, 1987); also Class. Quant. Grav. **4**, L125 (1987).

[2] Insisting that the velocity should be a continuous function of time would generically contradict the equations of motion if one adds a potential term to the Lagrangian, and thus, is not desirable. [This would occur, for instance, if one adds $-\int q\, dt$ to (1)].

[3] The elementary procedure of varying coordinates and velocities independently in the variational principle has a long history and is explained in many references. See, for instance, C. Lanczos, *The Variational Principles of Mechanics,* 4th ed. (University of Toronto, Toronto, 1970); also appendix of M. Henneaux, Ann. Phys. (N.Y.) **140**, 45 (1982).

[4] Note that (6) obeys the appropriate folding rule for transition amplitudes.

[5] J. W. Milnor, *Topology from the Differentiable Viewpoint* (University Press of Virginia, Charlottesville, 1965).

[6] The Brouwer degree is equal to unity for Lagrangians which are polynomials of odd degree in the velocity, while it vanishes for polynomials of even degree. These are thus excluded from the present treatment [Eqs. (15) and (16b) below are ill defined for $D = 0$].