Energy Quantisation and Time Parameterisation

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Abstract

We show that if space is compact, then trajectories cannot be defined in the framework of quantum Hamilton–Jacobi equation. The starting point is the simple observation that when the energy is quantized it is not possible to make variations with respect to the energy, and the time parameterisation \(t - t_0 = \partial E S_0\), implied by Jacobi’s theorem and that leads to group velocity, is ill defined. It should be stressed that this follows directly from the quantum HJ equation without any axiomatic assumption concerning the standard formulation of quantum mechanics. This provides a stringent connection between the quantum HJ equation and the Copenhagen interpretation. Together with tunneling and the energy quantization theorem for confining potentials, formulated in the framework of quantum HJ equation, it leads to the main features of the axioms of quantum mechanics from a unique geometrical principle. Similarly to the case of the classical HJ equation, this fixes its quantum analog by requiring that there exist point transformations, rather than canonical ones, leading to the trivial hamiltonian. This is equivalent to a basic cocycle condition on the states. Such a cocycle condition can be implemented on compact spaces, so that continuous energy spectra are allowed only as a limiting case. Remarkably, a compact space would also imply that the Dirac and von Neumann formulations of quantum mechanics essentially coincide. We suggest that there is a definition of time parameterisation leading to trajectories in the context of the quantum HJ equation having the probabilistic interpretation of the Copenhagen School.
1 Introduction

The validity of quantum mechanics is indisputable, but leaves many conceptual problems unresolved. For this reason over the years numerous schemes have been proposed to address such issues. Among those, the quantum HJ theory is one of the most investigated topics (see [1] for a partial list of papers). These studies involve the foundation of quantum mechanics, in particular its interpretation, cosmology, the analysis of quantum dynamics, molecular trajectories, etc. It has been suggested that the Quantum Hamilton–Jacobi Equation (QHJE) yields a trajectory representation of quantum mechanics (see e.g. [2] and references therein). The absence of trajectories is, however, inherent in the Copenhagen probabilistic interpretation of the quantum mechanical wave function. There appears, therefore, to be a fundamental dichotomy between the two approaches. In this paper we offer a solution to this puzzle. We demonstrate the absence of trajectories in the derivation of the QHJE from point transformations leading to the trivial hamiltonian [3][4]. The basic point is that trajectories can only be defined by time parameterisation of them, and include the Bohm–de Broglie pilot wave representation and Floyd’s time parameterisation [5] by using Jacobi theorem. We show in this paper that these time parameterisations are ill defined. This resolves the dichotomy with the Copenhagen interpretation.

In [6] we considered a Legendre duality in the framework of the Schrödinger equation. Consistency of this mathematical structure in the context of the phase–space reveals that classical mechanics must be modified [3]. The main idea has been to implement, as in the derivation of the classical HJ equation, the transformations leading to the free state. The difference is that we did not consider the usual canonical transformation with the space coordinate \( q \) and the conjugate momentum \( p \) considered as independent variables. Rather, we performed the transformation on \( q \) and considered the transformation on \( p \) as the one induced by the coordinate transformation, by assuming that the analog of the Hamilton characteristic function transforms as a scalar field. Such a transformation leads to a basic cocycle condition which, in turn, implies that the analog of the Hamilton characteristic function must satisfy the quantum analog of the stationary HJ equation. The derivation extends to the higher dimensional non–stationary case and to the relativistic case as well [4].

A basic theorem in [3] is that energy quantisation for bound states follows as a consistency condition. We stress that whereas in the standard approach energy quantisation is a direct consequence of the wave–function interpretation, here it follows from the cocycle condition without any assumption on the meaning of the wave–function.

The quantum Hamilton-Jacobi equation is

\[
\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S)^2 + V - \frac{\hbar^2}{2m} \Delta R = 0 ,
\]

\[
\frac{\partial R^2}{\partial t} + \frac{1}{m} \nabla \cdot (\nabla R^2 S) = 0 ,
\]

which can be obtained by identifying a solution of the Schrödinger equation with \( Re^{iS} \). Note that \( S \) is the quantum analog of Hamilton’s principal function. Let us now consider
a particle in a stationary state with energy $E$. We have

$$S = \int p \cdot dq - E(t - t_0),$$

where the first term, that we denote by $S_0$, is the quantum analog of Hamilton’s characteristic function. Let now assume that such a particle admits a trajectory $q = q(t)$. Performing a variation of time and energy, keeping fixed the initial and final spatial coordinates of the trajectory, we have

$$\delta S = \frac{\delta S_0}{\delta E} \delta E - (t - t_0) \delta E - E \delta t,$$

and by (3)

$$t - t_0 = \frac{\partial S_0}{\partial E}.$$

This is the time parametrization of particle trajectories that, as first observed by Floyd [5], should be used in considering the quantum HJ equation. This is just how trajectories are defined in classical mechanics as it implies the group velocity.

A simple but basic initial observation is that in the case of quantized spectra it is not possible to make the variation of the energy. In particular, the trajectories $q = q(t)$, that would follow by inverting Eq. (1), do not exist in the case of discrete energy spectra. Consistency arguments also show that this excludes the possibility of using (1) even in the case of continuous energy spectra. It is clear that the non existence of trajectories suggests that also the probabilistic interpretation may be derived without imposing it as a basic axiom.

As we will see, there is a connection between the non existence of trajectories and the cocycle condition. In particular, we will see that the implementation of the cocycle condition fixes gluing conditions on the ratio of two linearly independent solutions of the wave–function that can be satisfied only on compact spaces, so that continuous energy spectra arise only in the decompactification limit. The fact that such gluing conditions are a basic step in the geometrical formulation of [3][4], related to Legendre duality [5], and that led to the quantisation of the energy in the case of confining potentials, suggests that they should be always satisfied. It should be observed that in the case of a free particle the level spacing of the energy spectrum will be determined by the geometry of our three–dimensional space, essentially of the order $R^{-2}$, where $R$ is some characteristic cosmological length, and therefore extremely tiny. This, of course, does not mean that such a spacing could not be detected a priori. The fact that trajectories cannot be well–defined provides an intriguing relation between quantum HJ theory and the Copenhagen interpretation. However, the reason why they do not exist in the quantum HJ theory is that it is just the time parameterisation that does not exist. In some sense a similar view is also the one of the Copenhagen interpretation. Actually, time is not a (self–adjoint) operator, so that also in standard quantum mechanics time is not an observable.

There are additional reasons to consider the possibility that a free particle may have a quantized energy spectrum, even if the level spacing is extremely tiny. A rigorous treatment of continuous spectra requires elaborated structures and the probability of finding the particle in a given volume cannot be defined. Furthermore, it should be observed that there are two formulations of quantum mechanics in the framework of the
Copenhagen interpretation. The one by von Neumann [7], where quantum states are always rays in the Hilbert space \( L^2(\mathbb{R}) \), and the one by Dirac [8] that in general requires the rigged Hilbert space and the eigenfunctionals. In particular, in the Dirac formulation the wave–function of a free particle in \( \mathbb{R}^3 \) is seen as a tempered distribution, that is an element in \( S'(\mathbb{R}^n) \), the dual space of the Schwarz space \( \mathcal{S}(\mathbb{R}^n) \). In the case of compact spaces the Helmholtz equation
\[
-\frac{\hbar^2}{2m}\Delta \psi = E\psi,
\]
has only a discrete spectrum, so that the two formulations would essentially coincide. More generally, a compact space would fix some natural cutoff that may play an important rôle. We also consider the problem of defining a sort of probabilistic time such that the resulting trajectories in the quantum HJ theory reproduce the probabilistic interpretation of the Copenhagen School.

## 2 The cocycle condition and energy quantization

We define
\[
\mathcal{W}(q) = V(q) - E,
\]
where \( V \) is the potential energy and \( E \) the energy level. The main point of [3] is to assume the existence transformations leading any system to the one with trivial Hamiltonian, that is with \( \mathcal{W}(q) = 0 \). Doing this in classical mechanics leads to the classical HJ equation. The difference in the approach of [3] is that whereas in classical mechanics one considers the canonical transformations, where \( p \) and \( q \) are considered independent, we considered point transformations. More precisely, we considered the transformation of \( q \) and fixed the transformation on the conjugate momentum as the one induced by the relation
\[
p = \partial_q S_0,
\]
by considering \( S_0 \), the analog of the Hamilton characteristic function, as a scalar function under such a transformation of \( q \). The derivation can be extended to the non–stationary case and to the relativistic version as well [4]. Therefore, the derivation of [3, 4] is based on the principle that all physical state labeled by the function \( \mathcal{W}(q) \) can be connected by a coordinate transformation,
\[
q^a \rightarrow q^b = q^b(q^a),
\]
defined by
\[
S^b_0(q^b) = S^a_0(q^a).
\]
This implies that there always exists a coordinate transformation connecting any physical state to the one with \( \mathcal{W}^0(q^0) = 0 \). Inversely, this means that any physical state can be reached from the one with \( \mathcal{W}^0(q^0) = 0 \) by a coordinate transformation. This cannot be consistent with Classical Mechanics (CM). The reason being that in CM the physical system with \( \mathcal{W}^0(q^0) = 0 \) remains a fixed point under coordinate transformations. Thus, in CM it is not possible to generate all systems by a coordinate transformation from the trivial one. This implies the modification of CM, which is analyzed by a adding a still unknown function \( Q(q) \) to the classical HJ equation. Consistency conditions then fix the transformation properties for \( \mathcal{W}(q) \),
\[
\mathcal{W}^v(q^v) = (\partial_q q^a)^2 \mathcal{W}^a(q^a) + (q^a; q^v),
\]
and

$$Q^v(q^v) = (\partial_{q^a}q^a)^2 Q^a(q^a) - (q^a; q^v) ,$$

which fixes the cocycle condition

$$(q^a; q^v) = (\partial_{q^b}q^b)^2 [(q^a; q^b) - (q^c; q^b)] .$$  \hfill (5)

The cocycle condition is invariant under Möbius transformations and fixes the functional form of the inhomogeneous term. Furthermore, the cocycle condition fixes the identification

$$W(q) = -\frac{\hbar^2}{4m} \{e^{2iS_0/\hbar}, q\} ,$$

and

$$Q(q) = \frac{\hbar^2}{4m} \{S_0, q\} ,$$

where $\{f, q\} = f''/f' - \frac{3}{2}(f''/f')^2$ denotes the Schwarzian derivative. The cocycle condition, that generalizes to higher dimensions [4], implies that $S_0$ is solution of the Quantum Stationary HJ Equation (QSHJE),

$$\frac{1}{2m} (\partial_q S_0)^2 + V(q) - E + \frac{\hbar^2}{4m} \{S_0, q\} = 0 .$$  \hfill (6)

The equivalence with the one-dimensional stationary version of Eqs. (1) and (2) follows by observing that by Eq. (2) one gets

$$R = c \frac{1}{\sqrt{S_0}} ,$$

with $c$ a non–zero constant, so that

$$\frac{\Delta R}{R} = -\frac{1}{2} \{S_0, q\} .$$

It is easy to check that the solution of (6) can be expressed in terms of solutions of the Schrödinger equation. In particular,

$$e^{\frac{2iS_0}{\hbar}} = e^{i\alpha} \frac{w + i\ell}{w - i\ell} ,$$

where $\ell = \ell_1 + i\ell_2$, with $\ell_1$ and $\ell_2 \neq 0$ two arbitrary constant, and $w = \psi^D/\psi$, with $\psi^D$ and $\psi$ two real linearly independent solutions of the Schrödinger equation

$$\left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} + V(q) - E \right) \psi(q) = 0 .$$

A distinguished feature of the formalism in [3] is that both solutions of the Schrödinger equation, $\psi$ and $\psi^D$, are kept in the formalism. This can be seen from the properties of the Schwarzian derivative that show that the trivialising transformation is

$$q \to q^0 = \gamma(\psi^D/\psi) ,$$
where $\gamma(\psi^D/\psi)$ is an arbitrary Möbius transformation of $\psi^D/\psi$. In general the wave–function in the formulation of [3] is

$$
\psi(q) = R(q) \left( Ae^{iS_0} + Be^{-iS_0} \right).
$$

(7)

Furthermore, consistency conditions imply that $S_0(q)$ is never a constant. In particular, the quantum potential $Q(q)$ is never trivial and plays the rôle of intrinsic energy.

The formulation in [3] extends to higher dimensions and to the relativistic case as well [4]. Let us now review how energy quantisation arises in our formalism. The QSHJE is equivalent to the equation

$$
\{w, q\} = -4m(V(q) - E)/\hbar^2.
$$

This implies that $w \neq \text{const}$, $w \in C^2(R)$ and $w''$ differentiable on $R$. In addition from the properties of the Schwarzian derivative it follows that

$$
\{w, q^{-1}\} = q^4 \{w, q\},
$$

which can be seen as a direct consequence of the cocycle condition. However, such a relation is defined only if the conditions on $w$ hold on the extended real line $\hat{R} = R \cup \{\infty\}$. That is $w \neq \text{const}$, $w \in C^2(\hat{R})$ with $w''$ differentiable on $\hat{R}$ and

$$
w(-\infty) = \begin{cases} 
+w(+\infty) & \text{if } w(-\infty) \neq \pm \infty, \\
-w(+\infty) & \text{if } w(-\infty) = \pm \infty.
\end{cases}
$$

(8)

This means that $w$, and therefore the trivialising map, is a local homeomorphism of $\hat{R}$ into itself. This implies the continuity of $(\psi^D, \psi)$ and $(\psi^D', \psi')$ without assuming the probability interpretation of the wave–function. In particular, the QSHJE is defined only if the ratio $w = \psi^D/\psi$ of a pair of real linearly independent solutions of the Schrödinger equation is a local homeomorphism of the extended real line $\hat{R} = R \cup \{\infty\}$ into itself. This is an important feature as the $L^2(R)$ condition, which in the Copenhagen formulation is a consequence of the axiomatic interpretation of the wave–function, directly follows as a basic theorem which only uses the geometrical gluing conditions of $w$ at $q = \pm \infty$. In particular, denoting by $q_-$ (q_+) the lowest (highest) $q$ for which $V(q) - E$ changes sign, we have [3]

If

$$
V(q) - E \geq \begin{cases} 
P_-^2 > 0, & q < q_-, \\
P_+^2 > 0, & q > q_+,
\end{cases}
$$

(9)

then $w = \psi^D/\psi$ is a local self–homeomorphism of $\hat{R}$ iff the Schrödinger equation has an $L^2(\hat{R})$ solution.

Thus, since the QSHJE is defined if and only if $w$ is a local self–homeomorphism of $\hat{R}$, this theorem implies that energy quantisation directly follows from the QSHJE itself without further assumptions.
3 Time parameterisation

We emphasize that the present approach is fundamentally distinct from the Bohmian one [3]. Bohmian mechanics sets
\[ \psi(q) = R(q)e^{iS/\hbar}, \]
where \( \psi \) is the wave–function. On the other hand, implementation of the point transformations leading to the trivial hamiltonian necessitates that the wave–function is taken in the general form (7). Such a condition is reminiscent of the necessity in quantum field theories of using the two solutions of the relativistic quantum equations.

In Bohmian mechanics time parameterisation is defined by identifying \( p \) with the mechanical momentum
\[ p = \frac{\partial S}{\partial q} = m\dot{q}, \tag{10} \]
with \( S \) solution of the quantum HJ equation. In classical HJ theory time parameterisation is given by
\[ t - t_0 = \frac{\partial S^0}{\partial E}, \tag{11} \]
which leads to group velocity. In Classical Mechanics (CM) this is equivalent to identifying the conjugate and mechanical momenta. Namely, setting
\[ p = \frac{\partial S^0}{\partial q} = m\dot{q}, \]
yields (11). Bohmian mechanics therefore brings back the notion of trajectories for point particles, since we may solve for \( q(t) \). However, we note that the agreement between the definition of time parameterisation of trajectories by (10) and its definition by Jacobi theorem (11) is no longer true in quantum mechanics. The use of the latter definition in quantum mechanics, that is
\[ t - t_0 = \frac{\partial S_0}{\partial E}, \tag{12} \]
has been first proposed by Floyd [5]. In quantum HJ theory this leads to
\[ m\frac{dq}{dt} = \frac{\partial_q S_0}{1 - \partial_E(V + Q)}. \]
Therefore, in quantum mechanics the time parameterisation in (11) does not coincide with its definition via Jacobi theorem.

Floyd proposal (12) would in principle provide a trajectory representation of quantum mechanics which would seem to be in contradiction with the inherently probabilistic nature of quantum mechanics. We show that the definition (12) cannot be implemented. We emphasize, however, that this does not mean that the parameterisation provided by (12) cannot be useful. In fact, it is quite effective to perform semi–classical approximations. In this respect we note the successful application in studies of molecular dynamics [2].

It is clear that in the case of quantized energy spectra (12) is not defined. On the other hand, the concept of trajectory should be a universal one, so that one should consider a time parameterisation which is consistent in both cases of discrete and continuous spectra. This essentially would exclude (12) also in the case of continuous spectra.
is however a more stringent argument to show that (12) cannot be used to define time parameterisation of trajectories. In particular, we now show that the QSHJE is defined only in the case of discrete spectrum with the case of continuous spectrum arising only as a limiting case. We saw that the cocycle condition led to the QSHJE written as a Schwarzian equation. In particular, we established that the gluing conditions should always hold. Let us now consider the case of a continuous spectrum. Without loss of generality, we may consider the case when for large $q$ the potential is zero. For large $q$ two associated real independent solutions of the Schrödinger equation are
\[ \psi = \sin kq, \quad \psi^D = \cos kq. \]
This means that for large $q$ we have
\[ w = \tan kq. \]
On the other hand, whereas this function at finite distance is a local homeomorphism, it is not the case when considering the entire real axis. This can be also seen by considering a free particle in an infinitely deep well and considering the periodicity conditions. This is equivalent to consider the particle in $S^1$ and then sending its radius $R$ to infinity. For any finite $R$ the ratio of two linearly independent solutions is a local homeomorphism of $S^1$ and the spectrum is discrete. In the $R \to \infty$ limit the gluing condition is no longer under control. In the case of the free particle in an infinitely deep potential well of width $L$, the energy levels are
\[ E_n = \frac{\hbar^2 \pi^2}{2mL^2} n^2, \]
$n \in \mathbb{N}_+$. It follows that for any but finite value of $L$ the spectrum is discrete. We then conclude that imposing the cocycle condition requires a discrete spectrum which in turn implies that continuous variation of the energy is not possible. Equivalently, the time parameterisation by Jacobi theorem is not well defined. This can be generalized to the free particle in any space dimension leading to the same conclusion. On the other hand, it is a general theorem that the equation
\[ -\frac{\hbar^2}{2m} \Delta \psi = E\psi, \]
in bounded domains of $\mathbb{R}^n$, therefore including e.g. the $(n-1)$–sphere $S^{n-1}$, has only a discrete spectrum. At the level of the quantum HJ equation, this is just a consequence of the non–triviality of the quantum potential.

Therefore, without using any axiomatic interpretation of the wave–function, we have shown that trajectories cannot be derived from the quantum HJ equation. In particular, the concept of localized particle with a defined velocity does not exist. Since trajectories do not exist in the formulation of $\mathbb{R}$, one may try to consider finite differences instead of derivatives
\[ t_n = \frac{S_0(E_{n+1}) - S_0(E_n)}{E_{n+1} - E_n}. \quad (13) \]
This is a basic point since it leads to consider the superposition of different energy eigenstates, which is at the basis of the interference phenomena. In particular, whereas time
The evolution of a Hamiltonian eigenfunction corresponds to an overall phase, so that describing the same ray vector in the Hilbert space, the role of time is apparent, through interference, just when the physical system is the superposition of at least two energy levels. Eq. (13) indicates that the interference phenomena are deeply related to the concept of time.

Whereas Eq. (13) sheds light on the origin of interference in the Quantum Hamilton-Jacobi formulation, there is an interesting alternative which is suggested by Schrödinger equation. One may think that time parameterisation may be defined as a sort of random parameter whose distribution is fixed by the properties of the distribution of the energy eigenvalues. In other words, instead of considering finite difference, that gives $t = t(E)$, we may search for a more intrinsic definition. The idea is that the wave function depends on $E$, so one may formally invert this relation to $E = E(\psi)$. This leads to consider $t_\psi = t(\psi)$. In particular, consider a time independent potential. In this case the Schrödinger equation implies

$$\psi(q, t) = \sum_k c_k e^{-iE_k t} \psi_k(q),$$  

where the $\psi_k$ are the Hamiltonian eigenfunctions

$$H \psi_k = E_n \psi_k.$$

Next, recall that for one-dimensional bound states $\psi_n$ can be normalized in such a way that it takes real values. Multiplying (14) by $\psi_n$ and integrating over $\mathbb{R}$ one gets

$$t_\psi = \frac{i\hbar}{E_n} \left( \ln \int_{\mathbb{R}} \psi \psi_n dq - \ln \int_{\mathbb{R}} \psi(q, 0) \psi_n dq \right).$$  

(15)

Note however that $t_\psi$ is just the time experienced by the observer. This suggests that there exists a kind of time parameterisation leading to the probabilistic interpretation of trajectories in the framework of the quantum HJ equation.

## 4 Conclusions

Understanding the synthesis of quantum mechanics and general relativity remains the pivotal goal of fundamental physics. The main effort in this endeavour is in the framework of string theory. String theory provides a self-consistent perturbative approach to quantum gravity. The main achievement of string theory is that it gives rise to the gauge and matter ingredients of elementary particle physics, and predicts the number of degrees of freedom required to obtain a consistent theory. String theory therefore enables the development of a phenomenological approach to quantum gravity. The state of the art in this regard is the construction of Minimal Standard Heterotic String Models [9]. Over the past few years important progress has also been achieved in the understanding of the perturbative expansion of string theory for genus $g$ Riemann surfaces, see for example [10] and references therein. Despite its successes, string theory does not provide a conceptual starting point for formulating quantum gravity. What we seek is a fundamental hypothesis of which, possibly, string theories arise as perturbative limits. A basic property of string theory is T-duality [11], which may be viewed as phase-space duality in compact space.
In this paper we examined the definability of time parameterisation of trajectories in
the framework of the quantum HJ equation. We first observed that it is not possible
to perform infinitesimal variations of the energy when this is quantized. As such, the
quantum HJ equation does not lead to the concept of trajectory. Next, we discussed the
identification the mechanical momentum with the conjugate momentum

\[ m\dot{q} = \frac{\partial S}{\partial q}, \]

as done in Bohmian mechanics, and noticed that it is inconsistent with its derivation from
Jacobi’s theorem, which in turn cannot be applied in the case of systems with quantized
energy. On the other hand, consistency arguments show that if trajectories cannot be
deFINED in the case of of quantized energy, then trajectories do not exist even when the
energy spectrum is continuous.

In this respect it should be however stressed that quantum trajectories provide a
powerful approximation tool in quantum dynamics [2][12]. In particular, the method of
quantum trajectories has been developed as a computational tool to solve time-dependent
quantum mechanical problems by evolving ensembles of correlated quantum trajectories
through the integration of the hydrodynamic equations. These quantum trajectories serve
as a computational adaptive moving grid and from this perspective, these are not authentic
trajectories.

We then proposed that the above features of the quantum HJ equation are at the
heart of the probabilistic nature of quantum mechanics. In this respect, we considered
time as dependent on the wave–function getting an expression that suggests considering
time itself as having a probabilistic nature.

We also observed that the derivation of the quantum HJ equation from the cocycle
condition [3] is naturally formulated in compact spaces that can be extended considering
the decompactification limit. This suggests that our space is compact. In this case all the
possible energy spectra are quantized and would make essentially equivalent the Dirac
and von Neumann formulations of quantum mechanics. The compactness of space has
basic observational consequences and forthcoming evidence for it may exist in the cosmic
microwave background radiation [13].

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