A general formulation of discrete-time quantum mechanics, restrictions on the action and the relation of unitarity to the existence theorem for initial-value problems

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Abstract

A general formulation for discrete-time quantum mechanics, based on Feynman’s method in ordinary quantum mechanics, is presented. It is shown that the ambiguities present in ordinary quantum mechanics (due to noncommutativity of the operators), are no longer present here. Then the criteria for the unitarity of the evolution operator is examined. It is shown that the unitarity of the evolution operator puts restrictions on the form of the action, and also implies the existence of a solution for the classical initial-value problem.

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Introduction

Discrete-space-time physics is an old tradition originated in solid-state physics. This has been the starting point for lattice physics. On the other hand, continuous-space-time field theory has still some problems; not only from the mathematical point of view, but also from the computational point of view. The first kind of problems is, essentially, the lack of an exact definition for functional integration, and the problem of ultraviolet divergences in interacting field theories ([1], for example). The second kind of problems is related to the fact that most of the numerical results of field theory, are in fact perturbative results. A promising answer to this kind of problems seem to be lattice field theories, specially lattice gauge theories [2]. These theories, however, are interesting, not only as an approximation for continuous-space-time theories, but also as independent models [3-7].

Another problem, very much related to the above problems, is the lack of a consistent theory of quantum gravity. In the context of quantum gravity, there arises a natural scale for space-time, the plank scale, and it seems plausible that something new should happen at this scale. In string theories, this scale is the size, or the tension, of the string [8]. One can also use this scale as the size of a possible space-time lattice. In fact, there is no true reason for the continuousness of space-time: all of the measurements of space-time (direct or indirect) have a certain resolution, which is very much larger than the plank scale. On the other hand, there are examples for theories which force the time to be discrete ([9,10], for example).

Also, there has been attempts to discretize the time in quantum mechanics ([11], for example). In this paper, first a general formulation of discrete-time quantum mechanics is introduced (section I). This formulation is based on the action principle, or the Feynman’s path-integral formalism.

In section II the unitarity of the evolution operator is exploited to deduce restrictions on the form of the action. This section addresses a very old problem of classical mechanics: the problem of nonequivalent Lagrangians which give rise to same equations of motion [12,13]. It is shown that in one-dimensional space,
all possible forms of the Lagrangian are equivalent to the difference of a kinetic term and a potential term, where the potential is an arbitrary function of the position. This means that, at least in one dimension, any two Lagrangians (fulfilling the unitarity criteria and) giving the same equation of motion, must be equivalent, up to a constant multiplicative factor. At the end of this section, an example of an allowed action is presented, which gives rise to the Lagrangian of a charged particle moving in an electromagnetic field.

In section III, the equation of motion of the Hesinberg position operator is investigated. It is shown that this equation is, unambiguously, deduced from the classical equation of motion. In continuous-time quantum mechanics, this is not, generally, the case; that is, one can not, in a straightforward manner, deduce the equation of motion of the operators from the classical equation of motion. At the end of this section, it is shown that the unitarity criteria also guarantee the existence of a solution for the classical initial-value problem.

**I Formulation of discrete-time quantum mechanics (Schrödinger picture)**

Ordinary (continuous-time) quantum mechanics is based on two general parts: kinematics, which involves the definition of observables, state space, and measurements; and dynamics, which discusses the evolution of states. We need not change the kinematics. As for dynamics, we accept that a quantum system is a linear dynamical system, the evolution of which is a unitary one. In ordinary quantum mechanics, these among with the principle of correspondence lead to the Schrödinger equation:

$$\hat{H} |\psi\rangle = i\hbar \frac{d}{dt} |\psi\rangle . \tag{I.1}$$

In the case of discrete time, however, we do not have an infinitesimal time-translation. So the Hamiltonian, which is the generator of time-translation, does not arise naturally. One can of course write the single-step evolution operator $\hat{U}$ as

$$\hat{U}(\tau) = \exp \left( -\frac{i\tau \hat{H}}{\hbar} \right). \tag{I.2}$$
But if $\hat{H}$ is a well-defined Hermitian operator, this is not a real discretization of time; this is only a discrete sampling, because one can also define $\hat{U}(t)$ for arbitrary $t$ as

$$\hat{U}(t) = \exp \left( -\frac{it \hat{H}}{\hbar} \right), \quad \text{(I.3)}$$

and use it to find the solution of the Schrödinger equation (I.1).

There is an alternative which does not suffer from these artifacts, and that is to use the Feynman path-integral formulation. One only needs to translate the concept of path to discrete case, which is obvious. In ordinary quantum mechanics we have

$$U(x', x''; t', t'') = A \int [Dx(t)] \exp \left\{ \frac{i}{\hbar} S[x(t)] \right\}; \quad \text{(I.4)}$$

where $S$ is the action,

$$U(x', x''; t', t'') := \langle x'| \hat{U}(t', t'') | x'' \rangle, \quad \text{(I.5)}$$

and $|x'\rangle$ is the eigenvector of the position operator. Integration is over all paths which satisfy the boundary conditions

$$x(t') = x', \quad x(t'') = x'' \quad \text{(I.6)}$$

This means that we are dealing with a “multiple” integral, whose measure is (rather heuristically)

$$[Dx(t)] = \prod_{t' > t > t''} dx(t). \quad \text{(I.7)}$$

Although this description is rather ambiguous in continuous time, and must somehow be regularized, it is completely clear in discrete time. In this case we have

$$U_{n',n''}(x', x'') = A_{n',n''} \int dx_n \exp \left\{ \frac{i}{\hbar} S(x', \cdots, x_n, \cdots, x'') \right\}. \quad \text{(I.8)}$$

Equivalently, one can use the single-step evolution operator

$$U_{n+1/2}(x', x'') := U_{n+1,n}(x', x'') = A_{n+1/2} \exp \left\{ \frac{i}{\hbar} S(x', x'') \right\}. \quad \text{(I.9)}$$
We take this to be the axiom of time evolution, substituting (I.2). In (I.8) and (I.9), $A$ is a constant independent of $x'$ and $x''$.

Now, as we are dealing with a dynamical system, we have

$$U_{n',n''}(x',x'') = \int dx'' U_{n',n''}(x',x'') U_{n'',n'''}(x'',x'''),$$

which leads to a familiar result for the action:

$$S_{n',n''}[x] + S_{n'',n'''}[x] = S_{n',n'''}[x].$$

To summarize, we define an action for a unit-time interval as

$$S_{n+1/2}(x_{n+1}, x_n) := S_{n+1,n}(x_{n+1}, x_n).$$

Then, we generalize this to arbitrary intervals as

$$S_{n',n''}(x_{n'}, \cdots, x_{n''}) := \sum_{n' > n \geq n''} S_{n+1/2}(x_{n+1}, x_n).$$

The single-step evolution operator is then

$$U(x, y) := A \exp \left[ \frac{i}{\hbar} S(x, y) \right].$$

We have dropped the explicit time-dependence of the action for simplicity. But, as one can readily see, this does not alter our later results.

Until now, we have not exploited the unitarity condition of $\hat{U}$, and we have no restriction on the action. In the following section we will use this condition to restrict the form of the action.

**II Unitarity and restrictions on the action**

The unitarity condition for $\hat{U}$ is

$$\int dy U(x, y) U^*(z, y) = \delta(x - z),$$

We have dropped the explicit time-dependence of the action for simplicity. But, as one can readily see, this does not alter our later results.
or, in terms of the action,

$$|A|^2 \int dy \exp \left\{ \frac{i}{\hbar} [S(x, y) - S(z, y)] \right\} = \delta(x - z).$$  \hspace{1cm} (II.2)

Expanding the exponent as

$$S(x, y) - S(z, y) = (x - z) \cdot \nabla_x S(x, y) + O(|x - z|^2),$$  \hspace{1cm} (II.3)

and defining

$$u := \frac{1}{\hbar} (x - z),$$  \hspace{1cm} (II.4)

it is easy to see that (II.2), to lowest order in $\hbar$, gives rise to

$$|A|^2 \int dy \exp \left\{ i \frac{\hbar}{h} (x - z) \cdot \nabla_x S(x, y) \right\} = \delta(x - z).$$  \hspace{1cm} (II.5)

The action, itself, may depend on $\hbar$. So, to be more exact, the above equation holds for zeroth order (of $\hbar$) term of the action, i.e. the classical action. But, as we are going to restrict the form of the classical action, this does not mind.

Defining

$$Y := \nabla_x S(x, y),$$  \hspace{1cm} (II.6)

we have

$$|A|^2 \int dy \left| \det \left( \frac{\partial y}{\partial Y} \right) \right| \exp \left\{ i \frac{\hbar}{h} (x - z) \cdot Y \right\} = \delta(x - z).$$  \hspace{1cm} (II.7)

Now, the Jacobian is a function of $Y$ and $x$ only: It does not depend on $x - z$. So the left-hand side of (II.7) is the Fourier transform of this Jacobian, and is supposed to be the Dirac delta distribution. The Jacobian should, therefore, be independent of $Y$. Since $A$ is independent of $x$, the Jacobian should also be independent of $x$. We therefore have

$$\det \left( \frac{\partial y}{\partial Y} \right) = \text{const}.$$  \hspace{1cm} (II.8)
or

\[ \det \left( \frac{\partial Y}{\partial y} \right) = \text{const.} \]  

(II.8)’

This is a nontrivial differential equation, which restricts the form of \( S \). If the dimension of the space is more than one, it is not easy to determine the most general solution of this equation. But in one dimension the life is simpler and one can obtain such a solution.

**II.1 Action in one-dimensional space**

In one dimension, we have to solve

\[ \frac{\partial^2 S}{\partial x \partial y} = -\frac{m}{\tau}, \]  

(II.9)

where we have written the constant as above for later convenience. \( \tau \) is the time step parameter. This equation can easily be solved:

\[ S(x, y) = -\frac{m}{\tau} x y + f(x) + g(y), \]  

(II.10)

or

\[ S(x, y) = \frac{m}{2\tau} (x - y)^2 - \frac{\tau}{2} [V(x) + V(y)] + \left[ \phi(x) - \phi(y) \right], \]  

(II.10)’

The third part of this expression has no effect on the dynamics of the system. It is easy to see that addition of such a term to the action is equivalent to the following gauge transformation

\[ |x> \rightarrow \exp \left[ -\frac{i}{\hbar} \phi(x) \right] |x> . \]  

(II.11)

It is also easy to see that this term does not affect the equation of motion (which we will encounter in section III). We therefore conclude that the most general solution of (II.9) is equivalent to

\[ S(x, y) = \frac{m}{2\tau} (x - y)^2 - \frac{\tau}{2} [V(x) + V(y)] \]  

(II.12)

This form is a very familiar one. In fact, if we divide the action by \( \tau \) and let \( \tau \) tend to zero, we obtain

\[ L \left[ x(t) \right] := \lim_{\tau \to 0} \frac{S(x, y)}{\tau} = \frac{m}{2} \dot{x}^2 - V(x) \]  

(II.13)
which is the standard form of one-dimensional Lagrangians used in textbooks. This result is, however, an important one: First, in classical mechanics the general Lagrangian formulation does not restrict the form of Lagrangian as a function of position and velocity; one can have terms in Lagrangian which are, for example, quartic in $\dot{x}$. However, nobody has ever needed to consider such Lagrangians for real one-dimensional systems and it seems that nature has chosen the special form (II.13). This formulation provides an explanation for this fact, based on the general assumption of unitarity. Second, there are many nonequivalent Lagrangians that lead to a same equation of motion [12,13]. (By nonequivalent Lagrangians we mean Lagrangians, the difference of them is not a total derivative.) One essentially has no way to choose one of this Lagrangians for quantum theory. The discrete-time formulation characterizes only one single Lagrangian among these.

**II.II Action in multi-dimensional space**

It is easily seen that an action like (II.12) satisfies (II.8). To have a taste of other kinds of solutions, consider a perturbative approach:

$$S(x, y) = S_0(x, y) + s(x, y) := \frac{m}{2\tau} (x - y)^2 - \frac{\tau}{2} [V(x) + V(y)] + s(x, y).$$  \hspace{1cm} (II.14)

We want to solve the linearized equation, corresponding to (II.8)', in terms of $s$. This equation is readily seen to be

$$\text{tr} \left( \frac{\partial^2 s}{\partial x \partial y} \right) = \nabla_x \cdot \nabla_y s = 0.$$  \hspace{1cm} (II.15)

A special solution of this equation is of the form

$$s = \frac{1}{2} \{ [A_1(x_1, y_2, x_3, \cdots) - A_1(y_1, x_2, x_3, \cdots)] + [A_2(y_1, x_2, x_3, \cdots) - A_2(x_1, y_2, x_3, \cdots)] + \cdots \}. \hspace{1cm} (II.16)$$

In the limit $\tau \to 0$, we have

$$s = \frac{\tau}{2} \left\{ \left[ \frac{\partial A_1}{\partial x_1} \dot{x}_1 - \left( \frac{\partial A_1}{\partial x_2} \dot{x}_2 + \frac{\partial A_1}{\partial x_3} \dot{x}_3 + \cdots \right) \right] + \left[ \frac{\partial A_2}{\partial x_2} \dot{x}_2 - \left( \frac{\partial A_2}{\partial x_1} \dot{x}_1 + \frac{\partial A_2}{\partial x_3} \dot{x}_3 + \cdots \right) \right] + \cdots \right\}, \hspace{1cm} (II.17)$$

or

$$s = \tau \left( \frac{\partial A_1}{\partial x_1} \dot{x}_1 + \frac{\partial A_2}{\partial x_2} \dot{x}_2 + \cdots \right) - \frac{\tau}{2} \left( \frac{dA_1}{dt} + \frac{dA_2}{dt} + \cdots \right). \hspace{1cm} (II.18)$$
The second term is a total derivative. Defining

\[ qA_{\alpha} := \frac{\partial A_{\alpha}}{\partial x_{\alpha}}, \tag{II.19} \]

we see that this solution corresponds to the Lagrangian

\[ L = \frac{m}{2} \dot{x}^2 + q \dot{z} \cdot A - V(x), \tag{II.20} \]

which is the Lagrangian of a charged particle moving in the potential \( V(x) \) and a magnetic field, the vector potential of which is \( A(x) \).

**III Heisenberg picture, relation to classical mechanics, and existence theorem for the solution of the equation of motion**

Evolution of the operators in Heisenberg picture is just like the case of continuous time. We first define Heisenberg operators at time \( n \) in terms of their Schrödinger counterparts as

\[ \hat{\Omega}^H_n := (\hat{U}^\dagger)^n \hat{\Omega}^S_n \hat{U}^n. \tag{III.1} \]

Now, we want to discuss the equation of motion for these operators; to be more specific, we want to show that the Heisenberg position operator satisfies the “classical” equation of motion. In fact, the true classical equation of motion is (or can be) somehow ambiguous for operators, because it involves the position operator at three distinct times, and these operators do not commute with each other. But we will see that a certain ordering is dictated from the evolution governed by (III.1).

Consider the matrix element \( <x' | \frac{\partial S(\hat{x}^\dagger, w)}{\partial w} |x''> \), where we define

\[ \hat{x}^\dagger := \hat{U}^\dagger \hat{x} \hat{U}, \text{ and } \hat{x}^\dagger := \hat{U}^\dagger \hat{x} \hat{U}. \tag{III.2} \]

We have then

\[ <x' | \frac{\partial S(\hat{x}^\dagger, w)}{\partial w} |x''> = <x' | \hat{U}^\dagger \frac{\partial S(\hat{x}, w)}{\partial w} \hat{U} |x''> \]

\[ = \int dz <x' | \hat{U}^\dagger \frac{\partial S(\hat{x}, w)}{\partial w} |z> U(z, x'') \]

\[ = \int dz U^*(z, x') \frac{\partial S(z, w)}{\partial w} U(z, x'') \tag{III.3} \]
Now, setting $w = x''$, we come to
\[
< x' | \frac{\partial S(\hat{x}^\dagger, x'' )}{\partial x''} | x'' > = -i\hbar \frac{\partial}{\partial x''} \delta( x' - x'') = : - < x' | \hat{p} | x'' > :,
\]
where the momentum operator $\hat{p}$ is the generator of space translation, and its matrix element satisfies equation (III.4). To deduce (III.4) from (III.3), we have exploited the form of $U$ in terms of the action, and also unitarity of $\hat{U}$.

Equation (III.4) can be rewritten in terms of operators themselves:
\[
< x' | \frac{\partial S(\hat{x}^\dagger, x'')}{\partial x''} | x'' > = < x' | \frac{\partial S(\hat{x}^\dagger, \hat{x})}{\partial \hat{x}} \frac{\partial \hat{x}}{\partial x''} | x'' > \Rightarrow
\]
\[
\frac{\partial S(\hat{x}^\dagger, \hat{x})}{\partial \hat{x}} = -\hat{p},
\]
(III.5)
where the left-hand-side of (III.5) is an ordered form, in which $\hat{x}$s are at the right of $\hat{x}^\dagger$s.

By a similar argument, or by taking the Hermitian conjugate of (III.5), one concludes that
\[
\frac{\partial S(\hat{x}^\dagger, \hat{x})}{\partial \hat{x}} = -\hat{p},
\]
(III.6)
where the left-hand-side of (III.6) is in opposite ordering. Finally, since in this case both of these orderings lead to the same result, we can define a nonoriented ordering, which is equal to both of the above orderings:
\[
\frac{\partial S(\hat{x}^\dagger, \hat{x})}{\partial \hat{x}} = -\hat{p}.
\]
(III.7)

By a similar argument we come to
\[
\frac{\partial S(\hat{x}, \hat{x}^\dagger)}{\partial \hat{x}} = \hat{p}.
\]
(III.8)

Now, eliminating $\hat{p}$ from (III.7) and (III.8), we obtain
\[
\frac{\partial S(\hat{x}, \hat{x}^\dagger)}{\partial \hat{x}} + \frac{\partial S(\hat{x}^\dagger, \hat{x})}{\partial \hat{x}} = 0,
\]
(III.9)
or
\[
\frac{\partial S(\hat{x}_n, \hat{x}_{n-1})}{\partial \hat{x}_n} + \frac{\partial S(\hat{x}_{n+1}, \hat{x}_n)}{\partial \hat{x}_n} = 0.
\]
(III.10)
But this is the classical equation of motion for position operators (obtained by extremizing the action), except that it is time ordered (either in the forward, or in the reversed direction). It has no ambiguity and, once we know the classical action, everything is determined.

Now we come to the problem of existence of solution in classical mechanics. Suppose that we begin by an arbitrary action, which does not satisfy the unitarity criterion. One can not guarantee that the classical equation of motion has a solution for \(x_{n+1}\) for any choice of \(x_n\) and \(x_{n-1}\): this equation may be a nonlinear complicated one. This means that, not every initial-value lead to a path: there may be a time when the particle can not go anywhere.

Now suppose that the unitarity condition holds, so that the equation of motion for the operators, (III.7) through (III.9), hold. For any pair of initial values \(x_0\) and \(x_{-1}\), one can solve the classical counterpart of (III.8) for \(p_0\). Use a Gaussian wave packet with

\[
\langle \hat{x} \rangle = x_0, \quad \langle \hat{p} \rangle = p_0, \quad (III.11)
\]

and

\[
\Delta x = \alpha \sqrt{\frac{\hbar}{2}}, \quad \Delta p = \alpha^{-1} \sqrt{\frac{\hbar}{2}}, \quad (III.12)
\]

as an initial state for quantum mechanics. Then consider equation (III.9) in the limit \(\hbar \rightarrow 0\). In this limit, the uncertainties tend to zero, the operators commute, and we have

\[
\frac{\partial S(\langle \hat{x} \rangle, \langle \hat{x} \rangle)}{\partial \langle \hat{x} \rangle} + \frac{\partial S(\langle \hat{x} \rangle, \langle \hat{x} \rangle)}{\partial \langle \hat{x} \rangle} = 0. \quad (III.14)
\]

Notice that there always exists a \(\langle \hat{x} \rangle\), because one can compute it through the Schrödinger picture.

Now, we know that

\[
\frac{\partial S(x_0, x_{-1})}{\partial x_0} = p_0 = \langle \hat{p} \rangle = \frac{\partial S(\langle \hat{x} \rangle, \langle \hat{x} \rangle)}{\partial \langle \hat{x} \rangle}, \quad (III.15)
\]

where the last equality holds only in the limit \(\hbar \rightarrow 0\). Substituting \(x_0\) and \(x_{-1}\) for \(\langle \hat{x} \rangle\) and \(\langle \hat{x} \rangle\) in
(III.16), we will have

\[
\frac{\partial S(x_0, x_{-1})}{\partial x_0} + \frac{\partial S(< \hat{x}>, x_0)}{\partial x_0} = 0,
\]

which means that \(< \hat{x}^7 > \) (in the limit \( \hbar \to 0 \)) satisfies the classical equation of motion for the initial-values \( x_0 \) and \( x_{-1} \). Specially, if the dimension of space is one, we have seen that any action which satisfies the unitarity condition is of the form (II.10)', or equivalently (II.12). The equation of motion for such an action is linear in \( x_{n+1} \) and the coefficient of \( x_{n+1} \) is nonzero. Therefore every initial-value problem has one and only one solution.

In general, we have proved that the unitarity of the evolution operator, constructed through (I.14) from the action, is sufficient for the existence of a solution for classical initial-value problems.

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