EXTENSION OF QUANTUM MECHANICS TO THE CASE OF DISCRETE TIME

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Generalized equations of motion for the density matrix are constructed for the case of discrete time. The equations of motion for operators in the Heisenberg representation are generalized in an analogous way. Some properties of the equations of motion are studied, the treatment being conducted in a general form independent of any specific scheme for quantizing space-time. The most characteristic property of the equations considered is that they are not invariant under time reversal. This property can be expressed as a law of increase of an "entropy." In the limit of continuous time the equations go over into the usual equations of quantum mechanics; that is, they satisfy a correspondence principle.

1. INTRODUCTION

IN the present paper we consider one of the possible extensions of the equations of quantum mechanics to the case of discrete time. In the limit when time is made continuous the equations considered here go over into the usual Schrödinger equation for the density matrix. At the same time these equations have a number of characteristic peculiarities, the most interesting of which is the violation of time-reversal invariance.

We consider here the general form of the equations of motion and study their properties independent of any specific scheme for quantizing time. The combination of various particular ways of constructing quantized space-time with these equations will in general lead to different physical theories.

Certain well known attempts to introduce a quantized space-time into the modern theory of elementary particles, and the accompanying hopes of overcoming "ultraviolet" difficulties, are treated in [1-3].

2. CONSTRUCTION OF THE GENERALIZED EQUATIONS

We shall assume that the "time" in some reference system takes discrete values of the form $n\tau$, where n is an integer ($-\infty < n < \infty$) and τ is a fundamental constant of the dimensions of time. This sort of time quantization, not relativistically invariant in appearance, can actually be introduced in a completely relativistically invariant way, as Snider[1] has shown. The transition from the discrete time $n\tau$ to continuous time t is made formally by the substitution $n\tau \to t$ and $\tau \to 0$.

As is well known, quantum mechanics can be formulated either in terms of a ψ function (state vector) or in terms of a density matrix $\hat{\rho}$. Furthermore, if we confine ourselves to pure states (i.e., those describable by ψ functions) only, then the two formulations are completely equivalent. On the other hand, the description by means of the density matrix makes it possible to consider both pure and mixed states on an equal basis.

The first important difference between our proposed scheme and the usual one is that it permits the description of a quantum-mechanical system by means of the density matrix only, and does not permit a description by means of a ψ function.

The density matrix $\hat{\rho}$ must satisfy the following requirements, whose physical meaning is obvious: the requirement of Hermiticity

$$\hat{\rho}^+ = \hat{\rho}, \tag{2.1}$$

and those of positive definite character

$$\langle\psi\,|\,\hat{\rho}\,|\,\psi\rangle > 0, \tag{2.2}$$

where ψ is an arbitrary state vector, and of normalization

$$\mathrm{Tr}\,\hat{\rho} = 1. \tag{2.3}$$

On the other hand, every matrix which satisfies the requirements (2.1)—(2.3) can be regarded as a possible density matrix describing some state of the system. The mean value of a physical quantity $\hat{M}$ in the state described by a density matrix $\hat{\rho}$ is given by the relation

$$\langle\hat{M}\rangle = \mathrm{Tr}\,\{\hat{\rho}\hat{M}\}. \tag{2.4}$$

It is easy to see that the class of all possible density matrices satisfying the conditions (2.1)—

(2.3) is closed relative to the following two operations:

1) unitary transformations: if $\hat{\rho}$ is a density matrix and U is an arbitrary unitary operator, then the matrix $\hat{\rho}' = U\hat{\rho}U^+$ is also a possible density matrix.

2) formation of weighted averages: if $\hat{\rho}_1$ and $\hat{\rho}_2$ are density matrices, then the matrix $\hat{\rho} = \alpha_1 \hat{\rho}_1 + \alpha_2\hat{\rho}_2$ will also be a possible density matrix if α_1, α_2 are positive numbers and $\alpha_1 + \alpha_2 = 1$.

These remarks allow us to construct the equation of motion for the density matrix in the case of quantized time. The simplest analog of the usual equation of motion for the case of quantized time would be an equation of the form

$$\hat{\rho}[(n+1)\tau] = U\hat{\rho}(n\tau)U^+, \tag{2.5}$$

where U is some unitary operator. This equation satisfies the correspondence principle in an obvious way for $\tau \to 0$. By using the properties 1) and 2) of the density matrix, however, we can construct equations of much more general form.

Let us introduce two positive constants α and β, connected by the relation

$$\alpha + \beta = 1, \tag{2.6}$$

and two unitary operators U and V. We postulate for the density matrix $\hat{\rho}$ an equation of motion of the form

$$\hat{\rho}[(n+1)\tau] = \alpha U\hat{\rho}(n\tau)U^+ + \beta V\hat{\rho}(n\tau)V^+. \tag{2.7}$$

Equation (2.7) can be taken as the equation of motion for the density matrix, since because of the properties 1) and 2) this equation transforms the density matrix $\hat{\rho}(n\tau)$ into a matrix $\hat{\rho}[(n+1)\tau]$ which also satisfies all of the necessary conditions (2.1)–(2.3). We note that Eq. (2.7) could easily be subjected to a further generalization. The basic properties of this equation are also true for an equation of the form

$$\hat{\rho}[(n+1)\tau] = \Sigma\alpha_i U_i\hat{\rho}(n\tau)U_i^+. \tag{2.8}$$

Here the α_i are positive constants which satisfy the condition

$$\sum \alpha_i = 1,$$

and the U_i are unitary operators. The sum in the right member of Eq. (2.8) can contain any number of terms.

In what follows we confine ourselves to the study of the simple two-term equation (2.7), since it already shows a number of characteristic new properties which carry over easily to the more general equation (2.8). Besides this, in iterations of Eq. (2.7) we get a certain special form of Eq. (2.8). We shall note that the characteristic properties of equations of the form (2.7) or (2.8), which are associated with discreteness of the time, are absent for the "one-term" equation (2.5).

Let us now consider the passage to the limit of continuous time in Eq. (2.7). Since $\tau \to 0$, we must regard the unitary operators U and V as infinitely close to the unit operator. To and including terms of order τ we can write these operators in the form

$$U = 1 - iA\tau, \qquad V = 1 - iB\tau, \tag{2.9}$$

where A and B are Hermitian operators. Substituting the quantities (2.9) in (2.7) and keeping terms of first order in τ, we get the relation

$$\hat{\rho}[(n+1)\tau] = \hat{\rho}(n\tau) - i\tau[(\alpha A + \beta B), \hat{\rho}(n\tau)].$$

When we set $n\tau = t$ and $\tau \to 0$ in this equation, we get the equation of motion

$$i\partial\hat{\rho}/\partial t = [(\alpha A + \beta B), \hat{\rho}]. \tag{2.10}$$

Equation (2.10) is identical with the usual quantum-mechanical equation of motion for the density matrix $\hat{\rho}$, with the role of the Hamiltonian H played by the Hermitian operator $\alpha A + \beta B$ ($\hbar = 1$). It is extremely important that in this derivation no assumptions have been made about smallness of the constants α and β.

We see that when we pass to the limit of continuous time the equation of motion (2.7) and also the more general equation (2.8) go over in a natural way into known equations of quantum mechanics. This fact makes it plausible to consider Eq. (2.7) as the equation of motion for the case of continuous time.

3. EQUATIONS OF MOTION FOR OPERATORS. CONSERVATION LAWS

The equation of motion for operators in the Heisenberg representation can be generalized in a natural way for the case considered here. We shall start from the requirement that the changes of the mean values of any quantity owing to changes of the state in the Schrödinger picture must agree with the corresponding changes of mean value owing to changes of the operators in the Heisenberg picture. For discrete time this condition can be expressed in the form

$$\mathrm{Tr}\{\hat{\rho}[(n+1)\tau]\hat{M}(n\tau)\} = \mathrm{Tr}\{\hat{\rho}(n\tau)\hat{M}[(n+1)\tau]\}, \tag{3.1}$$

where $\hat{M}$ is the operator corresponding to some physical quantity. From (3.1) and the equation of motion (2.7) for $\hat{\rho}$ we get the equation of motion for $\hat{M}$:

$$\hat{M}[(n+1)\tau] = \alpha U^+\hat{M}(n\tau)U + \beta V^+\hat{M}(n\tau)V. \quad (3.2)$$

As in the preceding section, it is easy to show that in the limit of continuous time the equation (3.2) goes over into the usual quantum-mechanical equation of motion for an operator $\hat{M}$ with the Hamiltonian $\alpha A + \beta B$:

By means of the equation of motion (3.2) it is easy to extend the concept of constant of the motion to the discrete-time type of theory. A physical quantity $\hat{M}$ is a constant of the motion if it satisfies the condition

$$\hat{M} = \alpha U^+\hat{M}U + \beta V^+\hat{M}V. \quad (3.3)$$

Mean values of quantities that satisfy the condition (3.3) do not depend on the time.

If an operator $\hat{M}$ commutes with the operators U and V, $\hat{M}$ is obviously a constant of the motion. Besides such "trivial" constants of the motion there can also exist "nontrivial" constants of the motion, which satisfy only the condition (3.3) as a whole.

4. THE EQUATIONS OF MOTION TO ACCURACY τ^2

As we saw in Sec. 2, to first order in τ the properties of the equation (2.7) are extremely close to those of the usual quantum-mechanical equations. There are important deviations beginning with the terms of order τ^2. We shall consider this matter is somewhat more detail.

We represent the unitary operators U and V in the form

$$U = \exp(-iA\tau), \qquad V = \exp(-iB\tau), \quad (4.1)$$

where A and B are Hermitian operators. We then introduce operators H and W connected with A and B by the relations

$$A = H + 2\beta W, \qquad B = H - 2\alpha W \quad (4.2)$$

or

$$H = \alpha A + \beta B, \qquad W = \tfrac{1}{2}(A - B). \quad (4.3)$$

It can be seen from (2.10) that for $\tau \to 0$ the operator H goes over into the complete Hamiltonian of the system. The operator W has no classical analog for the case of continuous time.

Using the well known formula

$$e^a x e^{-a} = \sum_{n=0}^{\infty} \frac{1}{n!} [\overset{n}{a}, x], \quad (4.4)$$

where $[\overset{n}{a}, x]$ denotes the repeated commutator, and taking into account terms to and including τ^2, we can use (4.1) and (4.2) to put the equation of motion for the operators (3.2) in the form

$$\hat{M}[(n+1)\tau] = \hat{M}(n\tau) + i\tau[H, \hat{M}(n\tau)] - \tfrac{1}{2}\tau^2[H, [H, \hat{M}(n\tau)]] - 2\alpha\beta\tau^2[W, [W, \hat{M}(n\tau)]]. \quad (4.5)$$

It is clear from the form of this equation that the operators H and W occur in the equation of motion in entirely different ways. Let us now assume that the quantity $\hat{M}$ commutes with the operator H (is conserved in the "classical" sense). Then from (4.5) we get as the expression for the change of the quantity $\hat{M}$ in the time τ

$$\delta\hat{M} = -2\alpha\beta\tau^2[W, [W, \hat{M}]]. \quad (4.6)$$

We see that in the case now considered the change of the operator $\hat{M}$ in the time τ is proportional to τ^2 and depends only on the "nonclassical" operator W.

On the other hand, in some cases the contributions from H and W are of the same order. Let us consider, for example, the probability for transition of a system from one state to another in the time τ. We denote by λ a complete set of observable quantities of our system and consider a state for which the density matrix $\hat{\rho}$ at the initial time is diagonal in the λ representation:

$$\langle\lambda|\hat{\rho}(0)|\lambda'\rangle = \rho(\lambda)\delta_{\lambda\lambda'} \quad (4.7)$$

Using the condition (4.7), we can get from the equation of motion (4.7) an expression for the diagonal elements of the density matrix $\hat{\rho}(\tau)$,

$$\langle\lambda|\hat{\rho}(\tau)|\lambda'\rangle = \sum_{\lambda'} P(\lambda, \lambda')\rho(\lambda'), \quad (4.8)$$

where

$$P(\lambda, \lambda') = \alpha|\langle\lambda|U|\lambda'\rangle|^2 + \beta|\langle\lambda|V|\lambda'\rangle|^2. \quad (4.9)$$

Since the diagonal elements of the density matrix determine the distribution of probabilities for the given state of the system the quantity $P(\lambda, \lambda')$ can be regarded as the probability for transition of the system from state λ' to state λ in the time τ. Using the definitions (4.1) and (4.2) and confining ourselves to terms of order τ^2 in (4.9), we get for the transition probability for $\lambda \neq \lambda'$ the expression

$$P(\lambda, \lambda') = (|\langle\lambda|H|\lambda'\rangle|^2 + 4\alpha\beta|\langle\lambda|W|\lambda'\rangle|^2)\tau^2. \quad (4.10)$$

It can be seen from (4.10) that the operators H and W make contributions of the same order of magnitude to the probability of the system's making a transition in the time τ, and there is no interference between these contributions.

5. NONINVARIANCE OF THE EQUATION OF MOTION WITH RESPECT TO TIME REVERSAL

The arguments with which one establishes the time-reversal invariance of the equations of motion of quantum mechanics (cf. [4]) cannot be applied to the equation of motion (2.7). We shall show that Eq. (2.7) is actually not invariant with respect to time reversal, this noninvariance being an effect of the quantization of time and vanishing altogether in the limiting case of continuous time.

The most intuitive way to represent this irreversibility is to consider the "entropy" of the system, which we define by the relation

$$S(\rho) = -\operatorname{Tr}\{\hat{\rho}\ln\hat{\rho}\}. \tag{5.1}$$

The entropy so defined is a function of the state of the system, i.e., depends only on the density matrix $\hat{\rho}$. In the case of statistical equilibrium the definition (5.1) coincides with the generally accepted definition of entropy. We shall show that the quantity S increases monotonically with the time because of the equation of motion (2.7).

For brevity we introduce the notations

$$\hat{\rho}(n\tau) = \hat{\rho}, \qquad \hat{\rho}[(n+1)\tau] = \hat{\sigma}. \tag{5.2}$$

According to Eq. (2.7) the density matrices $\hat{\rho}$ and $\hat{\sigma}$ are connected by the relation

$$\hat{\sigma} = \alpha U\hat{\rho}U^+ + \beta V\hat{\rho}V^+. \tag{5.3}$$

Our general assertion will be proved if we show that

$$S(\sigma) > S(\rho). \tag{5.4}$$

By a suitable choice of the unitary transformations X and Y we can bring the matrices $\hat{\sigma}$ and $\hat{\rho}$ into diagonal form

$$\hat{\rho} = X\rho_D X^+, \qquad \hat{\sigma} = Y\sigma_D Y^+. \tag{5.5}$$

The index "D" in the relations (5.5) indicates that the matrix in question is diagonal. Substituting (5.5) in (5.3), we get the corresponding relation for the diagonal matrices:

$$\sigma_D = \alpha U'\rho_D U'^+ + \beta V'\rho_D V'^+, \tag{5.6}$$

where U′ and V′ are the unitary matrices

$$U' = Y^+UX, \qquad V' = Y^+VX. \tag{5.7}$$

From the equation (5.6) there follows a relation between the eigenvalues of the matrices $\hat{\rho}$ and $\hat{\sigma}$:

$$\sigma_\lambda = \Sigma a_{\lambda\mu}\rho_\mu, \tag{5.8}$$

where the coefficients $a_{\lambda\mu}$ are determined by the equation

$$a_{\lambda\mu} = \alpha|\langle\lambda|U'|\mu\rangle|^2 + \beta|\langle\lambda|V'|\mu\rangle|^2. \tag{5.9}$$

Owing to the unitarity of the matrices (5.7) the coefficients $a_{\lambda\mu}$ satisfy the relations

$$\sum_\lambda a_{\lambda\mu} = \sum_\mu a_{\lambda\mu} = 1. \tag{5.10}$$

It can be seen from the definition (5.1) that the entropy can be expressed in terms of the diagonal matrix elements by the equation

$$S(\rho) = -\sum_\lambda \rho_\lambda \ln \rho_\lambda. \tag{5.11}$$

The rest of the proof is based on the following simple inequality. Let $\varphi(x)$ be a function which satisfies the inequality

$$\varphi''(x) < 0. \tag{5.12}$$

Furthermore, let x_i be an arbitrary set of values of x. We define the average value $\bar{x}$ by the equation

$$\bar{x} = \sum a_i x_i, \tag{5.13}$$

where the a_i are positive numbers which satisfy the condition

$$\sum a_i = 1. \tag{5.14}$$

The average value of any function of κ is defined in an analogous way.

Then the inequality

$$\varphi(\bar{x}) \geqslant \overline{\varphi(x)} \tag{5.15}$$

holds for the function $\varphi(x)$.

To prove (5.15) we consider an expansion in Taylor's series with a remainder:

$$\varphi(x_i) = \varphi(\bar{x}) + (x_i - \bar{x})\varphi(\bar{x}) + {}^1/_2(x_i - \bar{x})^2\varphi''(\xi_i). \tag{5.16}$$

Multiplying both sides of (5.16) by a_i and summing over i, we get

$$\overline{\varphi(x)} = \varphi(\bar{x}) + \frac{1}{2}\sum a_i(x_i - \bar{x})^2\varphi''(\xi_i). \tag{5.17}$$

Because of the condition (5.12) the inequality (5.15) follows. We note that the equals sign in (5.15) is possible only in the case in which all of the quantities $x_i - \bar{x}$ are zero. This can happen only if there is only one nonvanishing coefficient a_i.

We consider the inequality (5.15) for the function $\varphi(x) = -x\ln x$, which satisfies the condition (5.12). From the relations (5.8) and (5.10) it follows that

$$-\sigma_\lambda \ln \sigma_\lambda \geqslant -\sum_\mu a_{\lambda\mu}\rho_\mu \ln \rho_\mu.$$

Then when we sum over λ and use (5.10) and (5.11) we find

$$S(\sigma) \geqslant S(\rho). \tag{5.18}$$

It is easy to show that there can be equality in (5.18) only in the following cases: if one of the coefficients α or β in the equation of motion (2.7) is equal to zero, or else if U = V. In both cases (2.7) reduces to the one-term equation (2.5). In the general case the relation (5.18) is strictly an inequality. This proves the inequality (5.4), and consequently also the general assertion that the entropy defined by the relation (5.1) increases monotonically.

Let us now consider the increase of entropy in the time τ, confining ourselves to terms of order τ^2. Using the notations (4.1) and (4.2), we can write the equation of motion (5.3) to this accuracy:

$$\hat{\sigma} = \hat{\rho} - i\tau [H, \hat{\rho}] - {}^1/_2 \tau^2 [H, [H, \hat{\rho}]] - 2\alpha\beta\tau^2 [W, [W, \hat{\rho}]].$$

By means of Eq. (4.4) we can write this relation with the same accuracy in the form

$$\hat{\sigma}' = e^{iH\tau} \hat{\sigma} e^{-iH\tau} = \hat{\rho} - 2\alpha\beta\tau^2 [W \ \ [W, \hat{\rho}]]. \qquad (5.19)$$

From (5.19) we get a relation between the eigenvalues of the matrices $\hat{\sigma}$ and $\hat{\rho}$, which is accurate to τ^2:

$$\sigma_\lambda = \rho_\lambda - 2\alpha\beta\tau^2 \langle\lambda | [W, [W, \hat{\rho}]] | \lambda\rangle. \qquad (5.20)$$

From this, when we use (5.11) and do some simple manipulations, we find the increase of the entropy in the time τ:

$$\delta S = 4\alpha\beta\tau^2 \operatorname{Tr} \{\hat{\rho} W [W, \ln \hat{\rho}]\}. \qquad (5.21)$$

As in the formula (4.6) for the changes of operators, the increase of the entropy in the time τ is proportional to τ^2 and depends only on W. When we go over to continuous time the effect of increase of entropy disappears, in accordance with the time-reversal invariance of ordinary quantum mechanics.

Summarizing, we can say that the equation of motion (2.7) considered in this paper has the property of dissipativity. This dissipativity is manifested only as a result of discreteness of the time, and disappears completely when we go to the limiting case of continuous time.

In conclusion we must point out that the increase of entropy considered in this section is not to be identified with the law of increase of entropy which holds for macroscopic systems. As is well known, the basis of the law of increase of entropy is a still unsolved problem, and attempts to derive this law, starting from the principles of classical or of quantum mechanics, have so far been unsuccessful. But the question whether the law of increase of entropy is connected with a possible quantization of space-time must in any case be the object of a special investigation, and is far beyond the scope of this paper.

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