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Dynamical Mappings of Density Operators in Quantum Mechanics. II. Time Dependent Mappings*

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The most general continuous time-dependent evolution of a physical system is represented by a continuous one-parameter semi-group of linear mappings of density operators to density operators. It is shown that if these dynamical mappings form a group they can be represented by a group of unitary operators on the Hilbert space of state vectors. This proof does not assume that the absolute values of inner products of state vectors or "transition probabilities" are preserved but deduces this fact from the requirement that density operators are mapped linearly to density operators. An example is given of a continuous one-parameter semi-group of dynamical mappings which is not a group.

I. INTRODUCTION

THE most general dynamical transformation of a physical system can be represented by a linear mapping of density operators to density operators. It was pointed out in an earlier paper¹ that there are many such dynamical mappings which are not Hamiltonian mappings, that is, there are linear mappings of the set of density operators into itself

which can not be represented by unitary transformations on the Hilbert space of state vectors. The present paper is a continuation of the investigation begun in reference 1, and answers some questions which were left open there. In particular, we consider whether there can be non-Hamiltonian dynamical mappings which represent a continuous time dependent evolution of a physical system.

In Sec. II the property that a family of dynamical mappings represent a continuous time dependent evolution of a system is formulated in the requirement that it forms a continuous one-parameter semi-group. The requirement that it form a con-

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¹ T. F. Jordan and E. C. G. Sudarshan, *J. Math. Phys.* 2, 772 (1961).

tinuous one-parameter group and the requirement that it is a continuous family of Hamiltonian mappings, i.e., that it is representable by a continuous group of unitary operators on the Hilbert space of state vectors, are apparently more restrictive conditions. In Sec. III it is shown that the latter two requirements are equivalent. Every continuous group of dynamical mappings is a continuous family of Hamiltonian mappings. But in Sec. IV an example is given of a continuous semi-group of dynamical mappings which is not a group and, therefore, is not a family of Hamiltonian mappings.

The one-parameter groups of dynamical transformations which we call "time dependent" can be used to represent other symmetry transformations on the system besides transformations in time. In fact, it is no problem to generalize our results from one-parameter groups to representations by dynamical mappings of many continuous groups such as the Lorentz group. That such representations must be generated by continuous unitary representations on the Hilbert space of state vectors² then follows in analogy to our proof in Sec. III that the group property implies that a time-dependent family of dynamical mappings is a family of Hamiltonian mappings. This proof does not require the assumption that the absolute values of inner products of state vectors or "transition probabilities" are preserved but proves this fact from the requirement that density operators are mapped linearly to density operators.

II. TIME-DEPENDENT DYNAMICAL MAPPINGS

In the quantum mechanical description of a physical system by operators on a separable Hilbert space \mathcal{H} , the state of the system can be represented by a density operator on \mathcal{H} . A density operator is a positive semi-definite, self-adjoint operator which has unit trace. These operators form a convex set. The extremal elements of this convex set are the pure state density operators; they are projection operators onto one-dimensional subspaces of \mathcal{H} . The properties of density operators were outlined in some detail in reference 1. It was shown that density operators belong to the Hilbert space \mathcal{L} of operators ρ on \mathcal{H} for which³ $\text{Tr}(\rho^\dagger\rho)$ is finite, the inner product in \mathcal{L} being defined by

$$(\rho, \sigma) = \text{Tr}(\rho^\dagger\sigma). \tag{2.1}$$

² E. P. Wigner, Ann. Math 40, 149 (1939).

³ It is sufficient for our purposes to consider only bounded operators which form a linear space without causing any problems of domains.

The pure state density operators span the space \mathcal{L} , so that a linear mapping on the density operators uniquely defines a linear mapping on \mathcal{L} . A dynamical transformation of the physical system may be represented by a linear transformation of \mathcal{L} which maps the convex set of density operators into itself. If A is a linear operator on \mathcal{L} such that, if ρ is a density operator, then

$$\rho' = A\rho \tag{2.2}$$

is also a density operator, we will call A a dynamical mapping.⁴

In order to represent dynamics in the usual sense, that is as a continuous time-dependent evolution of the state of the system, we must have a family of dynamical mappings $A(t)$,

$$\rho \rightarrow \rho(t) = A(t)\rho \tag{2.3}$$

depending on a real parameter t , such that

$$A(t)A(s) = A(t+s) \tag{2.4}$$

for non-negative values of t and s , and

$$A(0) = I. \tag{2.5}$$

In other words we must require that the dynamical mappings $A(t)$ form a one-parameter semi-group. In addition we must require that the expectation value

$$\langle \sigma \rangle_t = \text{Tr}(\sigma\rho(t)) = (\sigma, A(t)\rho) \tag{2.6}$$

of the self-adjoint operator σ belonging to \mathcal{L} , for the time dependent state $\rho(t)$, be a continuous function of the parameter t . Since the trace of the product is the inner product in \mathcal{L} , as is indicated in Eq. (2.6), this means that $A(t)$ must be weakly continuous as a function of t . The mathematical condition for a time dependent evolution of density operators is then that we have a family of linear transformations of the form (2.3) on \mathcal{L} , and that:

(I) $A(t)$, $0 \leq t < \infty$, is a weakly continuous one-parameter *semi-group* of dynamical mappings (linear transformations of \mathcal{L} that map the convex subset of density operators into itself).

If we want the dynamics to be reversible, that is if we require that every dynamical mapping have an inverse which is a dynamical mapping, then we need the stronger condition that:

(II) $A(t)$, $-\infty < t < +\infty$, is a weakly con-

⁴ We will use the same notational convention as in reference 1. Capital letters A will represent operators on \mathcal{L} and Greek letters ρ, ω, σ , operators on \mathcal{H} (elements of \mathcal{L}). Greek letters ϕ, ψ will denote vectors in \mathcal{H} , and small letters a, c will denote scalars.

tinuous one-parameter group of dynamical mappings ($A(t)^{-1} = A(-t)$).

Finally we are interested in time dependent Hamiltonian dynamical mappings which are defined by the condition that:

(III) There exists a (strongly or weakly) continuous one-parameter group of unitary operators $\omega(t)$ on \mathcal{H} , such that $A(t)\rho = \omega(t)\rho\omega^\dagger(t)$ for each ρ belonging to \mathcal{L} .

Clearly (III) implies (II) implies (I). We will see that conversely (II) implies (III), but that (I) does not imply (II).

III. HAMILTONIAN MAPPINGS

In this section we will show that a time dependent family of dynamical mappings is a family of Hamiltonian mappings whenever it is a one-parameter group. In reference 1 conditions were given which are necessary and sufficient for a dynamical mapping of the general form (2.2) to be a Hamiltonian mapping. However, no consideration was given to the time dependence of these mappings, or to the implications of time dependence which could possibly restrict the allowed dynamical mappings to Hamiltonian mappings. It is the purpose of this paper to consider these questions and thus complete the study of the relation of Hamiltonian quantum dynamics to the more general dynamics of density operators.

If a dynamical mapping takes pure state density operators to pure state density operators, then it defines a mapping of normalized vectors in \mathcal{H} to normalized vectors in \mathcal{H} . For each vector this mapping is defined up to a phase factor. If these phase factors can be chosen so as to yield a linear mapping on \mathcal{H} , we say that the dynamical mapping induces a linear mapping on \mathcal{H} . In the earlier paper¹ it was stated that if a dynamical mapping maps pure state density operators to pure state density operators and induces a linear mapping on \mathcal{H} , then it is a Hamiltonian mapping. This statement is true only for those dynamical mappings which map the set of pure state density operators onto itself. In Theorem 2 of reference 1, the possibility for a dynamical mapping to map the set of pure state density operators one-to-one onto a proper subset of itself was not given proper consideration. Before moving on to the new questions, we will give a corrected statement of this theorem, giving explicit attention to this particular feature:

Theorem. Equivalent necessary and sufficient conditions for a dynamical mapping to be a Hamiltonian dynamical mapping are:

(i) There exists a linear unitary operator ω on \mathcal{H} such that the dynamical mapping maps each operator ρ in \mathcal{L} to $\omega\rho\omega^\dagger$. (This can be taken as the definition of a Hamiltonian dynamical mapping.)

(ii) The dynamical mapping maps the set of pure state density operators onto itself and induces a linear mapping on \mathcal{H} .

(iii) For each member $\phi^{(i)}$ of any set of basis vectors in \mathcal{H} , there exists a normalized vector $\psi^{(i)}$, such that the set of these vectors spans \mathcal{H} , and the dynamical mapping maps $\phi^{(i)}\phi^{(j)\dagger}$ to $\psi^{(i)}\psi^{(j)\dagger}$.⁵

(iv) There exist linear operators ω and σ on \mathcal{H} , which have inverses, such that the dynamical mapping maps each operator ρ on \mathcal{L} to $\omega\rho\sigma^\dagger$.

Now we can proceed to the consideration of conditions under which time dependent dynamical mappings represent Hamiltonian dynamics.

Theorem. A time dependent family of dynamical mappings $A(t)$ is a family of Hamiltonian mappings (satisfying condition III) if it is a weakly continuous one-parameter group (satisfying condition II).

Proof. If the dynamical mappings $A(t)$ form a group, then for any value of t the dynamical mapping $A(t)$ has an inverse dynamical mapping $A(-t)$. Now $A(-t)$ can not map a density operator ρ which is not a pure state density operator to a pure state density operator. For let $\rho = a\rho_1 + (1-a)\rho_2$, where $0 < a < 1$, and ρ_1 and ρ_2 are distinct density operators. Then $A(-t)\rho = aA(-t)\rho_1 + (1-a)A(-t)\rho_2$ is not a pure state density operator unless $A(-t)\rho_1 = A(-t)\rho_2$, which can not be true, since $A(-t)$ must be one-to-one if it is to have an inverse. Hence, only pure state density operators can be mapped to pure state density operators by $A(-t)$. From this we can conclude that $A(t)$ must map all pure state density operators to pure state density operators, and must, in fact, map the set of pure state density operators one-to-one onto itself, since it has an inverse dynamical mapping. The group property, therefore, implies that we have an induced mapping of \mathcal{H} one-to-one onto itself. We need to determine that this induced mapping is linear.

Let ρ_ϕ be the projection operator whose range is the one-dimensional subspace of \mathcal{H} spanned by the normalized vector ϕ . Then,

$$\text{Tr}(\rho_\psi\rho_\phi) = |(\psi, \phi)|^2. \quad (3.1)$$

The density operators are the operators ρ on \mathcal{L} of

⁵ The notation is the same as in reference 1. $\psi\phi^\dagger$ is a linear operator defined on \mathcal{H} by its matrix elements with respect to any set of basis vectors $\phi^{(i)}$ in \mathcal{H} as $(\phi^{(i)}, \psi\phi^\dagger\phi^{(j)}) = (\phi^{(i)}, \psi)(\phi, \phi^{(j)})$.

the form

$$\rho = \sum_i a_i \rho_{\phi_i},$$

where $0 \leq a_i \leq 1$, $\sum_i a_i = 1$, and ϕ_i are a set of orthonormal vectors in \mathcal{H} . Since $A(t)$ maps the set of pure state density operators one-to-one onto itself, we can let

$$A(t)\rho_{\phi_i} = \rho_{\phi'_i},$$

where ϕ'_i form a set of distinct normalized vectors in \mathcal{H} . Then,

$$\rho' = A(t)\rho = \sum_i a_i \rho_{\phi'_i}$$

$$\text{Tr}(\rho'^2) = \sum_i a_i^2$$

$$\begin{aligned} \text{Tr}(\rho'^2) &= \sum_i a_i^2 + \sum_{i \neq j} a_i a_j |\langle \phi'_i, \phi'_j \rangle|^2 \\ &\geq \text{Tr}(\rho^2). \end{aligned}$$

By applying the same argument to $A(-t)$, which maps ρ' to ρ , we get that

$$\text{Tr}(\rho^2) \geq \text{Tr}(\rho'^2)$$

which, together with the previous result, implies that

$$\text{Tr}(\rho'^2) = \text{Tr}(\rho^2),$$

which can be true only if

$$\text{Tr}(\rho_{\phi_i} \rho_{\phi_j}) = |\langle \phi'_i, \phi'_j \rangle|^2 = 0$$

for $i \neq j$. Hence, we can conclude that orthogonal projections are mapped to orthogonal projections by $A(t)$, or in other words that sets of orthonormal vectors in \mathcal{H} are mapped to sets of orthonormal vectors by the mapping induced by $A(t)$. From this it follows that, if ρ is a completely continuous symmetric operator belonging to \mathcal{L} which is mapped to ρ' by $A(t)$, then

$$\text{Tr}(\rho'^2) = \text{Tr}(\rho^2)$$

since a completely continuous symmetric operator has a pure point spectrum. In particular, since $\rho_\psi - \rho_\phi$ is a completely continuous symmetric operator, we have that

$$\text{Tr}([\rho_\psi - \rho_\phi]^2) = 2 - \text{Tr}(\rho_\psi \rho_\phi + \rho_\phi \rho_\psi)$$

is equal to

$$\text{Tr}([\rho_{\psi'} - \rho_{\phi'}]^2) = 2 - \text{Tr}(\rho_{\psi'} \rho_{\phi'} + \rho_{\phi'} \rho_{\psi'}),$$

where $\rho_{\psi'}$ and $\rho_{\phi'}$ are the images under the mapping

$A(t)$ of ρ_ψ and ρ_ϕ , respectively, which implies, by Eq. (3.1), that

$$|\langle \psi, \phi \rangle|^2 = |\langle \psi', \phi' \rangle|^2.$$

The mapping induced on \mathcal{H} by $A(t)$ therefore preserves the absolute value of inner products.

Wigner⁶ has shown that if a mapping of a Hilbert space preserves the absolute value of inner products and is defined up to phase factors, then these phase factors can be chosen to make the mapping either linear and unitary or antilinear and antiunitary. The latter possibility is eliminated by the requirement that the dynamical mappings $A(t)$ form a weakly continuous one-parameter group with $A(0) = 1$.⁷ Hence, for each value of t we have that, for any operator ρ belonging to \mathcal{L} ,

$$A(t)\rho = \omega(t)\rho\omega^\dagger(t),$$

where $\omega(t)$ is a unitary linear operator on \mathcal{H} which is defined up to a phase factor. The operators $\omega(t)$ form a one-parameter group up to a phase factor, that is

$$\omega(t)\omega(s) = c(t, s)\omega(t + s),$$

where $c(t, s)$ is a complex number of absolute value one.

From the weak continuity of $A(t)$ it follows that, for any vectors ψ and ϕ in \mathcal{H} ,

$$\text{Tr}(\omega(t)\rho_\psi\omega^\dagger(t)\rho_\phi) = |\langle \omega(t)\psi, \phi \rangle|^2$$

is a continuous function of t . The operators $\omega(t)$, therefore, give a continuous unitary ray representation of the additive group of real numbers. It has been shown by Bargmann⁸ that in such a case the phase factors of the $\omega(t)$ can be chosen so that the $\omega(t)$ form a continuous one-parameter group of unitary operators on \mathcal{H} . This completes the proof of the theorem.

We notice that the proof of this theorem remains valid if, instead of a representation of the additive group of real numbers, we are interested in a representation by dynamical mappings of any locally compact topological group for which we can use the theorems of Bargmann⁸ to substitute a continuous unitary representation for a ray representation (representation up to a phase factor). For any symmetry group of this type, such as the Lorentz

⁶ E. P. Wigner, *Group Theory and its Application to the Quantum Mechanics of Atomic Spectra* (Academic Press Inc., New York, 1959).

⁷ The continuity condition is not needed here. That $\omega(t)$ is unitary is implied by the group property. For $\omega(t)$ is equal to within a phase factor to the square of $\omega(t/2)$, which is unitary whether $\omega(t/2)$ is unitary or antiunitary.

⁸ V. Bargmann, *Ann. Math.* 59, 1 (1954).

group, we can deduce the necessity of a representation by unitary transformations on the Hilbert space of state vectors.² The requirement that the induced mappings preserve the absolute values of inner products, or that "transition probabilities" be preserved by the symmetry transformations, need not be assumed; it can be *proved* from the requirement that each symmetry transformation maps density operators linearly to density operators.

IV. NON-HAMILTONIAN MAPPINGS

In this section we will show that the group property is necessary if a time dependent family of dynamical mappings is to be a family of Hamiltonian mappings. We present an example of a family of dynamical mappings $A(t)$ which have almost every property one might ask for except the group property. Let $\omega(t)$ be a continuous one-parameter semi-group of operators on \mathcal{H} which are isometric but not unitary. Examples of such semi-groups are well known.⁹ For each operator ρ belonging to \mathcal{L} , let

$$A(t)\rho = \omega(t)\rho\omega^\dagger(t). \quad (4.1)$$

It is easy to see that the $A(t)$ form a continuous one-parameter semi-group, and that, since pure state density operators are mapped to pure state density operators, each $A(t)$ is a dynamical mapping. Therefore, the $A(t)$ satisfy condition I.

⁹ F. Riesz and B. Sz. Nagy, *Functional Analysis*, translated from the second French edition by L. F. Boron; (F. Ungar Publishing Company, New York, 1955), p. 396.

But each $A(t)$ does not have an inverse dynamical mapping, so they do not satisfy condition II.

In addition to the property of time dependence, we have that for each t the $A(t)$ of this example is an extremal element of the convex set of dynamical mappings which maps the set of pure state density operators one-to-one onto a subset of itself, induces a linear mapping on \mathcal{H} , preserves the entropy or the trace of the square of density operators, and preserves the multiplication of operators on \mathcal{H} .

Every continuous one-parameter semi-group of isometric operators is generated by a maximal symmetric operator,¹⁰ so the transformation (4.1) can be thought of as the solution of a "Schrödinger equation" for the pure states with a maximal symmetric Hamiltonian operator. It is also known that such a semi-group can be made into a unitary group by extending the Hilbert space. The extension of the maximal symmetric generator of the semi-group is the self-adjoint generator of the unitary group.⁹ Hence, the dynamical mappings defined by the isometric semi-group can be thought of as the restriction of a family of Hamiltonian dynamical mappings to a subspace of the pure states.

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¹⁰ J. L. B. Cooper, *Ann. Math* 48, 827 (1947); *Proc. London Math Soc.* 50, 11 (1948).