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What is a Gauge Transformation in Quantum Mechanics?

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In classical theory, a physical state is an equivalence class under gauge transformations. Is the same true in quantum theory? The physical quantum states are the solutions of Dirac's quantum constraint equation. They cannot be constructed as equivalence classes under the "simple" gauge transformations generated by the Dirac constraints. However, we show here that they can be constructed as equivalence classes under suitably defined "complete" gauge transformations. The complete gauge transformations are generated by the action of the quantum constraints on arbitrary individual components of the state. [S0031-9007(98)06161-4]

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In classical mechanics, a gauge invariant state can be seen as an equivalence class of gauge-non-invariant states. Two gauge-non-invariant states are equivalent if there is a gauge transformation sending one into the other. In the canonical theory, the gauge transformations are generated by the first-class constraints. The same fails to be true in quantum mechanics: Dirac's quantum constraints C generate the gauge transformation $\psi \rightarrow e^{itC}\psi$ on the quantum states, but physical states cannot be seen as equivalence classes under the equivalence relation

$$\psi \sim e^{itC}\psi\,. \tag{1}$$

Rather, physical states are the states which are annihilated by the Dirac constraints [1].

We show in this Letter that one can see physical states as equivalence classes of gauge-non-invariant states in the quantum theory as well. But the equivalence relation is more complicated than (1). We call this alternative equivalence relation a "complete" quantum gauge transformation. Roughly, a complete quantum gauge transformation is defined as follows. $\phi \sim \psi$ if and only if there are states ρ_i and real numbers t_i such that

$$\psi = \sum_i \rho_i\,, \qquad \phi = \sum_i e^{it_iC}\rho_i\,. \tag{2}$$

That is, a complete gauge transformation is obtained by gauge transforming linear components independently. We show below that the space of the solutions of Dirac's constraints is (naturally identified with) the space of the equivalence classes defined by the equivalence relation (2).

Quantum gauge transformations in a finite dimensional Hilbert space.—Let us assume that we have a unitary representation U of a (gauge) group G in a Hilbert space $\mathcal{H}$. In this section we disregard all complications due to the infinite dimensionality of $\mathcal{H}$. The generators of the representation are the Dirac constraints, and the space of physical states $\mathcal{H}_{\rm Ph}$ is defined as the kernel of the Dirac constraints [1], namely, as the trivial representation of G in $\mathcal{H}$. Vectors in $\mathcal{H}_{\rm Ph}$ are gauge invariant, and represent physical states. A gauge-non-invariant state can roughly be seen as a state in a particular gauge. Physical predictions of a classical gauge theory are given by gauge invariant quantities; but in concrete calculations, we usually employ a gauge-non-invariant description—leaving the task of extracting the physical quantities at the end. It would be nice to be able to do the same in the quantum theory, namely, to work on $\mathcal{H}$ without recurring to $\mathcal{H}_{\rm Ph}$, keeping track of gauge equivalence. Therefore, the problem we pose here is to see if $\mathcal{H}_{\rm Ph}$ can be viewed as (is naturally isomorphic to) a space of equivalence classes in $\mathcal{H}$, under suitable gauge transformations generated by G.

Since $\mathcal{H}_{\rm Ph}$ is a linear subspace of H, the orthogonal projection π on $\mathcal{H}_{\rm Ph}$ provides a natural definition of quantum gauge equivalence in $\mathcal{H}$: $\phi \sim \psi$ if and only if

$$\pi(\phi) = \pi(\psi). \tag{3}$$

We have $\mathcal{H}_{\rm Ph} = \frac{\mathcal{H}}{\sim}$. Thus, our problem is to understand the precise relation between this equivalence and the transformations generated by U in $\mathcal{H}$. Can we interpret this equivalence as the possibility of being gauge transformed, as we do for the classical theory? More precisely, can we construct the equivalence relation ($\sim$) directly from U without having to solve for the invariant states first? Clearly, if there exists a $g \in G$ such that

$$\phi = U[g]\psi, \tag{4}$$

then $\phi \sim \psi$. However, the converse is not true in general. Namely, ϕ and ψ can be equivalent under (3) even if there is no $U[g]$ that maps one into the other. Therefore, the equivalence relation (3) is different than the equivalence relation (1).

To get some intuition on how this may come about, consider the following simple example. Let the group $U(1)$ act on R^3 by generating rotations around the z axis. (We consider here a real, rather than complex, Hilbert space, for simplicity.) The invariant subspace is the one-dimensional z axis. The equivalence classes under (3) are the planes $z = \text{const}$. On the other hand, the equivalence classes under (1) are the orbits of the action of the group, which are the circles ($z = \text{const}$, $x^2 + y^2 = \text{const}$), parallel to the $z = 0$ plane and centered on the z axis.

Clearly, it is the linear structure of quantum mechanics that differentiates gauge equivalence (being on the same z plane) from the fact of belonging to the same orbit (being on the same circle): Two distinct orbits on the same z plane are in the same gauge equivalence class.

This example suggests that two quantum states are quantum gauge equivalent not only if they can be transformed into each other by a finite rotation, but also if they can be decomposed into a linear combination of vectors which can be independently rotated into each other (it is easy to see that by rotating components independently, any two vectors on the same z plane can be transformed into each other). We make this intuition concrete as follows.

Theorem.—ψ and ϕ are equivalent [that is, (3) holds] if and only if there exist vectors $\rho_i \in \mathcal{H}$ and group elements $g_i \in G$ such that

$$\psi = \sum_i \rho_i, \qquad \phi = \sum_i U[g_i]\rho_i. \tag{5}$$

Demonstration.—To prove that (5) implies (3) is immediate: It suffices to notice that $\pi U[g] = \pi$. To prove the converse, we begin by proving that any vector ρ in the kernel K of π can be written as

$$\rho = \sum_i (U[g_i]\rho_i - \rho_i). \tag{6}$$

Let L be the space of all vectors that can be written as in (6). L is a linear subspace, it is invariant under $U[g]$ and is contained in K. Let S be the subspace of K orthogonal to L. S is a linear subspace, and it is invariant under $U[g]$ as well. A vector ρ in S cannot be U invariant because it is in K, therefore $\chi = U[g]\rho - \rho$ is different from zero. But since S is linear and U invariant, χ is also in S. But χ is also in L, by definition of L. Since L and S are orthogonal, ρ has to be zero. Therefore S is empty, $K = L$ and all vectors in K can be written as in (6). Now, if $\pi(\phi) = \pi(\psi)$, then $(\phi - \psi) \in K$; therefore, there are g_i and ρ_i such that

$$\phi - \psi = \sum_i (U[g_i]\rho_i - \rho_i). \tag{7}$$

It follows that

$$\phi - \sum_i U[g_i]\rho_i = \psi - \sum_i \rho_i \equiv \rho. \tag{8}$$

By adding ρ to both sums (with a corresponding $g =$ identity), we have (5), Q.E.D.

Thus, we can *define* the equivalence relation: $\phi \sim \psi$ if and only if there exist $\rho_i \in \mathcal{H}$ and $g_i \in G$ such that (5) holds. And we have

$$\mathcal{H}_{\rm Ph} = \frac{\mathcal{H}}{\sim}. \tag{9}$$

Intuitively, a quantum state is a linear quantum superposition of classical configurations (a wave function over configuration space). It is therefore reasonable that we may gauge transform each individual component of the superposition independently, without changing the gauge invariant quantum state.

We call the transformation $\psi \rightarrow U[g]\psi$ a "simple" quantum gauge transformation, and the transformation

$$\psi = \sum_i \rho_i \rightarrow \phi = \sum_i U[g_i]\rho_i \tag{10}$$

a complete quantum gauge transformation. We have proven that physical quantum states cannot be viewed as equivalence classes under simple quantum gauge transformations, but they can be viewed as equivalence classes under complete quantum gauge transformations.

Infinite-dimensional issues.—Let us sketch how the above is realized in a simple example of infinite-dimensional Hilbert space. Let $\mathcal{H}$ be the space $L_2[T^2]$ of functions $\psi(\alpha, \beta)$ on a two-torus, and let us have a single constraint $C = \iota \frac{\partial}{\partial \beta}$. We know what goes on in this case: The α variable is physical, the β variable is gauge. The physical information is contained in the α dependence of the state, while the β dependence is arbitrary. Two states must be gauge equivalent if they have, in a suitable sense, the same α dependence. Thus, arbitrarily "moving pieces of $\psi(\alpha, \beta)$ around in β" is a gauge transformation. The group G, however, acts on $\mathcal{H}$ by rotating states *rigidly* in the β direction: $U(\gamma)\psi(\alpha,\beta) = \psi(\alpha,\beta+\gamma)$. This is only a small fraction of the physical gauge equivalence. Simple gauge transformations are rigid displacements of the state in β; complete gauge transformations are arbitrary deformations of the state in the β direction. It is easy to see that, in this case, L is formed by all of the states such that $\int \psi(\alpha,\beta)d\beta = 0$, namely, by all of the β harmonics higher than zero. Indeed, harmonics higher than zero can all be set to zero with a complete gauge transformation of the form (5): It is sufficient to write the harmonic as the sum of two equal terms, and rotate one of the two by half a wavelength.

In infinite-dimensional spaces the well-known infinite subtleties of quantum mechanics may also appear. Zero can be in the continuum spectrum of the Dirac constraints and therefore physical states appear as generalized states. This happens, for instance, if in the example above we replace the two-torus with R^2. We have then to use continuum-spectrum techniques, such as Gel'fand triples [2] or something similar. In particular, $\mathcal{H}_{\mathrm{Ph}}$ is not a linear subspace of $\mathcal{H}$, but a linear subspace of a suitable closure $\overline{\mathcal{H}}$ of $\mathcal{H}$, which can be defined as the dual of a suitable dense subspace of $\mathcal{H}$.

In this case, the analysis of the previous section can be repeated with minor modifications, using $\overline{\mathcal{H}}$. U acts on $\overline{\mathcal{H}}$ by duality. $\mathcal{H}_{\mathrm{Ph}}$ is the U-invariant subspace of $\overline{\mathcal{H}}$. Let L be the subspace of $\overline{\mathcal{H}}$ formed by the vectors that can be written in the form (6), where now the sum may contain an infinite numbers of terms, and the required convergence is in $\overline{\mathcal{H}}$, not in $\mathcal{H}$. Consider $S = \frac{\overline{\mathcal{H}}}{\mathcal{H}_{\mathrm{Ph}} \oplus L}$. As before, it is easy to see that S is linear and U invariant. If ρ is a nonvanishing vector in S, it cannot be U invariant (because it would be in $\mathcal{H}_{\mathrm{Ph}}$) and $\chi = U[g]\rho - \rho$ is different from zero. But S is left invariant as well; therefore, $\chi \in S$ and not in L, but χ is also in L, by definition of L; therefore, S is empty and $\overline{\mathcal{H}} = \mathcal{H}_{\mathrm{Ph}} \oplus L$.

Notice that even if ψ and ϕ are in $\mathcal{H}$, in general the ρ_i's are in $\overline{\mathcal{H}}$ and not in $\mathcal{H}$. More precisely, the right-hand side of (7) is obviously in $\mathcal{H}$ if ψ and ϕ are; but when we split the sum into the two sums in (8), the individual sums need not converge in $\mathcal{H}$. Thus, ρ in (8) may be a generalized vector. Therefore we can still define $\mathcal{H}_{\mathrm{Ph}}$ as the space of the equivalence classes of vectors in $\mathcal{H}$ under the equivalence relation (5), but we must allow for decompositions in generalized vectors ρ_i as well.

However, the analysis above suggests that we can avoid the cumbersome introduction of $\overline{\mathcal{H}}$ and generalized vectors altogether. This follows from the fact that space L of the vectors that can be written in the form (6) is a proper subspace of $\mathcal{H}$. Thus, we can define L first, and construct the linear space $\mathcal{H}_{\mathrm{Ph}}$ as the space of the equivalence classes of vectors in $\mathcal{H}$, equivalent under the addition of vectors in L, namely, as $\frac{\mathcal{H}}{L}$. In other words, we can define the equivalence relation by (7) instead of by (5). This is done as shown below.

Given an infinite-dimensional Hilbert space $\mathcal{H}$ and a unitary representation U of a group G over it, we define L as the closed linear subspace of $\mathcal{H}$ formed by the vectors that can be written as

$$\rho = \sum_{i=1}^{\infty} (U[g_i]\rho_i - \rho_i). \tag{11}$$

We then call two states gauge equivalent if their difference is in L, and define

$$\mathcal{H}_{\mathrm{Ph}} = \frac{\mathcal{H}}{L}. \tag{12}$$

The space $\mathcal{H}_{\mathrm{Ph}}$ is defined in this way without recurring to generalized vectors or other extensions of $\mathcal{H}$. This space is naturally isomorphic to the space of generalized vectors that solve the Dirac constraints.

To clarify how this may happen, consider the following. In finite dimensions, if L is a proper subspace of $\mathcal{H}$, then $L_\perp$ the orthogonal complement of L (that is, the set of vectors orthogonal to L) is nontrivial, and

$$\mathcal{H} = L_\perp \oplus L. \tag{13}$$

We can thus identify $L_\perp$ with $\frac{\mathcal{H}}{L}$. In infinite dimensions, the orthogonal complement $L_\perp$ of a subspace L may be trivial (contain only the zero vector) even if L is smaller that $\mathcal{H}$. But $\frac{\mathcal{H}}{L}$ exists nevertheless, and it is naturally identifiable with the space of *generalized* vectors perpendicular to L. Gauge invariance of a generalized vector means being perpendicular to L. Therefore, if we construct $\mathcal{H}_{\mathrm{Ph}}$ by requiring gauge invariance (solving the Dirac constraints), we need generalized vectors. But if we construct $\mathcal{H}_{\mathrm{Ph}}$ as the space of the gauge equivalence classes, we may not need to introduce generalized states. We leave the analysis of this possibility for further work.

In conclusion, we have introduced the notion of "complete quantum gauge transformation." A complete gauge transformation is obtained by arbitrarily decomposing a vector in components and acting with the exponentiated constraints on each component independently. Namely, two vectors are gauge equivalent if Eq. (5) holds. We have shown that Dirac's physical state space $\mathcal{H}_{\mathrm{Ph}}$ can be obtained as the space of the equivalence classes of states, under complete quantum gauge transformations. Therefore, we suggest that the natural answer to the question in the title is provided by the complete gauge transformations.

In the classical Hamiltonian theory of constrained systems, one has to take two steps in order to reduce the full phase space Γ to the physical phase space Γ_{Ph}. First, solve the constraint; that is, find the constraint surface C in Γ. Second, factor away the gauge transformation; that is, define Γ_{Ph} as the space of the gauge orbits in C. Dirac showed that in the quantum theory a single step is sufficient: The physical states are the ones that solve the quantum constraints. Here we have shown that one can take this single step also by factoring away (complete) quantum gauge transformations. Thus, in the classical theory we find the physical states by solving the constraints *and* factoring away the gauge transformations. In the quantum theory we find the physical states by solving the constraints *or* factoring away the gauge transformations.

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