Quantum Canonical Transformations: Physical Equivalence of Quantum Theories

Arlen Anderson*
Blackett Laboratory
Imperial College
Prince Consort Road
London SW7 2BZ England

February 14, 1993

Abstract

Two quantum theories are physically equivalent if they are related, not by a unitary transformation, but by an isometric transformation. The conditions under which a quantum canonical transformation is an isometric transformation are given.

*arley@ic.ac.uk
One of the most powerful ways of solving a quantum theory is to make a canonical transformation to a simpler theory in different variables. Following Dirac[1, 2], there is a widespread belief that the unitary transformations are the analog of the classical canonical transformations in quantum theory. Quantum canonical transformations can however be defined without mentioning a Hilbert space structure, and they are in themselves neither unitary nor non-unitary. Furthermore, one finds that non-unitary transformations play an important role in the integrability of a theory[3].

Physically, one is often interested not only in solving a theory, but in finding when it is physically equivalent to another theory expressed in different variables. Two theories are physically equivalent if there is an isomorphism between their states which preserves the values of inner products, so that all physical amplitudes are the same. Certainly, two theories related by a unitary transformation are physically equivalent because a unitary transformation is defined as a linear norm-preserving isomorphism of a Hilbert space onto itself[4]. More generally, however, two theories are physically equivalent if they are related by an isometric transformation[4]: a linear norm-preserving isomorphism of one Hilbert space onto another.

A Hilbert space is a vector space together with an inner product satisfying certain conditions. Isometric transformations allow the inner product to change under the transformation. This freedom means that many non-unitary transformations define physically equivalent theories. Unitary equivalence has been exten-
sively studied from the standpoint of group representations[3]. Quantum canonical
transformations give a somewhat different perspective. This Letter will discuss the
conditions under which a quantum canonical transformation is an isometric trans-
formation. The discussion is made for the quantum mechanical case, but it is
anticipated that it can be generalized to field theory.

To allow for time-dependent transformations, the time $q_0$ and its conjugate
momentum $p_0$ ($[q_0, p_0] = i$) are adjoined to the usual canonical variables in phase
space. For notational convenience, the collection of extended phase space vari-
ables are denoted $(q, p)$, as if they were one-dimensional. The extension to higher
dimensions is straightforward.

Since quantum canonical transformations will be defined outside of a Hilbert
space structure, two unfamiliar definitions are made. First, the phase space vari-
ables $(q, p)$ are treated not as operators but as elements of an associative algebra
$\mathcal{U}$ containing all complex functions of $(q, p)$, consistent with the canonical com-
mutation relations, having Laurent expansions and their algebraic and functional
inverses (e.g. $(1 + q)^{-1}$, $\ln q$). Functions like $p^{-n}$ are well-defined in this alge-
bra. Second, when acting on functions on configuration space $\psi(q)$, the function
$C(q, p) \in \mathcal{U}$ has the representation $\hat{C}(\hat{q}, \hat{p})$, where $(\hat{q}, \hat{p}) \equiv (q, -i\partial_q)$. Since $\hat{C}$ is not
in general invertible as an operator, one takes the inverse in the algebra and then
represents it as an operator $(C^{-1})$. Operators involving $(p^{-1})$ are to be understood
in the sense of pseudo-differential operators[3]. For further discussion, see Ref. [3].

A quantum canonical transformation is defined[3, 7] to be a change of the phase
space variables \((q, p)\), induced by a function \(C(q, p) \in \mathcal{U}\),

\[
q \mapsto CqC^{-1} = q'(q, p),
\]

\[
p \mapsto CpC^{-1} = p'(q, p)
\]

which preserves the canonical commutation relations

\[
[q, p] = i = [q'(q, p), p'(q, p)].
\]

There is a clear analogy with the definition of a classical canonical transformation as a change of the (classical) phase space variables which preserves the Poisson bracket \(\{q_c, p_c\} = 1\). Note that this definition does not mention either Hilbert spaces or inner products. The quantum canonical transformations are neither unitary nor non-unitary.

For convenience, consider the case of non-relativistic quantum mechanics. The extension to relativistic quantum mechanics is immediate. The Schrödinger operator corresponds to a function \(\mathcal{H}(q, p) = p_0 + H(q_i, p_i, q_0)\) in \(\mathcal{U}\). The canonical transformation \(C\) transforms \(\mathcal{H}\) as

\[
\mathcal{H}'(q, p) = C\mathcal{H}(q, p)C^{-1} = \mathcal{H}(CqC^{-1}, CpC^{-1}).
\]

The solutions \(\psi'\) of \(\tilde{\mathcal{H}}'\psi' = 0\) then induce solutions \(\psi\) of \(\tilde{\mathcal{H}}\psi = 0\)

\[
\psi(q) = (C^{-1})^{\dagger}\psi'(q).
\]

Since no inner product has been specified, the transformation \((C^{-1})^{\dagger}\) acts on all solutions of \(\mathcal{H}'\), not merely the normalizable ones. There is some subtlety involving functions that lie in the kernels of \(\tilde{C}\) or \((C^{-1})^{\dagger}\), but it won’t be important.
for physical equivalence since an isometric transformation must be an isomorphism
between the states of the respective Hilbert spaces.

At this point, as we are interested in physical solutions, an inner product is
imposed on the solutions of $\mathcal{H}$

$$
\langle \phi | \psi \rangle_\mu \equiv \langle \phi | \mu(\tilde{q}, \tilde{p}) | \psi \rangle_1
$$

$$=
\int d\Sigma \phi^*(q) \mu(\tilde{q}, \tilde{p}) \psi(q),
$$

where the integration is over spatial configuration space. Physical solutions are
those which are normalized to either unity or the delta function. The “measure
density” $\mu(\tilde{q}, \tilde{p})$ may in general be operator valued and may involve the temporal
variables. This should not be surprising as the inner product for the Klein-Gordon
equation involves $\tilde{p}_0$.

When one makes a canonical transformation, in general the measure density
must transform to preserve the norm of states. Given a canonical transformation
$C$ from $\mathcal{H}$ to $\mathcal{H}'$ as in (3), the norm of states is preserved when

$$
\langle \psi | \psi \rangle_\mu = \langle (C^{-1})^\dagger \psi' | \mu | (C^{-1})^\dagger \psi' \rangle_1
$$

$$=
\langle \psi' | (C^{-1})^\dagger \mu(C^{-1})^\dagger \psi' \rangle_1
$$

$$=
\langle \psi' | \psi' \rangle_{\mu'}.
$$

The transformed measure density is

$$
\mu'(\tilde{q}, \tilde{p}) = (C^{-1})^\dagger \mu(\tilde{q}, \tilde{p})(C^{-1})^\dagger,
$$

or, in $\mathcal{U}$,

$$
\mu'(q, p) = C^{-1\dagger} C^{-1} \mu(CqC^{-1}, CpC^{-1}).
$$
Here, \((C^{-1})^\dagger\) is the “adjoint” of \((C^{-1})\) in the trivial measure density, \(\mu = 1\). From (7), one sees that the measure transforms as a function on \(\mathcal{U}\) multiplied by an inhomogeneous factor.

For functions of the spatial phase variables, the adjoint is computed by taking the complex conjugate and integrating by parts (assuming boundary terms to vanish—if they do not, the transformation is not a physical equivalence). The adjoint cannot be taken for \(p_0\) because the integration measure does not involve \(dq_0\). In some instances, a \(p_0\)-dependent factor in a canonical transformation only changes the time-dependence of the solutions in a unitary fashion. In this case, it can be allowed to act directly on the wave function and its effect will cancel between the two wave functions in the inner product. In other cases, canonical transformations involving \(p_0\) do not produce physically equivalent systems.

If the Hilbert space of the transformed system \(\mathcal{H}'\) has the measure given by (6) and is isomorphic to the original Hilbert space, the canonical transformation is isometric. The quantum theories defined by \(\mathcal{H}\) and \(\mathcal{H}'\) and their Hilbert spaces are then physically equivalent.

For isomorphisms of a Hilbert space onto itself, the measure density does not change. If the measure density is purely a function of the spatial coordinates, as it usually is in non-relativistic quantum mechanics, one finds from (7) the familiar condition for a unitary transformation: \(C^\dagger C = 1\), where \(C^\dagger = \mu^{-1}C^\dagger_1\mu\) is the adjoint in the measure density \(\mu\) of the Hilbert space.

An example will illustrate that (6) is sometimes used implicitly in common
practice. Consider the canonical transformation $C = e^{q^2/2}$ from the harmonic oscillator $H = p^2 + q^2$, to the operator for the Hermite polynomials $H' = p^2 + 2ipq + 1$. The harmonic oscillator energy eigenstates $\psi_n(q)$ are given in terms of the Hermite polynomials $H_n(q)$ by

$$\psi_n(q) = e^{-q^2/2}H_n(q).$$

(8)

The transformation is clearly an isomorphism, but the operator $\tilde{C}$ is not unitary because it is real. The harmonic oscillator energy eigenstates are normalized in the trivial measure $\mu = 1$. By (6), the transformation is an isometry and the theories are physically equivalent if the Hermite polynomials are normalized in the measure $\mu' = e^{-q^2}$. This is the familiar result.

A canonical transformation can fail to be an isometry in two ways. First, the transformation may not be an isomorphism. A canonical transformation or its inverse that involves a finite-order differential operator will have a non-trivial kernel. If the kernel of the transformation lies in one of the Hilbert spaces, the transformation is not an isomorphism. This often happens with raising and lowering or intertwining operators.

The simplest example is the canonical transformation given by the lowering operator $p$ for the Hermite polynomials. This transformation annihilates the ground state $\psi = 1$ as it steps all the eigenfunctions down by one. The mapping $p$ is not invertible on the space of Hermite polynomials. Such a situation can sometimes be handled by speaking of partial isometries, physical systems which are equivalent on a subsystem of states.
The second way that a canonical transformation can fail to be an isometry is if the inner product in the transformed Hilbert space does not have the measure \( (3) \), so that the norms of states are not preserved. If \( C \) involves a finite-order differential operator, the norm-preserving inner product will have an operator-valued measure density. In non-relativistic quantum mechanics, measure densities are almost exclusively coordinate-valued. If one does not use the norm-preserving inner product, the normalization of states must have changed during the transformation.

The simplest example is again given using the lowering operator for the Hermite polynomials. The measure density which preserves the norm of states after the transformation \( \psi = \psi' \) is \( \mu' = p e^{-q^2} \). If one uses the measure density \( \tilde{\mu}' = e^{-q^2} \) appropriate to Hermite polynomials, one finds an operator \( e^{q^2} p e^{-q^2} \) acting on one of the states in the inner product. The Hermite polynomials are eigenfunctions of this operator, so the form of the inner product is the same as it was originally but with a state-dependent renormalization factor (the eigenvalue). The norm of the states has changed. This is familiar because the recursion operator between normalized \( H_n \) depends on \( n \). This example is generic.

As a final example illustrating the broader application of isometric canonical transformations to physical equivalence than of unitary transformations, consider two harmonic oscillators of different frequency, \( \mathcal{H} = p_0 + p^2 + \omega^2 q^2 \) and \( \mathcal{H}' = p_0 + p^2 + \omega'^2 q^2 \). Perhaps unexpectedly, these are physically equivalent. Their spectra are different, so there can be no unitary transformation between them. The action of a canonical transformation \( C \) in \( (3) \) on the function \( \mathcal{H} \) corresponding
to the Schrodinger operator must be slightly generalized. Solutions of $\mathcal{H}'$ are still mapped to solutions of $\mathcal{H}$ if

$$\mathcal{H}' = DC\mathcal{H}C^{-1}$$

(9)

where $D$ is taken in the present instance to be a constant, but could more generally be a function of $q$ or any operator with a trivial kernel. The canonical transformation

$$C = e^{i\ln(\omega'/\omega)q_0p_0} e^{i\ln(\omega'/\omega)qp}$$

(10)

relates the two harmonic oscillators through (9) with the factor $D = \omega'/\omega$. The harmonic oscillator energy eigenstates of frequency $\omega$ are given by

$$\psi'_n = \left(\frac{\omega'}{\pi}\right)^{1/4} e^{-\omega'q^2/2} H_n(\omega'^{1/2}q) e^{-i(2n+1)\omega'q_0}. \quad (11)$$

The transformed solutions are

$$\psi_n = (C^{-1})^\dagger \psi'_n = \left(\frac{\omega}{\pi}\right)^{1/4} e^{-\omega q^2/2} H_n(\omega^{1/2} q) e^{-i(2n+1)\omega q_0}. \quad (12)$$

Note that the normalization constant did not change. This is because the measure density transforms by (6) to give

$$\mu' = e^{i\ln(\omega'/\omega)p_0q_0} e^{i\ln(\omega'/\omega)qp} = \left(\frac{\omega}{\omega'}\right)^{1/2}, \quad (13)$$

so that the normalization of states is preserved. (In computing the transformed measure density, the $p_0$ dependent part of $C$ is allowed to act on the states to change their time-dependence, and only the adjoint of the $p$ dependent term is taken.) Since the transformed measure is independent of $n$, it can be absorbed
into the definition of the wave function to make the measure in the inner product trivial. That two harmonic oscillators of different frequency should be physically equivalent should not be counter-intuitive. Note that they are present in isolation so that nothing is setting a time-scale. If one had a single system containing two harmonic oscillators of different frequency, there would not be a canonical transformation that would make both frequencies the same.

In summary, the definition of a general canonical transformation does not involve the specification of a Hilbert space. Canonical transformations therefore are not of themselves unitary or non-unitary. Two theories are physically equivalent if the canonical transformation between them is an isometric transformation. Upon specifying the initial and final Hilbert spaces, a canonical transformation is an isometry if it is an isomorphism and the measure densities in the inner products defining the Hilbert spaces are related by (6).

I would like to thank J. Friedman and C.J. Isham for discussions of this work.

References

[1] P. A. M. Dirac, The Principles of Quantum Mechanics, 4th. ed., (Oxford Univ. Press: Oxford, 1958).

[2] See, e.g., M. Moshinsky and C. Quesne, J. Math. Phys. 12 1772 (1971); P.A. Mello and M. Moshinsky, J. Math. Phys. 16 2017 (1975); J. Deenen, M. Moshinsky, and T.H. Seligman, Ann. Phys. (NY) 127, 458 (1980).
[3] A. Anderson, Imperial College preprint Imperial-TP-92-93-19/hep-th-9302nnn (1993).

[4] N. Dunford and J.T. Schwartz, *Linear Operators, Part 1*, (Wiley: New York, 1963).

[5] G.W. Mackey, *Unitary Group Representations in Physics, Probability, and Number Theory*, (Benjamin/Cummings Publ. Co.: Reading, MA, 1978); A. Wawrzyńczyk, *Group Representations and Special Functions*, (D. Reidel Publ. Co.: Dordrecht, 1984).

[6] L. Hörmander, *The Analysis of Linear Partial Differential Operators, vol. III*, (Springer-Verlag: Berlin, 1985).

[7] M. Born, W. Heisenberg and P. Jordan, Ztschr. f. Phys. 35, S. 557 (1926); W. Heisenberg, Math. Ann. 95, 683 (1926).