Quantum Canonical Transformations and Integrability: Beyond Unitary Transformations

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Abstract

Quantum canonical transformations are defined in analogy to classical canonical transformations as changes of the phase space variables which preserve the Dirac bracket structure. In themselves, they are neither unitary nor non-unitary. A definition of quantum integrability in terms of canonical transformations is proposed which includes systems which have fewer commuting integrals of motion than degrees of freedom. The important role of non-unitary transformations in integrability is discussed.

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Unitary transformations are a cornerstone of quantum theory. Despite Dirac’s assertion, however, they fall short of being the analog of the classical canonical transformations. Quantum canonical transformations can be defined without specifying a Hilbert space structure, and in themselves they are neither unitary nor non-unitary.

Canonical transformations play essentially three distinct roles: in evolution, in physical equivalence and in integrability. Evolution is described by unitary canonical transformations—this is the source of the analogy between unitary and classical canonical transformations. Physically equivalent theories are related by isometric transformations, of which the unitary transformations are an important subclass. This Letter will define general quantum canonical transformations and will illustrate the importance of non-unitary transformations for quantum integrability.

Using quantum canonical transformations, the wave equation for a system of interest can be transformed to a simpler equation whose general solution is known. Because the transformation is defined outside the Hilbert space structure of the theory, it transforms all solutions of the wave equation, not just the normalizable ones. As well, the norm of states may not be preserved by the transformation.

The argument is made below that a general quantum canonical transformation can be decomposed as a product of elementary canonical transformations of known behavior, as conjectured by Leyvraz and Seligman. Each of the elementary canonical transformations corresponds to a familiar tool used in solving differential
equations: extracting a function of the independent variables from the dependent variable, change of independent variables, and Fourier transform. The significance of this is that the procedure of solving a linear differential equation is systematized by the canonical transformations. More sophisticated tools, including raising and lowering operators\[6\], intertwining operators\[7, 8\], and differential realizations of Lie algebras\[9\], are easily shown to be canonical transformations in this sense. Few of these are unitary transformations, yet together they solve nearly all known integrable models in quantum mechanics.

As this approach takes place outside of a Hilbert space context, there are two unfamiliar distinctions that must be made\[10\]. First, the non-commuting phase space variables \((q, p)\) are to be understood not as operators but as elements of an associative algebra \(\mathcal{U}\) generated by complex functions\[11\] of \(q, p, q^{-1}, p^{-1}\), consistent with the canonical commutation relations. As elements of this algebra, functions like \(p^{-n}\) are well-defined. The variables \((q, p)\) have a representation as operators \((\hat{q}, \hat{p}) \equiv (q, -i\partial_q)\) acting on functions \(\psi(q)\) on configuration space. These are not to be thought of as self-adjoint operators in the standard inner product because no Hilbert space has been specified (and in particular the functions \(\psi(q)\) need not be square-integrable).

Functions \(C(q, p) \in \mathcal{U}\) are represented by operators \(\hat{C}(\hat{q}, \hat{p})\). Operators involving \((p^{-1})\) are to be understood in the sense of pseudo-differential operators\[12\]. To avoid technical detail, the domains of operators are not given, but are to be inferred from their behavior. There is a subtlety in the correspondence of functions
in $\mathcal{U}$ and their representation as operators: the operator $(C^{-1})^\dagger$ corresponding to $C^{-1}$ is not always inverse to $\hat{C}$ because the kernels of $\hat{C}$ or $(C^{-1})^\dagger$ may be non-trivial. While this prevents one from rigorously speaking of the operator $\hat{C}^{-1}$, except when $\hat{C}$ is invertible, by using $(C^{-1})^\dagger$, one effectively defines the inverse for all functions lying outside the kernels of the respective operators.

To allow for time-dependent transformations, it is useful to extend the phase space to include time $q_0$ and its conjugate momentum $p_0$, with $[q_0, p_0] = i$. For notational convenience, let $(q, p)$ denote all of the extended phase space variables: equations will be given as if $(q, p)$ were one-dimensional; the extension to higher dimensions is straightforward.

A classical canonical transformation is a change of the classical phase space variables $(q_c, p_c) \mapsto (q'_c(q_c, p_c), p'_c(q_c, p_c))$ which preserves the Poisson bracket $\{q_c, p_c\} = 1 = \{q'_c, p'_c\}$. A general quantum canonical transformation may be defined in direct analogy as a change of the (non-commuting) phase space variables which preserves the Dirac bracket

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

These transformations are generated by an arbitrary complex function $C(q, p) \in \mathcal{U}$ (cf. [13])

$$CqC^{-1} = q'(q, p), \quad CpC^{-1} = p'(q, p).$$

The $C$ producing a given pair $(q', p')$ is unique (up to a multiplicative constant). Note that factor ordering is built into the definition of the canonical transformation in the ordering of $C$. No Hilbert space is mentioned in this definition.
The Schrödinger operator corresponds to the function $\mathcal{H}(q, p) = p_0 + H(q, p, q_0)$ in $\mathcal{U}$. The canonical transformation $C$ transforms this as

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

(Generalizing the notion of canonical transformation, one could consider inhomogeneous transformations $\mathcal{H}' = D\mathcal{H}C^{-1}, D \in \mathcal{U}; D = 1$ is assumed here.) Solutions of $\mathcal{H}'\psi' = 0$ induce solutions of $\tilde{C}\mathcal{H}(C^{-1})\psi' = 0$. If the kernel of $\tilde{C}$ is trivial, then

$$\psi = (C^{-1})\psi'$$

are solutions of $\mathcal{H}$. Note that since no inner product has been specified, the transformation $(C^{-1})\tilde{}$ acts on all solutions of $\mathcal{H}'$, not merely the normalizable ones. If $\ker (C^{-1})\tilde{}$ (or $\ker \tilde{C}$) is non-trivial, then additional canonical transformations between $\mathcal{H}$ and $\mathcal{H}'$ may be needed to construct all the solutions of $\mathcal{H}$. The uniqueness of the transformation $C$ is discussed below.

When the kernel of $\tilde{C}$ is non-trivial, the situation is less simple and requires further discussion. In this case, there may be solutions $\psi'$ of $\mathcal{H}'$ which by (4) produce a $\psi$ which is not a solution of $\mathcal{H}$, but instead lead to

$$\psi'' = \mathcal{H}\psi,$$

where

$$\psi'' \in \ker \tilde{C}.$$

To illustrate the problem in a simple case, consider $\mathcal{H} = p^3$, $\mathcal{H}' = p^3$. Clearly, $C = p$ is a canonical transformation, $C\mathcal{H}C^{-1} = \mathcal{H}'$. Consider the solution $\psi' = q^2$.
of $\tilde{H}'\psi' = 0$. By (4), this gives $\psi = (p^{-1})\psi' = iq^3/3$. This is not a solution of $\tilde{H}$: $\tilde{H}\psi = -2 \notin \ker \tilde{C}$. One has $\hat{p}\psi = q^2 = \psi'$ so that $\tilde{C}$ is invertible on the solution $\psi$, so this is not the source of the problem.

The problem is that when $\ker \tilde{C}$ is non-trivial, the transformation $(C^{-1})_\tilde{C}$ can take one outside the solution space of $\tilde{H}$. To deal with this, one must always check that $\tilde{H}\psi = 0$ for candidate $\psi = (C^{-1})_\tilde{C}\psi'$. If $\psi$ is not a solution, it has a decomposition $\psi = \psi_s + \psi_n$, as the sum of a solution $\psi_s$ and a non-solution $\psi_n$. If the intersection of $\ker \tilde{C}$ and $\ker (\tilde{H}^{-1})_\tilde{C}$ is empty, then $\tilde{H}$ is invertible on $\psi_n$. Thus, one may remove it from $\psi$ by the projection

$$\psi_s = (1 - (\tilde{H}^{-1})_\tilde{C}\tilde{H})\psi.$$  

If $\ker \tilde{C} \cap \ker (\tilde{H}^{-1})_\tilde{C} \neq \emptyset$, one must work harder. A completely general method of handling the non-trivial kernel of $\tilde{C}$ is not yet worked out.

Consider the uniqueness of the canonical transformation $C$ between $\mathcal{H}$ and $\mathcal{H}'$. A symmetry of $\mathcal{H}$ is a transformation $S_\lambda$ such that $S_\lambda \mathcal{H} S_\lambda^{-1} = \mathcal{H}$. The symmetries of $\mathcal{H}$ form a group. If $\mathcal{H}$ has a symmetry $S_\lambda$ and $\mathcal{H}'$ a symmetry $S'_\mu$, then the function $S'_\mu^{-1}CS_\lambda$ is also a canonical transformation from $\mathcal{H}$ to $\mathcal{H}'$. Conversely, if $C_a$ and $C_b$ are two canonical transformations from $\mathcal{H}$ to $\mathcal{H}'$, then $C_b^{-1}C_a$ is a symmetry of $\mathcal{H}$ and $C_aC_b^{-1}$ is a symmetry of $\mathcal{H}'$. This implies that the collection $\mathcal{C}$ of canonical transformations from $\mathcal{H}$ to $\mathcal{H}'$ are given by one transformation $C$ between them and the symmetry groups of $\mathcal{H}$ and $\mathcal{H}'$.

An observable (integral of motion) $A$ is a function in $\mathcal{U}$ which commutes with $\mathcal{H}$, $[A, \mathcal{H}] = 0$. Since canonical transformations preserve the commutation relations,
they induce transformations on the observables of a theory. The observables $A$ which commute with $\mathcal{H}$ are obtained from the $A'$ that commute with $\mathcal{H}'$ by

$$A = C^{-1}A'C.$$  \hspace{1cm} (6)

The eigenvalues of a complete set of commuting observables are often used to characterize quantum states. The observables which characterize the states of $\tilde{\mathcal{H}}$ are thus induced from those which characterize the states of $\mathcal{H}'$. Suppose that $\mathcal{H}'$ has a complete set of commuting observables. Then if $\tilde{C}$ is invertible, this set is transformed to a complete set for $\mathcal{H}$. This is the familiar situation that one is accustomed to call “integrable”: $\mathcal{H}$ has a complete set of commuting observables.

An unexpected form of integrability is possible in the case that more than one canonical transformation is needed to obtain all the solutions of $\tilde{\mathcal{H}}$. This may happen if $\tilde{C}$ is not invertible. Suppose that two canonical transformations $C_1$ and $C_2$ suffice to obtain all the solutions of $\tilde{\mathcal{H}}$. By assumption, there are solutions $\psi_1 = (C_1^{-1})\tilde{\psi}'_1$ of $\tilde{\mathcal{H}}$ which cannot obtained from any solution $\psi'_2$ of $\mathcal{H}'$ using $(C_2^{-1})\tilde{\psi}'$. For example, the state of $\mathcal{H}'$ that should correspond to $\psi_1$ may lie in ker$(C_2^{-1})\tilde{\psi}'$, or possibly $\psi_1 \in \ker \tilde{C}_2$. Similarly, there are solutions $\psi_2 = (C_2^{-1})\tilde{\psi}'_2$ which cannot be obtained using $(C_1^{-1})\tilde{\psi}'$. Together, however, all solutions of $\mathcal{H}$ are encompassed by solutions of the form $\psi_1$ and $\psi_2$.

Let $A'_k$ denote a complete set of commuting observables which characterize the states of $\mathcal{H}'$. Two sets of observables $A_{1k}$ and $A_{2k}$ are obtained from $A'_k$,

$$A_{1j} = C_1A'_jC_1^{-1}, \quad A_{2k} = C_2A'_kC_2^{-1}. \hspace{1cm} (7)$$
In general, $A_{1j}$ and $A_{2k}$ will not commute for all $j, k$. The result is that while all the states of $\mathcal{H}$ have been constructed from those of $\mathcal{H}'$, the states of $\mathcal{H}$ are not characterized by a single complete set of commuting observables. Instead, the states $\psi_1$ and $\psi_2$ are characterized by different sets of commuting observables. This is a more general form of integrability than has been traditionally considered. In a system of this kind having $n$ degrees of freedom, when considering all states of the system, there would appear to be fewer than $n$ quantum integrals of the motion (observables). On suitably restricted subsets of states, however, there would be different collections of $n$ integrals.

Consider now the construction of canonical transformations. Classically, the infinitesimal generating functional $F(q_c, p_c)$ generates the finite canonical transformation \[ u'(q_c, p_c) = \exp(\epsilon v_F)u(q_c, p_c). \] (8)

where $v_F = F_{,q_c}\partial_{q_c} - F_{,p_c}\partial_{p_c}$ is the Hamiltonian vector field generated by $F$. The algebra of the canonical group is

\[ [v_F, v_G] = -v_{\{F,G\}}, \] (9)

and it is generated by the Hamiltonian vector fields obtained from $F \in \{h(q_c), h(q_c)p_c, h(p_c), h(p_c)q_c\}$. In principle then a general classical canonical transformation can be expressed as a product of finite transformations with these $v_F$.

Quantum mechanically, each of these classical transformations has a quantum implementation as $C = e^{iF}$ (note that $F$ is in general complex). Introducing the operation $I$ which interchanges the coordinate and momentum, $(q, p) \mapsto (-p, q)$,
the transformations which are nonlinear in the momentum can be expressed in terms of the other two. There are then three elementary canonical transformations(cf. [13]):

1) similarity (gauge) transformations, $C = e^{-f(q)}$

\[(q, p) \mapsto (q, p - if, q), \quad \psi'(q) = e^{-f(q)}\psi(q) \quad (10)\]

2) point canonical transformations, $C = P_{f(q)}$

\[(q, p) \mapsto (f(q), \frac{1}{f(q)}p), \quad \psi'(q) = \psi(f(q)) \quad (11)\]

and, 3) interchange, $C = I = (2\pi)^{-1/2} \int_{-\infty}^{\infty} dq e^{iqp'}$

\[(q, p) \mapsto (-p', q'), \quad \psi'(q') = I\psi(q) \quad (12)\]

The point canonical transformation is denoted by $P_{f(q)}$ because in general a finite product of terms of the form $\exp(ig(q)p)$ is required to represent such a transformation[17]. The transformations non-linear in the momentum are the composite elementary transformations:

4) $C = e^{-f(p)} = I e^{-f(q)}I^{-1}$

\[(q, p) \mapsto (q + if, p), \quad \psi'(q) = e^{-f(p)}\psi(q) \quad (13)\]

and, 5) $C = P_{f(p)} = IP_{f(q)}I^{-1}$

\[(q, p) \mapsto (\frac{1}{f, p}q, f(p)), \quad \psi'(q') = P_{f(p)}\psi(q) = (f^{-1}(p), p)\exp(if^{-1}(\hat{p})q')\psi(q)|_{q=0}. \quad (14)\]
It is important to emphasize that all functions are complex and may have zeroes or singularities. All expressions are ordered as written. The functions in the transformations may be many-variable. Since coordinates and momenta of differing index commute, a variable participates only as a constant parameter in any transformation which does not involve its conjugate.

Since a general classical canonical transformation can be expressed as a product of elementary canonical transformations, one expects that the same is true for quantum canonical transformations. This is equivalent to the assertion that any function $C(q, p)$ can be decomposed as a product of the elementary canonical transformations. There are functions $C$ which cannot decomposed into a finite product, and their action on a wavefunction cannot be realized explicitly.

This motivates the following definition of quantum integrability:

Definition. A quantum system $\mathcal{H}(q, p)$ is integrable (in the sense of homogeneous canonical transformations) if its general solution $\psi$ can be obtained from arbitrary time-independent functions $\psi^{(0)}$ using a collection of finitely decomposable canonical transformations $C_{\lambda} \in C$ which trivialize the wave operator

$$C_{\lambda} \mathcal{H}(q, p)C_{\lambda}^{-1} = p_0.$$  \hspace{1cm} (15)

Note that the $C_{\lambda}$ can be expressed as $CS_{\lambda}$ where $C$ is a particular canonical transformation to triviality and $S_{\lambda}$ is a symmetry of $\mathcal{H}$. If $A'_k$ are a complete set of commuting observables for $\mathcal{H}' = p_0$, then $A_{k\lambda} = C_{\lambda}A'_kC_{\lambda}^{-1}$ are sets of commuting
observables for $\mathcal{H}$ for each $\lambda$. The $A_{k,\lambda}$ may not commute for different $\lambda$. As discussed above, the system is nevertheless integrable, even though there is not a single set of commuting observables which serves to characterize all states of $\mathcal{H}$.

The condition of finite decomposability is necessary to have explicit representations for the solutions of $\mathcal{H}$. It raises the question of characterizing the class of Hamiltonians that can solved with a finite number of elementary transformations. This is reminiscent of the basic question addressed by Galois theory of which polynomials can be factored using a finite combination of the operations of addition, subtraction, multiplication, division and the taking of $n^{th}$ roots. Just as there are polynomials whose roots cannot be expressed in terms of a finite combination of the algebraic operations, one expects there are equations which cannot be solved by a finite number of elementary canonical transformations.

Having established the basic formalism, consider some illustrative examples. The time-independent Schrödinger equation, with $\mathcal{H} = p_0 + H(q_i, p_i)$, is clearly trivialized by $C = e^{iH(q_0 - t)}$ (where $t$ is a constant). In general, this is not an elementary transformation, and its action on the wavefunction is not immediately evident. By finding a (finitely decomposable) canonical transformation $\tilde{C}$ such that, say, $\tilde{C}H\tilde{C}^{-1} = p$, the action of $C$ is determined because

$$e^{iH(q_0 - t)} = \tilde{C}^{-1} e^{i\tilde{p}(q_0 - t)} \tilde{C}$$

is now a finite product of elementary canonical transformations. Applying the operator representation of this to $\delta(q - q')$, one can compute the propagator $K(q, q_0 | q', t)$. 

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This procedure may be used in general to simplify functions of operators. Consider the one-dimensional point canonical transformation \( e^{iag(q)p} \). Let \( G(q) = \int dq/g(q) \). For \( C = P_{G(q)} \), one has \( CpC^{-1} = g(q)p \). The action of \( e^{iag(q)p} \) on \( q \) is then computed

\[
\exp(iag(q)p)q \exp(-iag(q)p) = Ce^{iap}C^{-1}qCe^{-iap}C^{-1} = G^{-1}(G(q) + a).
\] (17)

This result is found by a more laborious method in [16].

Canonical transformations involving polynomial functions of \( p \) are non-unitary in inner products with coordinate-valued measure density[3]. As they underlie raising and lowering operators, the recursion operators for the special functions, intertwining and Lie algebraic transformations, they are undeniably important in the solution of many problems. As an illustration, consider the Darboux transformation[8, 18] from a Hamiltonian \( H_0 = p^2 + V_0 \) to another \( H_1 = p^2 + V_0 - 2g, q \), where \( g \) satisfies the Ricatti equation \( g, q + g^2 = V_0 + \lambda \). The canonical transformation from \( H_0 \) to \( H_1 \) is \( C = \exp(\int gdq)p \exp(-\int gdq) \). The key step in the transformation is that performed by \( p \) which transforms

\[
q \mapsto q - \frac{i}{p} = pq \frac{1}{p}.
\] (18)

This has the remarkable property

\[
g(q - \frac{i}{p}) = pg(q)\frac{1}{p} = g(q) - ig(q)_q \frac{1}{p}.
\] (19)

The Taylor expansion of \( g \) terminates at the first term; classically, there would be an infinite series.
From (10)-(12), it is clear as discussed in the introduction that the elementary canonical transformations correspond to the standard tools used in the solution of differential equations. The discovery and implementation of transformations to solve an equation is made more transparent when looked at from the perspective of canonical transformations. The practical gain is largely through a reduction in the technical demands of implementing a trial transformation.

The integrability of a quantum system by (15) corresponds to the existence of a sequence of standard manipulations which solve the wave equation. This notion of integrability is different than the standard one of the existence of a complete set of commuting observables. The possibility exists that all the solutions of a Hamiltonian can be found using canonical transformations, but there will not be a single complete set of commuting observables valid for all states. Rather there will be collections of commuting observables which apply to different sets of states.

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