Quantum canonical transformations are defined algebraically outside of a Hilbert space context. This generalizes the quantum canonical transformations of Weyl and Dirac to include non-unitary transformations. The importance of non-unitary transformations for constructing solutions of the Schrödinger equation is discussed. Three elementary canonical transformations are shown both to have quantum implementations as finite transformations and to generate, classically and infinitesimally, the full canonical algebra. A general canonical transformation can be realized quantum mechanically as a product of these transformations. Each transformation corresponds to a familiar tool used in solving differential equations, and

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1   Introduction

Canonical transformations are a powerful tool of classical mechanics whose strength has not been fully realized in quantum mechanics. Canonical transformations are already widely used, at least implicitly, because as Dirac[1] and Weyl[2] emphasized the unitary transformations are canonical. Aside from the linear canonical transformations, which have been well understood for many years[3], comparatively little work (but see, e.g., [4, 5, 6]) has been done directly on quantum canonical transformations as nonlinear changes of the non-commuting phase space variables. Progress has been inhibited because of the mistaken belief that quantum canonical transformations must be unitary.

Classically, a canonical transformation is a change of the 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 $\{q_c, p_c\} = 1 = \{q'_c, p'_c\}$. Born, Heisenberg, and Jordan[7] propose as the natural definition of a quantum canonical transformation: a change of the non-commuting phase space variables

$$q \mapsto q'(q, p), \qquad p \mapsto p'(q, p), \tag{1}$$

which preserves the Dirac bracket (canonical commutation relations)

$$[q, p] = i = [q'(q, p), p'(q, p)]. \tag{2}$$

Such a transformation is implemented by a function $C(q, p)$ such that

$$q'(q, p) = CqC^{-1}, \qquad p'(q, p) = CpC^{-1}. \tag{3}$$

This definition applies at the purely algebraic level, and no Hilbert space or inner product need be mentioned. As a consequence, the transformation is itself neither unitary nor non-unitary. The immediate implication is that quantum canonical transformations may be non-unitary, a generalization beyond Dirac's and Weyl's consideration.

Canonical transformations serve three primary purposes: for evolution, to prove physical equivalence, and to solve a theory. Classically, these blur together. Quantum mechanically, however, they are distinct. Evolution is produced by unitary transformations[1, 2]. Physical equivalence is proven with isometric transformations, which extend the definition of unitary transformations to norm-preserving isomorphisms between different Hilbert spaces[8]. (It is useful to distinguish unitary and isometric because for many physicists the working definition of a unitary transformation U is $U^{\dagger}U = 1$, and this is not true of isometric transformations.) Solution of a theory is accomplished with general canonical transformations and may involve non-unitary transformations[9].

Mello and Moshinsky[4] raise three issues concerning the definition (1) of a quantum canonical transformation. First, the ordering of $q'(q, p)$ and $p'(q, p)$ must be given, so that they are well-defined. Second, when the transformation is represented by operators,

inverse and fractional powers of differential operators may appear, and these must be defined. Third, the transformation may be non-unitary, and the sense of this must be understood. This paper addresses these concerns.

A quantum phase space is introduced which consists of pairs of canonically conjugate elements of a non-commutative algebra $\mathcal{U}$ constructed from the phase space variables q, p. Objects like the Hamiltonian which are ordered combinations of q, p are elements of $\mathcal{U}$. Each element of $\mathcal{U}$ defines a canonical transformation, so $\mathcal{U}$ may be identified as the quantum canonical group. It is assumed to be a topological transformation group which acts transitively on itself by the adjoint action. Expressions like $p^{-\alpha}$ (α an arbitrary complex number) are well-defined as elements of $\mathcal{U}$. Because the canonical commutation relations are imposed as relations on $\mathcal{U}$, every function in the algebra has a well-defined ordering. The quantum phase space is thus defined algebraically without specifying an inner product or Hilbert space structure—canonical transformations made upon it preserve the quantum structure of the canonical commutation relations, but these transformations are neither unitary nor non-unitary.

The phase space variables (q, p) are represented as operators $(\check{q}, \check{p}) \equiv (q, -i\partial_q)$ which act on functions $\psi(q)$ on configuration space, again without specifying the Hilbert space structure. Inverse and fractional powers are understood in a sense analogous to that of pseudo-differential operators[10]. The ordering implicit in elements of $\mathcal{U}$ gives a well-defined ordering to the corresponding quantum operators. Since the operators are defined outside of a Hilbert space, they define a transformation on all solutions of the Schrödinger equation, including non-normalizable ones.

Once the Hilbert space of physical states is specified, one may find that the kernel of a particular canonical transformation lies in the Hilbert space or that the normalization of states changes under the transformation. In these cases, the canonical transformation is non-unitary, but nevertheless it may have proven useful in constructing the explicit representation of solutions of the Schrödinger equation.

Classically, a theory is solved with canonical transformations by transforming the Hamiltonian to a simpler one whose equations of motion can be solved. The implementation of this same program quantum mechanically is the most significant application of the approach to quantum canonical transformations described here and will be the focus. It will be shown that a general quantum canonical transformation can be constructed as a product of elementary canonical transformations of known behavior, as conjectured by Levyraz and Seligman[5]. These elementary canonical transformations each correspond to a familiar tool used in solving differential equations: change of variables, extracting a function of the independent variables from the dependent variable, and Fourier transform. The procedure of solving a differential equation is systematized by the use of the elementary canonical transformations. More sophisticated tools for solving differential equations, including raising and lowering operators[11], supersymmetry[12], intertwining

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operators[13, 14], and Lie algebraic methods[15], may also be shown to be canonical transformations.

The quantum canonical transformations provide a unified approach to the integrability of quantum systems. One may define as quantum integrable ("in the sense of canonical transformations") those problems whose general solution can be constructed as a finite product of elementary canonical transformations. In view of the fact that the standard tools for integrating differential equations are among the canonical transformations, most if not all of the known soluble equations are in this class.

The unifying nature of the canonical transformations is a consequence of the size of the canonical group. The canonical group provides the maximum freedom to transform the form of a differential equation while preserving the relation between the derivative and the coordinate. The approach of Lie to the solution of differential equations involves constructing symmetries that transform an equation into itself. These finite dimensional Lie groups are subgroups of the canonical group. Generalized symmetries, which preserve the broad form of an equation, say that it remain a second order derivative plus a potential (such as appears in the Lax formulation of the Korteweg-deVries equation), give rise to infinite-dimensional symmetry groups whose algebras are Kac-Moody algebras. These are subgroups of the canonical group as well.

The outline of the paper is as follows. The treatment begins with the definition of the quantum phase space and the algebra $\mathcal{U}$ (Section 2.1). An effort is made to be precise about the definition of $\mathcal{U}$ as this determines the class of functions that may be used for making canonical transformations. Next, the elements of $\mathcal{U}$ are represented as operators acting on functions on configuration space (Section 2.2). The definition of a quantum canonical transformation is then reviewed, and some basic properties established (Section 2.3). The conditions under which a canonical transformation defines a physical equivalence are found (Section 2.4).

This is followed by a discussion of classical infinitesimal canonical transformations. Three elementary canonical transformations are introduced, and two additional composite elementary transformations are constructed. It is shown that, classically, the infinitesimal forms of these transformations generate the full algebra of canonical transformations. The inference is drawn that in principle by using their quantum implementations, any quantum canonical transformation can be made (Section 2.5). Next, the quantum implementation of the elementary canonical transformations is given. An example illustrating their use is given by computing the exponential of the infinitesimal generator of point canonical transformations (Section 2.6).

The next section is devoted to examples. First, the linear canonical transformations are constructed as products of elementary transformations (Section 3.1). The free particle and the harmonic oscillator are then done to illustrate various aspects of the use of canonical transformations (Sections 3.2-3.4). Of note is the solution of the time-dependent har-

monic oscillator by an approach which suggests that many time-independent integrable potentials can be generalized to contain time-dependent parameters without sacrificing integrability (Section 3.5). The first order intertwining operator is shown to be a canonical transformation; this allows the construction of the recursion relations and Rodrigues' formulae for all equations that are essentially hypergeometric (Section 3.6). An example involving a form of Bessel's equation is done to emphasize the difference between the classical and quantum canonical transformations which simplify a Hamiltonian to a given one (Section 3.7). Finally, the problem of a particle propagating on a higher-dimensional sphere is solved as an illustration of the use of intertwining operators as canonical transformations (Section 3.8).

Readers primarily interested in applications may focus on the sections giving the definition of quantum canonical transformations (Sec. 2.3) and the implementation of the elementary canonical transformations (Sec. 2.6) before moving to the examples of Sec. 3.

2   Formal aspects

2.1   The Quantum Phase Space

Before discussing quantum canonical transformations, it is important to define the space on which they will act, that is, the quantum phase space. To set the stage, consider the classical phase space for an unconstrained system of n degrees of freedom. Classically, the phase space is the vector space R^{2n} with coordinates $(q_1, \ldots, q_n, p_1, \ldots, p_n)$. The phase space can be extended to include time q_0 and its conjugate momentum p_0[16]. The Hamiltonian $H(q_1, \ldots, q_n, p_1, \ldots, p_n, q_0)$ is a function on the extended phase space, as are all possible observables, such as the position of the center of mass, the total angular momentum, the momentum of the kth degree of freedom, etc. On the phase space, there is a symplectic form $\sum_{k=0}^{n} dq_k \wedge dp_k$ which is reflected in the Poisson bracket of functions on phase space

$$\{f, g\} = \sum_{k=0}^{n} \partial_{q_k} f \partial_{p_k} g - \partial_{p_k} f \partial_{q_k} g.$$

A canonical transformation is a change of coordinates on extended phase space which preserves the symplectic form, or equivalently, the Poisson bracket relations.

Quantum mechanically, there is a parallel structure but with several crucial differences. The phase space variables $\{q_k\}$, $\{p_k\}$ ($k = 0, \ldots, n$) are members of a non-commutative algebra $\mathcal{U}$. As such, they cannot be thought of as coordinates on a vector space in the usual sense. Instead the parallel to the classical case is drawn one level higher between classical observables and elements of $\mathcal{U}$. Broadly speaking, the elements of $\mathcal{U}$ are sums of ordered products of the $\{q_k\}$, $\{p_k\}$ (and their algebraic inverses $\{q_k^{-1}\}$,

$\{p_k^{-1}\}$) which may be expressed $f<q_0, \ldots, q_n, p_0, \ldots, p_n>$. Two expressions related by repeated application of the canonical commutation relations are equivalent and represent the same element in $\mathcal{U}$. Objects like the quantum Hamiltonian are the analog of the classical observables. The $\{q_k\}$, $\{p_k\}$ act in a sense as coordinates as they label the elements of $\mathcal{U}$ with respect to a set of preferred elements, namely themselves. The quantum phase space $\mathcal{M}$ is defined to be the set of canonically conjugate quantum variables

$$\mathcal{M} = \{(\{x_j\}, \{p_{x_k}\}) \in \bigoplus_1^{2n+2} \mathcal{U} \,|\, [x_j, p_{x_k}] = i\delta_{jk}, \ [x_j, x_k] = 0, \ [p_{x_j}, p_{x_k}] = 0\}. \quad (4)$$

The specification of the commutation relations is analogous to defining the Poisson bracket structure or symplectic form. A canonical transformation is a mapping $C \in \mathcal{U}$ from $\mathcal{M}$ to $\mathcal{M}$ given by

$$C : (\{x_j\}, \{p_{x_k}\}) \mapsto (\{Cx_jC^{-1}\}, \{Cp_{x_k}C^{-1}\}). \quad (5)$$

By construction, the mapping C preserves the canonical commutation relations.

Classically, any function of the classical variables

$$F(q_1, \ldots, q_n, p_1, \ldots, p_n, q_0, p_0)$$

is an observable. Precisely what class of functions is allowed is vague, but intuitively one wants smooth (C^∞) functions on R^{2n+2}, with possibly a countable set of singularities. The task at hand is to characterize the elements of $\mathcal{U}$.

First a point of terminology: quantum mechanically, the word "observable" cannot be used to refer to an element of $\mathcal{U}$ because it is already defined in an incompatible way. The word "function" is also inappropriate because strictly speaking a function is a mapping from a domain to a range, and the elements of $\mathcal{U}$ do not take values in some domain and are not themselves mappings. The natural choice would be the term "symbol," denoting an element of a ring, but this word is already in common usage in a related but distinct way for pseudo-differential operators[10].

With reluctance, the new term "notion" is proposed. The generators q_k, p_k ($k = 0, \ldots, n$) are called "notes," marking certain elements of $\mathcal{U}$ as significant. An element $f \in \mathcal{U}$ having an expression $f<q_0, \ldots, q_n, p_0, \ldots, p_n>$ as an ordered combination of notes is a "notion." The angle brackets are used to emphasize that f is not a function of the notes, but an ordered expression in terms of them. Angle brackets and this terminology will only be used in this section. In later sections, the convenient fiction that elements of $\mathcal{U}$ like the Hamiltonian are functions of the phase space variables will be maintained in conformance with common practice. When a notion is represented as an operator, it is called a "notable"—observables are a subset of the notables.

For convenience, let (q, p) denote the phase space variables. The extension to the many-variable case is straightforward.

Begin with an intuitive description of $\mathcal{U}$. First, it must contain all possible Hamiltonians, as well as all the notions corresponding to observables. In particular, since every classical potential is a possible analog of a quantum potential, $\mathcal{U}$ must contain the notion expressions for the C^∞ functions of q, with singularities, that are allowed classically. Classically, this space of functions is topologized by defining a family of seminorms on open sets of the domain of the functions[17]. Quantum mechanically, there is no underlying domain from which to induce the topology. One must work directly with the abstract algebraic expression—the notion—corresponding to a function. Nevertheless one expects that a topology persists, even if it is difficult to define it precisely. The existence of this topology will be assumed.

Secondly, $\mathcal{U}$ must be closed under canonical transformations. This means that if $x, C \in \mathcal{U}$ then $CxC^{-1} \in \mathcal{U}$. The stronger assumption is made that the adjoint action of C is transitive, that is, for every $x, y \in \mathcal{U}$, there exists a $C \in \mathcal{U}$ such that $CxC^{-1} = y$. This property is important for defining functions on $\mathcal{U}$[18].

Define a notion of q to be those $x \in \mathcal{U}$ such that $[x, q] = 0$, denoted $x<q>$. There is a subgroup $\mathcal{D} \subset \mathcal{U}$ which transforms a notion of q to a notion of q. The notions $x<q>$ form a normal subgroup $\mathcal{Q}$ of $\mathcal{D}$. The quotient group $\mathcal{D}/\mathcal{Q}$ is the abstract analog of the diffeomorphism group. Part of the difficulty in topologizing $\mathcal{U}$ can be traced to the fact that it contains the diffeomorphism group as a subgroup, and the topology of the diffeomorphism group is a deep subject in itself[19].

From this discussion, it is clear that the algebra $\mathcal{U}$ is assumed to be a topological transformation group[20] which acts transitively on itself by the adjoint action. A more precise definition of $\mathcal{U}$ may be given by describing a construction of it. One begins with the Weyl algebra[21] of polynomials in the notes q, p, with the relation

$$qp - pq = i. \tag{6}$$

One adjoins the elements q^{-1}, p^{-1}, together with the relations

$$q^{-1}q = qq^{-1} = 1, \qquad p^{-1}p = pp^{-1} = 1. \tag{7}$$

Additional relations like

$$q^{-1}p - pq^{-1} = -iq^{-2}$$

follow from those given already, as, for example, this one is $-q^{-1}[q,p]q^{-1}$.

The core $\mathcal{U}_c$ of the algebra $\mathcal{U}$ is given by the ring over the complex field of formal Laurent expansions in q, p having only a finite number of non-vanishing coefficients of negative powers. A general element $f \in \mathcal{U}_c$ can be expressed as the notion

$$f<q,p> = \sum_{\{n_j, m_j\}} a_{\{n_j, m_j\}} q^{n_1} p^{m_1} q^{n_2} p^{n_2} \cdots . \tag{8}$$

These notions could be topologized in terms of open sets in a space coordinatized by the expansion coefficients.

Using the relations, the notion (8) can be reordered to put all of the p's on the right. Representing the p's as differential operators, the symbol $f(q, \xi)$ of the corresponding pseudodifferential operator is obtained by taking the Fourier transform[10]. One can go on to prove that the pseudodifferential operators form an algebra, and the class of symbols has a topology as C^∞ functions. This procedure is not followed here because it is useful not to insist on reordering a notion to obtain the symbol, and indeed for many notions that will be used, it is not obvious what their reordering is nor what growth properties their symbols would have.

The algebra $\mathcal{U}$ is completed by closing $\mathcal{U}_c$ under an action of functional composition. The space of canonically conjugate variables is the set

$$\mathcal{M} = \{(x, p_x) \in \mathcal{U} \oplus \mathcal{U} \mid xp_x - p_x x = i\}. \tag{9}$$

Each notion $f{<}q, p{>}$ induces a function $\tilde{f}$ from $\mathcal{M}$ to $\mathcal{U}$ by

$$\tilde{f}(x, p_x){<}q, p{>} = f{<}x{<}q, p{>}, p_x{<}q, p{>>}. \tag{10}$$

As an example, the induced action of the notion $f{<}q, p{>} = qp^3$ on a pair (x, p_x) is

$$\tilde{f}(x, p_x) = xp_x^3. \tag{11}$$

When this action is evaluated on the pair

$$(x{<}q, p{>}, p_x{<}q, p{>}) = (q^2, (2q)^{-1}p),$$

one has

$$\tilde{f}(x, p_x){<}q, p{>} = q^2 \left(\frac{1}{2q}p\right)^3. \tag{12}$$

By the transitivity of the adjoint action of $\mathcal{U}$ on itself, this function has the important property

$$\tilde{f}(CxC^{-1}, Cp_x C^{-1}) = C\tilde{f}(x, p_x)C^{-1}, \tag{13}$$

which defines the value of the function everywhere in $\mathcal{M}$ in terms of its value at (q, p). Dirac grappled with the issue of defining a function of non-commuting variables in the early days of quantum mechanics[18], and this was one of his requirements. From (10), one sees that the function $C\tilde{f}(x, p_x)C^{-1}$ is induced by the notion CfC^{-1}.

On the subgroup $\mathcal{Q}$ of notions of q, there is a similar induced mapping from $\mathcal{U}$ to $\mathcal{U}$

$$\tilde{f}(x){<}q, p{>} = f{<}x{<}q, p{>>}. \tag{14}$$

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Clearly, closure above induces closure on this subgroup. Focussing on this subgroup, one can see the nature of the extension of $\mathcal{U}_c$ produced by the repeated action of the induced mapping of $\mathcal{M}$ on $\mathcal{U}$.

The requirement of closure introduces three new types of elements. First, the induced action of $f = q^{-1}$ on $x \in \mathcal{U}$ gives the algebraic inverse elements x^{-1}. Acting on q, one has $\tilde{f}(q) = q^{-1}$. Given C such that $x = CqC^{-1}$, one has

$$Cq^{-1}C^{-1} = C\tilde{f}(q)C^{-1} = \tilde{f}(x) \equiv x^{-1}. \tag{15}$$

But applying C to $q^{-1}q = qq^{-1} = 1$ gives

$$Cq^{-1}C^{-1}x = xCq^{-1}C^{-1} = 1. \tag{16}$$

Therefore $x^{-1} \equiv Cq^{-1}C^{-1}$ is the algebraic inverse of x. Uniqueness of the inverse in $\mathcal{U}$ then establishes correspondences like

$$(1 - q)^{-1} = \sum_{n=0}^{\infty} q^n$$

Secondly, the induced action of a formal Laurent expansion having an infinite number of non-vanishing coefficients of positive powers on q^{-1} gives a formal expansion having an infinite number of non-vanishing coefficients of negative powers. For example, the induced action of $\exp(-q^2) \equiv \sum_{n=0}^{\infty}(-1)^n q^{2n}/n!$ on q^{-1} gives the notion $\exp(-q^{-2})$.

Finally, since for $f \in \mathcal{Q}$, one has $x = CqC^{-1}$ for some $C \in \mathcal{U}$, there exists the functional inverse $g = C^{-1}qC \in \mathcal{Q}$ such that

$$\tilde{f}(g) = q. \tag{17}$$

The C is not unique, but the non-uniqueness does not affect the notion $g<q>$, only that of its conjugate $p_g<q,p>$. This means that notions like $\ln q$ and $q^{1/2}$ are in $\mathcal{Q}$ as inverses in the sense of (17) to the mappings induced by e^q and q^2. Each of these could also be defined in terms of formal Laurent expansions about points other than zero.

One might be concerned about possible branch structure of the inverses. The algebra $\mathcal{U}$ is defined over the field of complex scalars. Considering elements in $\mathcal{U}$ which involve these explicitly, one has for example

$$(\alpha q)^{1/2} = \alpha^{1/2} q^{1/2}. \tag{18}$$

The branch structure is determined by the functions of the complex scalars. There is no additional branch structure associated with the generators themselves.

In the more general case of $f \in \mathcal{U}$, one must define the functional inverse on the induced mapping of $\mathcal{M}$ to $\mathcal{M}$. Given $(f, p_f) \in \mathcal{M}$, there exists $(g, p_g) \in \mathcal{M}$ such that

$$(\tilde{f}(g, p_g), \tilde{p}_f(g, p_g)) = (q, p) \tag{19}$$

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If $(f, p_f) = (CqC^{-1}, CpC^{-1})$, then $(g, p_g) = (C^{-1}qC, C^{-1}pC)$. This inverse is unique.

This completes the construction of $\mathcal{U}$. One can see that it is quite large, consisting essentially of all formal Laurent expansions and their algebraic and functional inverses. A description of what is not included is perhaps more succinct: one does not allow expressions that involve distributions, in themselves or in their derivatives. This is because the algebraic and functional inverses of a distribution are undefined. The possibility exists that one might exclude distributions from $\mathcal{U}$ and $\mathcal{M}$, which constitute the quantum canonical group and quantum phase space, but allow them as part of an extended class of notions on which the canonical transformations act. In this way, one might treat Hamiltonians that involve distributions. This will not be considered here.

2.2   Representation as Operators

The elements of the quantum canonical group $\mathcal{U}$ must be represented by operators before they may act on the states of a Hilbert space. For notational convenience here and in the sequel, let (q, p) denote all of the phase space variables (q_k, p_k) $(k = 0, \ldots, n)$. The variables (q, p) will be represented by the operators $(\check{q}, \check{p}) \equiv (q, -i\partial_q)$ acting on functions $\psi(q)$ on configuration space. These operators are not to be thought of as self-adjoint operators in the standard inner product because a Hilbert space has not yet been specified, and in particular $\psi(q)$ need not be square-integrable. Functions $C(q, p) \in \mathcal{U}$ are represented by operators $\check{C}(\check{q}, \check{p})$. (As discussed above, to conform with common usage, the convenient fiction is used from here on that elements $C(q, p) \in \mathcal{U}$ are functions of (q, p) rather than their more precise characterization as the "notions" $C{<}q, p{>}$ expressed in terms of q, p.)

There is a subtlety in the correspondence of functions in $\mathcal{U}$ and their representations as operators. The operator $(C^{-1})^{\check{}}$ corresponding to C^{-1} is not always inverse to $\check{C}$ because the kernels of $\check{C}$ or $(C^{-1})^{\check{}}$ may be non-trivial. This prevents one from rigorously speaking of the operator $\check{C}^{-1}$, except when $\check{C}$ is invertible. Given a function ψ on which one will apply $\check{C}$, it may be decomposed as a sum of three parts

$$\psi = \psi_0 + \psi_1 + \overline{\psi},$$

where $\psi_0 \in \ker\check{C}$; ψ_1 in the pre-image of the kernel of $(C^{-1})^{\check{}}$, i.e., $\check{C}\psi_1 \in \ker(C^{-1})^{\check{}}$; and the remainder $\overline{\psi}$. The function

$$\overline{\psi}' = \check{C}\overline{\psi}$$

is then in the class $\mathrm{Im}\check{C}/\ker(C^{-1})^{\check{}}$ while $\overline{\psi} \in \mathrm{Im}(C^{-1})^{\check{}}/\ker\check{C}$. One has the desired properties

$$(C^{-1})^{\check{}}\check{C}\overline{\psi} = \overline{\psi}, \tag{20}$$

and

$$\check{C}(C^{-1})^{\check{}}\overline{\psi}' = \overline{\psi}'. \tag{21}$$

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By using $\check{C}$ and $(C^{-1})\check{\,}$, one has a definition of the inverse that applies for all functions that lie outside the kernels of the respective operators. As an example, the action of $(p^{-1})\check{\,}$ is indefinite integration modulo an element of $\ker \check{p}$, that is, modulo an additive constant.

It is believed that this definition agrees with that of the pseudo-differential operators, up to infinite smoothing operators[10]. As will be seen below, operators corresponding to functions of p are often evaluated in terms of the Fourier transform of a function of q, similar to the treatment of pseudo-differential operators.

2.3   Quantum Canonical Transformations

A quantum canonical transformation is defined[7] as a change of the phase space variables which preserves the Dirac bracket

$$[q, p] = i = [q'(q, p), p'(q, p)]. \tag{22}$$

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

$$CqC^{-1} = q'(q, p), \quad CpC^{-1} = p'(q, p). \tag{23}$$

Factor ordering is built into the definition of the canonical transformation through the ordering of C. No Hilbert space is mentioned in this definition.

The C producing a given pair $(q', p') \in \mathcal{M}$ is unique (up to a multiplicative constant). Suppose that there were two canonical transformations C_1 and C_2 implementing the same change of variables

$$\begin{aligned} C_1 q C_1^{-1} &= \quad q' \quad = C_2 q C_2^{-1} \\ C_1 p C_1^{-1} &= \quad p' \quad = C_2 p C_2^{-1}. \end{aligned} \tag{24}$$

Multiplying by C_2^{-1} on the left and C_1 on the right, one sees that $C_2^{-1} C_1$ simultaneously commutes with both q and p and therefore must be a multiple of the identity.

The Schrödinger operator corresponds to the function

$$\mathcal{H}(q, p) = p_0 + H(q_1, \ldots, q_n, p_1, \ldots, p_n, q_0) \tag{25}$$

in $\mathcal{U}$—this will be referred to as the "Schrödinger function." The canonical transformation C transforms the Schrödinger function

$$\mathcal{H}'(q, p) = C\mathcal{H}(q, p)C^{-1} = \mathcal{H}(CqC^{-1}, CpC^{-1}). \tag{26}$$

(The action of canonical transformations can be generalized by considering inhomogeneous transformations $\mathcal{H}' = DC\mathcal{H}C^{-1}$, $D \in \mathcal{U}$. This can be useful in certain applications. $D = 1$ is assumed here; the case with $\check{D}$ invertible requires only minor modification.)

Solutions of the Schrödinger equation $\check{\mathcal{H}}'\psi' = 0$ are solutions of $\check{C}\check{\mathcal{H}}(C^{-1})\check{\,}\psi' = 0$. If the kernel of $\check{C}$ is trivial, then

$$\psi = (C^{-1})\check{\,}\psi' \tag{27}$$

are solutions of the Schrödinger equation $\check{\mathcal{H}}\psi = 0$. Note that since no inner product has been specified, the transformation $(C^{-1})\check{\,}$ acts on all solutions of $\check{\mathcal{H}}'$, not merely the normalizable ones. When the kernel of $\check{C}$ is non-trivial, the situation is less simple and requires further discussion.

Before addressing this, consider the uniqueness of the canonical transformation C between $\mathcal{H}$ and $\mathcal{H}'$. A symmetry of $\mathcal{H}$ is a transformation S_λ 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_λ and $\mathcal{H}'$ a symmetry S'_μ, then the function $S'^{-1}_\mu C S_\lambda$ 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 $C_a C_b^{-1}$ 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 $\mathcal{H}'$.

In constructing the solutions of $\check{\mathcal{H}}$ from those of $\check{\mathcal{H}}'$, one must take care when the kernel of $\check{C}$ is non-trivial. In this case, there may be solutions ψ' of $\check{\mathcal{H}}'$ which by (27) produce a ψ which is not a solution of $\check{\mathcal{H}}$, but instead lead to

$$\psi'' = \check{\mathcal{H}}\psi, \tag{28}$$

where

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

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 $\check{\mathcal{H}}'\psi' = 0$. By (27), this gives $\psi = (p^{-1})\check{\,}\psi' = iq^3/3$. This is not a solution of $\check{\mathcal{H}}$: $\check{\mathcal{H}}\psi = -2 \in \ker\check{C}$. One has $\check{p}\psi = q^2 = \psi'$ so that $\check{C}$ is invertible on the solution ψ, so this is not the source of the problem.

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

$$\psi_s = (1 - (\mathcal{H}^{-1})\check{\,}\check{\mathcal{H}})\psi.$$

If $\ker\check{C} \cap \ker(\mathcal{H}^{-1})\check{\,} \neq \emptyset$, one must work harder.

2.4 Physical Equivalence and Isometric Transformations

One of the central features of the approach described here is that canonical transformations need not be unitary. It is important however to determine the circumstances under which they are. Both in evolution and for establishing the physical equivalence of two theories, unitary transformations play a key role. Strictly speaking a unitary transformation is defined as a linear norm-preserving isomorphism of a Hilbert space onto itself[22]. For evolution this is fine, but for physical equivalence it is too restrictive.

Two theories are physically equivalent if the values of all transition amplitudes are the same in both theories. This may be true even if the theories are formulated in different Hilbert spaces, that is, with different inner products. It would be a physically and mathematically sound generalization to extend the definition of a unitary transformation to this case because this is the spirit in which unitary is meant. Unfortunately, the secondary definition of a unitary transformation U as one for which $U^\dagger U = 1$ follows from the assumption that U maps the Hilbert space onto itself. This definition is so embedded in the collective consciousness of physicists that it would be foolish to try to modify it.

A linear norm-preserving isomorphism from one Hilbert space onto another is also known as an isometric transformation[22]. The prudent course is to distinguish this from a unitary transformation for which $U^\dagger U = 1$. Then, two theories are physical equivalent if they are related by an isometric transformation. The phrase "unitary equivalence" is often used as a synonym for "physical equivalence." This usage while perhaps mildly misleading is acceptable because it tends to call to mind the notion that norms are preserved and not a specific formula which is violated.

To determine the conditions under which a canonical transformation is isometric, consider two Schrödinger functions $\mathcal{H}$ and $\mathcal{H}'$ related by a canonical transformation C (26). For C to define a physical equivalence, it must be an isomorphism between the Hilbert spaces of $\mathcal{H}$ and $\mathcal{H}'$ and is therefore invertible on them. The solutions ψ of $\check{\mathcal{H}}\psi = 0$ are thus given in terms of the solutions ψ' of $\check{\mathcal{H}}'\psi' = 0$ by (27).

The inner product on the solutions of $\mathcal{H}$ has the form

$$\begin{aligned}\langle\phi|\psi\rangle_\mu &\equiv \langle\phi|\check{\mu}(\check{q},\check{p})|\psi\rangle_1 &(29)\\ &= \int d\Sigma\,\phi^*(q)\check{\mu}(\check{q},\check{p})\psi(q),\end{aligned}$$

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" $\check{\mu}(\check{q},\check{p})$ 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 $\check{p}_0$.

When one makes a canonical transformation, in general the measure density must transform to preserve the norm of states. This is why one must consider isometric

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transformations. Given the canonical transformation C from $\mathcal{H}$ to $\mathcal{H}'$, the norm of states is preserved when

$$
\begin{aligned}
\langle\psi|\psi\rangle_\mu &= \langle(C^{-1})^\vee\psi'|\check{\mu}|(C^{-1})^\vee\psi'\rangle_1 \\
&= \langle\psi'|(C^{-1})^{\vee\dagger_1}\check{\mu}(C^{-1})^\vee|\psi'\rangle_1 \\
&= \langle\psi'|\psi'\rangle_{\mu'}.
\end{aligned}
$$

The transformed measure density is

$$
\check{\mu}'(\check{q},\check{p}) = (C^{-1})^{\vee\dagger_1}\,\check{\mu}(\check{q},\check{p})(C^{-1})^\vee, \tag{30}
$$

or, in $\mathcal{U}$,

$$
\mu'(q,p) = C^{-1\,\dagger_1}C^{-1}\mu(CqC^{-1},CpC^{-1}). \tag{31}
$$

Here, $(C^{-1})^{\vee\dagger_1}$ is the "adjoint" of $(C^{-1})^\vee$ in the trivial measure density, $\check{\mu}=1$. From (31), one sees that the measure transforms as a function on $\mathcal{U}$ multiplied by an inhomogeneous factor.

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 (30) the familiar condition for a unitary transformation: $\check{C}^\dagger\check{C}=1$, where $\check{C}^\dagger=\check{\mu}^{-1}\check{C}^{\dagger_1}\check{\mu}$ is the adjoint in the measure density $\check{\mu}$ of the Hilbert space.

The possibility exists for one to redefine the states by absorbing a factor from the measure-density. This is an additional canonical transformation. For example, if $\check{\mu}$ and $\check{\mu}'$ are self-adjoint in the trivial measure density, i.e., $\check{\mu}^{\dagger_1}=\check{\mu}$, $\check{\mu}'^{\dagger_1}=\check{\mu}'$, by redefining the wavefunction

$$
\psi'' = \check{\mu}^{-1/2}\check{\mu}'^{1/2}\psi', \tag{32}
$$

the measure density reverts to the original $\check{\mu}$. The transformation from ψ to ψ'' then preserves the measure density and so may be unitary. This redefinition can be useful in many circumstances, but there are times when it is desirable to work with a transformed measure density.

To summarize, if the Hilbert space of the transformed system $\mathcal{H}'$ has the measure given by (30) 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 further discussion, see Ref. [8].

2.5 Infinitesimal Canonical Transformations

Having explored the general features of quantum canonical transformations, turn now to consider their connection with classical canonical transformations and the basis for

their explicit construction. Classically, an infinitesimal canonical transformation is generated by an (infinitesimal) generating function $F(q, p)$[23]. Associated to this generating function is the Hamiltonian vector field

$$v_F = F_{,p}\partial_q - F_{,q}\partial_p \tag{33}$$

whose action on a function u on phase space is the infinitesimal transformation

$$\delta_F u = \epsilon v_F u = -\epsilon\{F, u\} \tag{34}$$

where $\{F, u\}$ is the classical Poisson bracket. Through the correspondence between classical and quantum theory in which Poisson brackets times i go over into commutator brackets, this canonical transformation can be expressed in terms of the quantum operator $\exp(i\epsilon \breve{F})$

$$e^{i\epsilon\breve{F}}\breve{u}e^{-i\epsilon\breve{F}} = \breve{u} + i\epsilon[\breve{F}, \breve{u}] + O(\epsilon^2). \tag{35}$$

Because of operator ordering ambiguities in defining the quantum versions of $\breve{F}$ and $\breve{u}$, the classical and quantum expressions for the infinitesimal transformation can differ by higher order terms in $\hbar$ (at the same order of ϵ).

There are three elementary canonical transformations in one-variable which have well-known implementations as finite quantum transformations. They are similarity (gauge) transformations, point canonical (coordinate) transformations and the interchange of coordinates and momenta. It is natural to ask what class of transformations is reached by products of them[5]. By finding the algebra generated by the infinitesimal versions of these transformations, this can be determined. The somewhat surprising result is that classically they generate the full canonical algebra. (A partial result in this direction was found by Deenen[6] who did not consider the interchange operation.)

Since the infinitesimal elementary canonical transformations generate the full classical canonical algebra, in principle, any finite classical canonical transformation can be decomposed into a product of elementary canonical transformations. Since each of the elementary canonical transformations has a quantum implementation as a finite transformation, the implication is that products of the quantum implementations of the elementary canonical transformations span the quantum analog of the classical canonical group. Thus, any quantum canonical transformation can be decomposed as a product of elementary quantum canonical transformations. In practice at present, one is limited to finite products of the transformations. Nevertheless, as will be shown, this is a very powerful tool for solving problems in quantum mechanics.

It is important to emphasize that the claim is not made that one can "quantize" a classical canonical transformation by decomposing it into elementary canonical transformations and then replacing each elementary transformation with its quantum implementation. This is not true. Given an ordered function of quantum phase space variables and

a classical version obtained by letting the variables commute, if one applies a sequence of elementary canonical transformations to both, the resulting quantum and classical expressions will in general not be related by simply letting the quantum phase space variables commute. This is consistent with van Hove's theorem[24].

A simple example will cement the point. The transformation

$$p \mapsto p - q^2, \qquad q \mapsto q \tag{36}$$

is a canonical transformation both classically and quantum mechanically. If this transformation is applied to p^2, then classically one has

$$\text{classical}: \qquad p^2 \mapsto (p - q^2)^2 = p^2 - 2q^2 p + q^4, \tag{37}$$

while quantum mechanically one has

$$\text{quantum}: \qquad p^2 \mapsto (p - q^2)^2 = p^2 - 2q^2 p + q^4 + 2iq. \tag{38}$$

These are not the same. The difference is the term $2iq$ which arose from ordering the latter expression with all of the p's on the right. One might think that there is some other ordering which would preserve the correspondence with the classical result. A consequence of van Hove's theorem[24] is that there is no factor ordering prescription that will preserve the correspondence of the classical and quantum expressions for all functions on phase space.

The conclusion one draws from this is that one is to put the classical theory aside and work exclusively within an ordered quantum theory. The role of the classical theory here is solely to motivate the definition of the elementary canonical transformations. Quantum canonical transformations are constructed directly in the quantum theory. The examples below illustrate how they may be used to solve a theory by transforming to a simpler one whose solution is known without reference to the classical theory. In Section 3.7, a second example emphasizing the difference between classical and quantum canonical transformations is done.

Return to the details of the classical elementary canonical transformations. Similarity (gauge) transformations are infinitesimally generated by $F_S = f(q)$. Point canonical transformations are infinitesimally generated by $F_P = f(q)p$. The discrete transformation I interchanging the role of coordinate and momentum is

$$I : p \mapsto -q, \qquad I : q \mapsto p. \tag{39}$$

Using the interchange operator, composite elementary transformations which are nonlinear in the momentum can be formed. They are the composite similarity transformation, infinitesimally generated by

$$F_{CS} = I F_S I^{-1} = f(p),$$

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and the composite point canonical transformation, infinitesimally generated by

$$F_{CP} = I F_P I^{-1} = -f(p)q.$$

Each of these corresponds to a finite transformation through application of the interchange operator to the finite forms of the similarity and point canonical transformations.

The many-variable generalization of the similarity transformation is straightforward. It is infinitesimally generated by $F_S = f(q_1, \ldots, q_n)$. Interchanging any set of coordinates with their conjugate momenta gives the composite many-variable similarity transformations. For example, in two variables, one has the infinitesimal generating functions $F_{CS1} = f(p_1, q_2)$, $F_{CS2} = f(q_1, p_2)$ and $F_{CS12} = f(p_1, p_2)$.

The observation is now made that classically the algebra generated by the elementary and composite elementary transformations is the full canonical algebra

$$[v_F, v_G] = -v_{\{F,G\}}. \tag{40}$$

where F, G are arbitrary functions on phase space. It is to be expected that Hamiltonian vector fields will have this algebraic structure. More surprising is that the above collection of generating functions produce a general function on phase space through the Poisson bracket operation. This is verified by taking commutators of the different types of transformations.

Consider the two-variable case—the many-variable case follows similarly. Introducing the monomial generating functions

$$F_{nm}^{jk} = q_1^{j+1} q_2^{k+1} p_1^{n+1} p_2^{m+1}, \tag{41}$$

where $j, k, n, m \in Z$, the Poisson bracket of two of these is

$$\{F_{n_1 m_1}^{j_1 k_1}, F_{n_2 m_2}^{j_2 k_2}\} = ((j_2 + 1)(n_1 + 1) - (j_1 + 1)(n_2 + 1)) F_{n_1+n_2 \ m_1+m_2+1}^{j_1+j_2 \ k_1+k_2+1} \tag{42}$$
$$+ ((k_2 + 1)(m_1 + 1) - (k_1 + 1)(m_2 + 1)) F_{n_1+n_2+1 \ m_1+m_2}^{j_1+j_2+1 \ k_1+k_2}.$$

Inspection shows that a general monomial can be constructed by beginning with the monomial forms which generate the elementary and composite elementary canonical transformations.

By taking linear combinations, one can form any function having a Laurent expansion about some point (not necessarily the origin). To avoid having to use formal Laurent expansions about nonzero points for functions like $q^{1/2}$ or $\ln q$, greater generality is obtained by working with generating functions of the form

$$F = f_1(q_1) f_2(q_2) g_1(p_1) g_2(p_2). \tag{43}$$

This produces any function which can be represented as a sum of separable products.

2.6 Quantum Implementations

Each of the elementary canonical transformations can be implemented quantum mechanically as a finite transformation. Their action is collected in Fig. 1, and each will be reviewed below.

The interchange of coordinates and momenta

$$p \mapsto IpI^{-1} = -q, \qquad q \mapsto IqI^{-1} = p. \tag{44}$$

is implemented through the Fourier transform operator

$$\check{I} = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} dq' e^{iqq'} \tag{45}$$

for which it is evident that

$$\check{I}q' = -i\partial_q \check{I}, \qquad \check{I}p' = -q\check{I}. \tag{46}$$

The wavefunction is transformed

$$\psi^{(1)}(q) = \check{I}\psi^{(0)}(q) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} dq' e^{iqq'} \psi^{(0)}(q'). \tag{47}$$

The inverse interchange is

$$p \mapsto q, \qquad q \mapsto -p. \tag{48}$$

It is implemented by the inverse Fourier transform

$$(I^{-1})\check{} = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} dq' e^{-iqq'}. \tag{49}$$

The similarity transformation in one-variable is implemented by

$$e^{-f(q)}, \tag{50}$$

where $f(q)$ is an arbitrary complex function of the coordinate(s). While the coordinate is unchanged, the momentum transforms

$$p \mapsto e^{-f(q)} p e^{f(q)} = p - if_{,q}, \tag{51}$$

The wavefunction is transformed

$$\psi^{(1)}(q) = (e^{-f(q)})\check{}\psi^{(0)}(q). \tag{52}$$

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The composite similarity transformation is implemented by applying the interchange transformation to $e^{-f(q)}$ to exchange coordinates for momentum in f. In the one-variable case, the composite similarity transformation operator is

$$e^{-f(p)} = I e^{-f(q)} I^{-1}. \tag{53}$$

It produces the canonical transformation

$$q \mapsto e^{-f(p)} q e^{f(p)} = q + i f_{,p}, \tag{54}$$

while leaving the momentum unchanged. The wavefunction is transformed

$$\psi^{(1)}(q) = (e^{-f(p)})\check{}\psi^{(0)}(q) = (I e^{-f(q)} I^{-1})\check{}\psi^{(0)}(q). \tag{55}$$

Note that the operator corresponding to $e^{-f(p)}$ is defined in terms of the Fourier transform of a function of q, similar to its definition as a pseudodifferential operator[10].

In the many-variable case, the function f may involve either the coordinate or its conjugate momentum for each variable. Because variables of different index commute, each variable responds to the (composite) similarity operator as if it were a one-variable operator in that variable with the other variables treated as parameters. Thus, for each coordinate (momentum) of which f is a function, the corresponding conjugate momentum (coordinate) is shifted as in the one-variable case.

For reasons discussed below, it is convenient to represent the finite point canonical transformation not explicitly as the exponential of the infinitesimal form, but symbolically as $P_{f(q)}$. The effect of the point canonical transformation $P_{f(q)}$ is to implement the change of variables

$$q \mapsto P_{f(q)} q P_{f^{-1}(q)} = f(q), \tag{56}$$
$$p \mapsto P_{f(q)} p P_{f^{-1}(q)} = \frac{1}{f_{,q}} p.$$

The effect of $P_{f(q)}$ on the wavefunction is

$$\psi^{(1)}(q) = \check{P}_{f(q)} \psi^{(0)}(q) = \psi^{(0)}(f(q)). \tag{57}$$

The composite point canonical transformation is formed by composition with the interchange operator

$$P_{f(p)} = I P_{f(q)} I^{-1}. \tag{58}$$

It has the effect of making a change of variables on the momentum

$$q \mapsto \frac{1}{f_{,p}} q, \tag{59}$$
$$p \mapsto f(p).$$

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The operator ordering of the transformed q is determined by the action of the interchange operator on the coordinate point canonical transformation. The transformed wavefunction is

$$
\begin{aligned}
\psi^{(1)}(q) &= \check{P}_{f(p)}\psi^{(0)}(q) = (IP_{f(q)}I^{-1})\check{\,}\psi^{(0)}(q) \\
&= \left((f_{,p}(p)e^{if(p)q})\check{\,}\psi^{(0)}(q)\right)|_{q=0}.
\end{aligned}
\tag{60}
$$

The behavior of the finite transformation obtained by exponentiating the infinitesimal generating function of the point canonical transformations, $F = g(q)p$, can be computed using the above transformations. Let $G(q) = \int dq/g(q)$. For $C = P_{G(q)}$, one has $CpC^{-1} = g(q)p$, so that

$$
e^{iag(q)p} = Ce^{iap}C^{-1}.
\tag{61}
$$

The action of $e^{iag(q)p}$ on q taking $q \mapsto f(q)$ is then

$$
\begin{aligned}
f(q) = \exp(iag(q)p)q\exp(-iag(q)p) &= Ce^{iap}C^{-1}qCe^{-iap}C^{-1} \\
&= Ce^{iap}G^{-1}(q)e^{-iap}C^{-1} \\
&= CG^{-1}(q+a)C^{-1} \\
&= G^{-1}(G(q)+a).
\end{aligned}
\tag{62}
$$

This result is found by a more laborious method in [6].

As an explicit example, take $g = q^m$. The infinitesimal transformation is then that of the Virasoro generators. The finite transformation is (for $m \neq 1$)

$$
f(q) = e^{iaq^m p}qe^{-iaq^m p} = (q^{1-m} + (1-m)a)^{1/1-m}.
\tag{63}
$$

while for $m = 1$

$$
f(q) = e^a q.
\tag{64}
$$

For $m = 0, 1, 2$ the transformations $e^{i\alpha p}$, $e^{i(\ln\beta)qp}$, and $e^{i\gamma q^2 p}$ produce translations $q + \alpha$, scalings βq and special conformal transformations $q/(1 - \gamma q)$. These are well-known to generate the group $SL(2, C)$.

Eq. (62) gives the finite transformation $q \mapsto f(q)$ produced by the infinitesimal generating function $F = g(q)p$. It can also be read as a functional equation

$$
G(f(q)) = G(q) + a
\tag{65}
$$

which is to be solved for G given f. Not surprisingly, this equation does not have a solution for all f. The implication is that not all point canonical transformations can be expressed as the exponential of an infinitesimal transformation. This is an explicit demonstration of the well-known property of the diffeomorphism group that the exponential

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map does not cover a neighborhood of the identity[19]. This is a property of infinite-dimensional Lie groups and stands in contrast to the situation in finite-dimensional Lie groups.

A corollary is that the product of the exponentials of two generators cannot always be expressed as an exponential of a third generator. For this reason, it is generally not useful to express point canonical transformations in exponential form, but rather to note directly the change of coordinate they produce. (As reassurance, it is true that every point canonical transformation can be expressed as a finite product of exponentials[19].)

3 Applications

3.1 Linear Canonical Transformations

The linear canonical transformations form a finite-dimensional subgroup of all canonical transformations, and there has been much interest in them in the context of coherent states[3, 25]. As canonical transformations, they can be constructed from a product of elementary transformations.

Consider the case of a single variable. A linear composite similarity transformation

$$q \mapsto q - i\alpha p.$$

transforms the wavefunction

$$\psi^{(a)} = (e^{\alpha p^2/2})^{\vee}\psi^{(0)}.$$

(A superscript is used to indicate the generation of the transformation. Subscripts are used to distinguish variables when necessary.) A linear similarity transformation

$$p \mapsto p^b - i\beta q^b$$

makes the change

$$\psi^{(b)} = (e^{-\beta q^2/2})^{\vee}\psi^{(a)}.$$

Finally a scaling of the coordinate

$$p \mapsto \frac{1}{\gamma}p, \qquad q \mapsto \gamma q$$

gives

$$\psi^{(1)} = (e^{i \ln \gamma\, qp})^{\vee}\psi^{(b)}.$$

The full transformation is

$$p \mapsto \frac{1}{\gamma}p - i\beta\gamma q, \qquad q \mapsto \frac{-i\alpha}{\gamma}p + \gamma(1 - \alpha\beta)q, \tag{66}$$

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with

$$\psi^{(1)}(q) = (e^{i \ln \gamma\, qp} e^{-\beta q^2/2} e^{\alpha p^2/2})\check{}\,\psi^{(0)}(q). \tag{67}$$

A general $SL(2,C) \equiv Sp(2,C)$ transformation is of the form $p = ap' + bq'$, $q = cp' + dq'$ where $ad - bc = 1$. This gives the correspondence $\alpha = ic/a$, $\beta = iab$, $\gamma = 1/a$ $(a \neq 0)$.

By expressing $\psi^{(0)}$ as the Fourier transform of $\tilde{\psi}^{(0)}$, an integral representation is found for $\psi^{(1)}$ which does not explicitly involve exponentials of differential operators

$$\psi^{(1)}(q) = \frac{1}{(2\pi)^{1/2}} \int dq'\, e^{i\gamma q'q - \beta\gamma^2 q^2/2 + \alpha q'^2/2} \tilde{\psi}^{(0)}(q'). \tag{68}$$

A related result is given by Moshinsky[4].

The interchange transformation taking $(q, p) \mapsto (p, -q)$ can be constructed similarly as a linear canonical transformation. It is found to be

$$I = e^{iq^2/2} e^{ip^2/2} e^{iq^2/2}. \tag{69}$$

Using this, one can modify the derivation of (67) to handle the case where $a = 0$.

The operators representing the functions p^2, q^2, $(qp+pq)/2$ in $\mathcal{U}$ generate a realization of the $SL(2,C)$ algebra. Since $SL(2,C)$ is a finite-dimensional Lie group, every element of the group in the neighborhood of the identity can be expressed as an exponential of an element of the algebra. As well, a given linear canonical transformation may be expressed in many ways as a product of elementary transformations. Each will give an expression analogous to (67) or (68).

The generalization to many-variables is straightforward. The group of linear canonical transformations is $Sp(2n, C)$, and a realization of it is found from the linear similarity, composite similarity and scaling transformations. Realizations of other finite-dimensional Lie groups in terms of canonical transformations are found by treating them as subgroups of $Sp(2n, C)$.

By expressing the coordinates and momenta in terms of harmonic oscillator creation and annihilation operators, one finds the expressions for the action of linear canonical transformations on coherent states[3]. These are useful for handling squeezed states in quantum optics[25].

3.2 Non-relativistic Free Particle

The non-relativistic free particle is an easily solved problem which doesn't require any sophisticated machinery. It may however serve to illustrate a number of features of the use of canonical transformations, and, for this reason, it will be treated somewhat exhaustively.

The free particle Schrödinger function is

$$\mathcal{H}^{(0)} = p_0 + p^2. \tag{70}$$

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It may be immediately trivialized

$$\mathcal{H}^{(1)} = p_0 \tag{71}$$

by the two-variable similarity transformation

$$p_0 \mapsto p_0 - p^2, \qquad q \mapsto q + 2pq_0. \tag{72}$$

(Variables left unchanged by a transformation will be suppressed.) The original wavefunction is given in terms of the transformed one by

$$\psi^{(0)}(q, q_0) = (e^{-ip^2 q_0})\breve{\psi}^{(1)}(q). \tag{73}$$

where the solution of the trivialized Schrödinger equation $\mathcal{H}^{(1)}\breve{\psi}^{(1)} = 0$ is any q_0-independent function. This formula is just the formal expression for the evolution of an initial wavefunction in terms of the exponential of the Hamiltonian. In general, this formal result is insufficiently explicit, but for the free particle, it can be used to find more useful forms of the wavefunction.

For example, if the initial wavefunction is taken to be a plane wave $\psi^{(1)} = \exp(ikq)$, one finds the plane wave stationary solution

$$\psi^{(0)} = e^{ikq - ik^2 q_0}. \tag{74}$$

If the initial wavefunction is a delta function at x, then using the Fourier integral representation of the delta function, the wavefunction is

$$\psi^{(0)} = (e^{-ip^2 q_0/2})\breve{\frac{1}{2\pi}} \int_{-\infty}^{\infty} dq' e^{i(q-x)q'}. \tag{75}$$

Acting with the operator inside the integral and integrating the resulting Gaussian gives

$$\psi^{(0)} = (4\pi i q_0)^{-1/2} e^{i(q-x)^2/4q_0}. \tag{76}$$

This is the free particle Green's function.

It is clear that the nature of the wavefunction depends on the initial wavefunction used to generate it. This obvious comment is important to bear in mind because the "natural" solution of a transformed problem will not always correspond to the desired solution. To see this, consider a second approach to the free particle. The interchange transformation

$$p \mapsto -q, \qquad q \mapsto p$$

is equivalent to taking the Fourier transform of the original Schrödinger equation and gives

$$\mathcal{H}^{(a)} = p_0 + q^2. \tag{77}$$

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The original wavefunction is given by the inverse Fourier transform

$$\psi^{(0)}(q) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} dq' e^{-iqq'} \psi^{(a)}(q'). \tag{78}$$

The new equation $\check{\mathcal{H}}^{(a)} \psi^{(a)} = 0$ can be solved "naturally" in two ways. The first is simply to integrate with respect to q_0. This gives

$$\psi^{(a)} = f(q) e^{-iq^2 q_0} \tag{79}$$

where $f(q)$ is an arbitrary q_0-independent function that arises as an integration constant. One finds the wavefunction

$$\psi^{(0)} = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} dq' e^{-iqq' - iq'^2 q_0} f(q'). \tag{80}$$

This is a less familiar form of the wavefunction—it is of course just a momentum space representation—and it is perhaps not immediately obvious how to obtain the solutions above. Inspection shows that if $f = \delta(q' + k)$ one finds the plane wave stationary solution. Alternatively, if f is taken to be

$$f = \frac{1}{(2\pi)^{1/2}} e^{ixq'}, \tag{81}$$

then, at $q_0 = 0$, one has $\psi^{(0)} = \delta(q - x)$ and, evaluating the integral, one finds again the Green's function (76).

The second "natural" approach is to separate variables

$$\psi^{(a)} = \phi^{(a)}(q) e^{-ik^2 q_0}. \tag{82}$$

This results in the equation

$$(q^2 - k^2) \phi^{(a)} = 0, \tag{83}$$

which has as its solution

$$\phi^{(a)} = \delta(q - k) \tag{84}$$

(k can have either sign). Now inverting the interchange operation gives the familiar plane wave solution

$$\psi^{(0)} = \frac{1}{(2\pi)^{1/2}} e^{ikq - ik^2 q_0}. \tag{85}$$

The Green's function solution is however no longer obtainable.

The first of these approaches can itself be implemented as a canonical transformation. The similarity transformation

$$p_0 \mapsto p_0 - q^2, \qquad p \mapsto p - 2qq_0 \tag{86}$$

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trivializes the Schrödinger function

$$\mathcal{H}^{(1)} = p_0$$

and gives the wavefunction

$$\psi^{(a)} = (e^{-q^2 q_0})\check{\psi}^{(1)}. \tag{87}$$

The wavefunction $\psi^{(1)}$ is any q_0-independent function. The result for the original wavefunction is then (80).

The second approach of separation of variables is not so much a canonical transformation as a realization of the assertion that the solution space of the Schrödinger operator has a product structure.

3.3   Harmonic Oscillator

The harmonic oscillator is the paradigmatic problem in quantum mechanics, and it is a test piece for any method. Its solution by canonical transformation reemphasizes how the form of a solution is affected by the details of evaluating the product of operators representing the canonical transformation. Also, it is observed that more than one canonical transformation to triviality is needed to obtain both independent solutions of the original Hamiltonian.

The Hamiltonian for the harmonic oscillator is

$$H^{(9)} = p^2 + \omega^2 q^2. \tag{88}$$

A similarity transformation $\exp(\omega q^2/2)$, taking

$$p \mapsto p + i\omega q,$$

will cancel the quadratic term in the coordinate leaving

$$H^{(a)} = p^2 + 2i\omega qp + \omega.$$

This is recognized as corresponding to the operator for the Hermite polynomials. The transformation $\exp(\omega q^2/2)$ is real and therefore not unitary. It is however an isometric transformation. From (30), the measure density in the transformed inner product is $\check{\mu}^{(a)} = e^{-\omega q^2}$, which is the measure density in which the operator for the Hermite polynomials is self-adjoint.

Since solution by power series expansion is not a canonical transformation, so much as a method of approximation, additional transformations are needed. The composite similarity transformation $\exp(-p^2/4\omega)$ takes

$$q \mapsto q + ip/2\omega$$

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and cancels the quadratic term in the momentum, giving the Hamiltonian

$$H^{(b)} = 2i\omega qp + \omega. \tag{89}$$

Finally, the point canonical transformation P_{e^q}, taking

$$p \mapsto e^{-q}p, \qquad q \mapsto e^q,$$

transforms the Hamiltonian to action-angle form

$$H^{(1)} = 2i\omega p + \omega. \tag{90}$$

In terms of the full Schrödinger function, this is

$$\mathcal{H}^{(1)} = p_0 + 2i\omega p + \omega. \tag{91}$$

A final two-variable similarity transformation produced by $\exp(-\omega(2p - i)q_0)$,

$$p_0 \mapsto p_0 - 2i\omega p - \omega, \qquad q \mapsto q + 2i\omega q_0,$$

trivializes this, leaving

$$\mathcal{H}^{(2)} = p_0. \tag{92}$$

The wavefunction $\psi^{(1)}$ is given in terms of $\psi^{(0)}$ by

$$\psi^{(1)}(q) = \big(P_{e^q} e^{-p^2/4\omega} e^{\omega q^2/2}\big)^{\vee} \psi^{(0)}(q),$$

which may be inverted to find

$$\psi^{(0)}(q) = \big(e^{-\omega q^2/2} e^{p^2/4\omega} P_{\ln q}\big)^{\vee} \psi^{(1)}(q). \tag{93}$$

From the eigenfunctions of $H^{(1)}$

$$\psi_n^{(1)}(q) = e^{nq - i(2n+1)\omega q_0},$$

one has

$$\psi_n^{(0)}(q) = e^{-\omega q^2/2} e^{-(\partial_q)^2/4\omega} q^n e^{-i(2n+1)\omega q_0}. \tag{94}$$

This is the correct (unnormalized) harmonic oscillator eigenfunction. This formula is valid for complex n. Requiring that the wavefunction be normalizable fixes n to be a non-negative real integer. For other n, one finds an infinite power series in $1/q$ which is divergent at $q = 0$.

As remarked above, $\check{H}^{(a)}$ is the Hamiltonian whose solutions are the Hermite polynomials. This implies

$$H_n(q) \propto e^{-(\partial_q)^2/4} q^n \tag{95}$$

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Given this form, it is immediate that ∂_q is the lowering operator

$$\partial_q H_n(q) \propto n H_{n-1}(q). \tag{96}$$

This result could also be found by observing that p is a canonical transformation from $H^{(a)}$ to $H^{(a)} + 2\omega$. This transformation has a non-trivial kernel: the constant solution $H_0(q)$ is annihilated by the transformation. This means that p is not an isomorphism from the Hilbert space of $H^{(a)}$ to that of $H^{(a)} + 2\omega$. It is therefore not a unitary transformation. Despite being non-unitary, the importance of the lowering operator cannot be denied.

Furthermore, if one computes the transformed measure density produced by p, one finds it is operator valued and not the familiar coordinate dependent expression. By absorbing the square-root of this operator valued measure density into the wavefunction by (32), one can recover the standard inner product. This produces an n-dependent renormalization of the wavefunctions. This renormalization factor is the n-dependent factor that is present in the lowering operator relating normalized harmonic oscillator wavefunctions.

The representation (95) of the Hermite polynomials is unfamiliar because of the operator produced by the composite similarity transformation between $H^{(a)}$ and $H^{(b)}$. If this transformation is decomposed into elementary canonical transformations, direct evaluation leads to the more familiar Rodriques' formula for the Hermite polynomials. The decomposed transformation is

$$\psi^{(a)}(q) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\bar{q}\, e^{i\bar{q}q} e^{\bar{q}^2/4\omega} \int_{-\infty}^{\infty} dq'\, e^{-i\bar{q}q'} q'^n. \tag{97}$$

This may be evaluated by first rewriting q'^n as $(i\partial_{\bar{q}})^n$ acting on the exponential $\exp(-i\bar{q}q')$. It may be extracted from the q' integral which then gives $\delta(\bar{q})$. Integrating by parts n times transfers the $i\partial_{\bar{q}}$ operators to act on the remaining exponential terms

$$\psi^{(a)}(q) = \int_{-\infty}^{\infty} d\bar{q}\, (-i\partial_{\bar{q}})^n e^{i\bar{q}q + \bar{q}^2/4\omega} \delta(\bar{q}). \tag{98}$$

Completing the square of the argument of the exponential gives

$$\frac{1}{4\omega}(\bar{q} + 2i\omega q)^2 + \omega q^2,$$

from which the purely q part can be extracted from the integral. The $-i\partial_{\bar{q}}$ derivatives act equivalently to $-\partial_q/2\omega$ derivatives, and after converting them, they can be removed from the integral. This leaves a Gaussian integrated against a delta function which is immediately evaluated. The result is

$$\psi^{(a)}(q) = e^{\omega q^2} \left(\frac{-\partial_q}{2\omega}\right)^n e^{-\omega q^2}. \tag{99}$$

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This is proportional to the Rodrigues' formula for the Hermite polynomials

$$H_n(\xi) = e^{\xi^2}(-\partial_\xi)^n e^{-\xi^2}. \tag{100}$$

From this form, it is immediate that $e^{\xi^2}(-\partial_\xi)e^{-\xi^2} = -\partial_\xi + 2\xi$ is the raising operator.

There is a second linearly-independent solution of the harmonic oscillator which was not obtained by this canonical transformation. This solution is not normalizable, but from the standpoint of simply solving the differential equation, this is not important. A second canonical transformation which trivializes the Schrödinger function in a different way produces the other solution. This solution is easily found by observing that the harmonic oscillator Hamiltonian is symmetric under $\omega \mapsto -\omega$. Making this symmetry transformation on the canonical transformation above gives the transformation to the action-angle Hamiltonian

$$H^{(1')} = -2i\omega p - \omega. \tag{101}$$

The Schrödinger function could be trivialized by a two-variable similarity transformation, but this is unnecessary.

The wavefunction $\psi^{(0')}$ is given in terms of $\psi^{(1')}$ by

$$\psi^{(0')}(q) = (e^{\omega q^2/2} e^{-p^2/4\omega} P_{\ln q}) \check{\psi}^{(1')}(q). \tag{102}$$

From the eigenfunctions of $H^{(1')}$

$$\psi_n^{(1')} = e^{-(n+1)q - i(2n+1)\omega q_0},$$

one has

$$\psi_n^{(0')}(q) = e^{\omega q^2/2} e^{(\partial_q)^2/4\omega} q^{-(n+1)} e^{-i(2n+1)\omega q_0}. \tag{103}$$

These are clearly not normalizable for any n.

The problem of the inverted harmonic oscillator with Hamiltonian

$$H^{(0)} = p^2 - \omega^2 q^2 \tag{104}$$

can be solved by the above canonical transformations after ω is replaced by $i\omega$. This is a scattering problem, so both independent solutions are delta-function normalizable, with no quantization of n. This emphasizes the importance of both canonical transformations to triviality.

3.4 Harmonic Oscillator Propagator

The propagator for the harmonic oscillator is formally given by

$$K(q, q_0|a, 0) = (e^{-iH^{(0)}q_0})\check{\delta}(q - a). \tag{105}$$

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This can be evaluated by canonical transformations. The Hamiltonian for the harmonic oscillator is transformed to the Hamiltonian in action-angle form

$$H^{(1)} = i2\omega p + \omega, \tag{106}$$

by the canonical transformation

$$H^{(1)} = CH^{(0)}C^{-1}, \tag{107}$$

where

$$C = P_{e^q}e^{-p^2/4\omega}e^{\omega q^2/2}. \tag{108}$$

This means that the propagator can be expressed by a product of elementary canonical transformations

$$
\begin{aligned}
K(q, q_0|a, 0) &= (C^{-1}e^{-iH^{(1)}q_0}C)\check{\delta}(q - a) \\
&= (e^{-\omega q^2/2}e^{p^2/4\omega}P_{\ln q}e^{(2\omega p - i\omega)q_0}P_{e^q}e^{-p^2/4\omega}e^{\omega q^2/2})\check{\delta}(q - a).
\end{aligned} \tag{109}
$$

Evaluate (109) starting from the right. The first product is

$$F_1 = e^{\omega q^2/2}\delta(q - a) = e^{\omega a^2/2}\delta(q - a).$$

The next product is

$$F_2 = (e^{-p^2/4\omega})\check{\ }F_1.$$

This can be evaluated in two ways. One can recognize that $(e^{-p^2/4\omega})\check{\ }$ is the unitary operator generating free-particle ($H = p^2$) propagation for time $t = -i/4\omega$ and use the propagator

$$K_{free}(q, t|q', 0) = (4\pi it)^{-1/2}e^{i(q-q')^2/4t}. \tag{110}$$

Or, one can express $e^{-p^2/4\omega}$ as

$$e^{-p^2/4\omega} = Ie^{-q^2/4\omega}I^{-1},$$

and, by evaluating the action of this on $\delta(q-a)$, derive the free particle propagator. This is essentially what is done in (75). The result is that

$$F_2 = (\omega/\pi)^{1/2}e^{-\omega(q-a)^2+\omega a^2/2}.$$

The third product is the application of the point canonical transformation

$$
\begin{aligned}
F_3 &= \check{P}_{e^q}F_2 \\
&= (\omega/\pi)^{1/2}\exp(-\omega(e^q - a)^2 + \omega a^2/2).
\end{aligned}
$$

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The fourth product is a translation of q by $-i2\omega q_0$

$$
\begin{aligned}
F_4 &= (e^{(2\omega p - i\omega)q_0})\check{}\, F_3 \\
&= (\omega/\pi)^{1/2} \exp(-\omega(e^{q-i2\omega q_0} - a)^2 + \omega a^2/2 - i\omega q_0).
\end{aligned}
$$

This is followed by another point canonical transformation

$$
\begin{aligned}
F_5 &= \check{P}_{\ln q} F_4 \\
&= (\omega/\pi)^{1/2} \exp(-\omega(q e^{-i2\omega q_0} - a)^2 + \omega a^2/2 - i\omega q_0).
\end{aligned}
$$

A second free particle evolution gives

$$
\begin{aligned}
F_6 &= (e^{p^2/4\omega})\check{}\, F_5 \\
&= i\omega/\pi \int dq'\, e^{\omega(q-q')^2} \exp(-\omega(q' e^{-i2\omega q_0} - a)^2 + \omega a^2/2 - i\omega q_0) \\
&= \left(\frac{\omega}{2\pi i \sin 2\omega q_0}\right)^{1/2} \exp(i\frac{\omega a^2}{2}\cot 2\omega q_0 - i\frac{\omega a q}{\sin 2\omega q_0} - \frac{\omega q^2}{e^{4i\omega q_0} - 1})
\end{aligned}
$$

Lastly, multiplying by $e^{-\omega q^2/2}$ gives the final result

$$
K(q, q_0|a, 0) = \left(\frac{\omega}{2\pi i \sin 2\omega q_0}\right)^{1/2} \exp(i\frac{\omega}{2\sin 2\omega q_0}\Big((a^2 + q^2)\cos 2\omega q_0 - 2aq\Big)). \quad (111)
$$

This is the familiar Green's function for the harmonic oscillator.

3.5 Time-Dependent Harmonic Oscillator

The time-dependent harmonic oscillator can also be solved by canonical transformation. This has been done previously with a different sequence of canonical transformations by Brown[26]. Here, the approach will be to parallel the solution of the time-independent harmonic oscillator in trivializing the Schrödinger function. This emphasizes the connection between the time-dependent and time-independent problems. It is conjectured that the parallel structure shown here carries over to time-dependent versions of other exactly soluble problems.

One begins with the Schrödinger function

$$
\mathcal{H}^{(0)} = p_0 + p^2 + \omega^2(q_0)q^2 \quad (112)
$$

where the angular frequency $\omega(q_0)$ is a function of time. The quadratic term in the coordinate is cancelled by making a two-variable similarity transformation, $\exp(-f(q_0)q^2/2)$. This gives the Schrödinger function

$$
\mathcal{H}^{(a)} = p_0 + p^2 - 2ifqp + (2\omega^2 - if_{,q_0} - 2f^2)q^2/2 - f. \quad (113)
$$

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The condition that the quadratic potential be cancelled is

$$if_{,q_0} + 2f^2 = 2\omega^2. \tag{114}$$

This Ricatti equation is linearized by the substitution

$$f = i\frac{\phi_{,q_0}}{2\phi} \tag{115}$$

which gives

$$\phi_{,q_0 q_0} = -4\omega^2\phi. \tag{116}$$

To go further requires the specific time-dependence of $\omega(q_0)$.

The next step is to cancel the quadratic term in the momentum with a second two-variable similarity transformation, $\exp(-g(q_0)p^2/2)$. This gives the Schrödinger function

$$\mathcal{H}^{(b)} = p_0 + (2 - ig_{,q_0} + 4fg)p^2/2 - 2ifqp - f \tag{117}$$

with the condition

$$ig_{,q_0} - 4fg = 2 \tag{118}$$

This equation can be integrated to find

$$g = \exp(-i4 \int f dq_0) \int -2i \exp(i4 \int f dq_0) dq_0. \tag{119}$$

The Schrödinger function is then

$$\mathcal{H}^{(b)} = p_0 - 2ifqp - f.$$

The coordinate change

$$p \mapsto e^{-q}p, \qquad q \mapsto e^q \tag{120}$$

eliminates the coordinate from the Schrödinger function

$$\mathcal{H}^{(c)} = p_0 - 2ifp - f. \tag{121}$$

Finally, the Schrödinger function is trivialized to

$$\mathcal{H}^{(1)} = p_0 \tag{122}$$

by the composite two-variable shift

$$\exp(-(-2p+i) \int f dq_0).$$

Since $\psi^{(1)}$ is any q_0-independent function, this gives the result

$$\psi^{(0)}(q, q_0) = (e^{f(q_0)q^2/2} e^{g(q_0)p^2/2} P_{\ln q} e^{(-2p+i) \int f(q_0) dq_0}) \psi^{(1)}(q). \tag{123}$$

The time-independent result is recovered when $f = -\omega$ and $\psi^{(1)}(q) = e^{nq}$.

3.6 Intertwining

Intertwining is the existence of an operator D which transforms between two operators

$$H^{(1)}D = DH^{(0)}. \tag{124}$$

It is a powerful method for solving differential equations because it gives the solutions of $H^{(1)}$ in terms of those of $H^{(0)}$. All of the recursion relations and Rodrigues' formulae for the classical special functions can be understood as a consequence of intertwining.

The most widely known example of intertwining is that of the Darboux transformation between two Hamiltonian operators in potential-form[14]

$$H^{(i)} = p^2 + V_i(q). \tag{125}$$

One would like to know what potentials can be reached from a given one by an intertwining transformation (124). In the usual approach, an ansatz is made that the intertwining operator D is a first order differential operator, and the operator is constructed by requiring that the intertwining relation (124) be satisfied. It is satisfactory to begin with first order operators because the intertwining transformation can be iterated.

Since the intertwining operator is a canonical transformation, it can be constructed as a sequence of elementary canonical transformations. The construction is interesting because it involves a transformation in which operator ordering makes the the quantum case simpler than the classical. This is the source of the power of the differential operator ansatz, and it is the first example of a transformation which favors the quantum problem over the classical.

Begin with a Hamiltonian with potential

$$H^{(0)} = p^2 + V_0(q). \tag{126}$$

The potential may be cancelled by making a similarity transformation

$$p \mapsto p - ig(q)$$

This gives the Hamiltonian

$$H^{(a)} = p^2 - 2igp - \lambda \tag{127}$$

together with the Ricatti equation

$$g_{,q} + g^2 = V_0 + \lambda. \tag{128}$$

The transformed wavefunction is

$$\psi^{(a)} = (e^{-\int g dq})\check{\psi}^{(0)}. \tag{129}$$

A composite similarity transformation is made on the coordinate with p

$$q \mapsto pq\frac{1}{p} = q - \frac{i}{p}. \tag{130}$$

This is the key step in an intertwining transformation. It has the very interesting property

$$g(q - \frac{i}{p}) = g(pq\frac{1}{p}) = g(q) - ig(q)_{,q}\frac{1}{p}. \tag{131}$$

Note that only the first term in the Taylor expansion of g appears—classically the full Taylor expansion would have arisen. After the transformation, the Hamiltonian becomes

$$H^{(b)} = p^2 - 2igp - 2g_{,q} - \lambda. \tag{132}$$

and the transformed wavefunction is

$$\psi^{(b)}(q) = (e^{\int dp/p})\check{\psi}^{(a)}(q) = \check{p}\psi^{(a)}(q). \tag{133}$$

Because the kernel of $\check{p}$ is non-trivial, this transformation may be non-unitary for the reasons discussed above in the context of the lowering operator for the Hermite polynomials. Nevertheless, it is useful.

The transformation

$$p \mapsto p + ig(q)$$

cancels the term linear in the momentum giving the Hamiltonian

$$H^{(1)} = p^2 + V_1(q), \tag{134}$$

with the new potential

$$V_1 = -g_{,q} + g^2 - \lambda. \tag{135}$$

The transformed wavefunction is

$$\psi^{(1)}(q) = (e^{\int g dq})\check{\psi}^{(b)}(q). \tag{136}$$

In terms of the original wavefunction, this is

$$\psi^{(1)}(q) = (e^{\int g dq} p e^{-\int g dq})\check{\psi}^{(0)}(q) = -i(\partial_q - g)\psi^{(0)}(q). \tag{137}$$

Comparing (128) and (135), the change in potential is

$$V_1 - V_0 = -2g_{,q}. \tag{138}$$

The Ricatti equation (128) [or (135)] can be solved to find that g is given by the logarithmic derivative of an eigenfunction of $H^{(0)}$ (or the negative logarithmic derivative of an eigenfunction of $H^{(1)}$) with eigenvalue λ. This is the standard result from intertwining[14].

If one inverts (137) to obtain $\psi^{(0)}$ in terms of $\psi^{(1)}$, one obtains the integral operator expression

$$\psi^{(0)}(q) = (e^{\int g dq} p^{-1} e^{-\int g dq})^{\check{}} \psi^{(1)}(q). \tag{139}$$

To obtain a differential operator relation, one may note that taking $g \to -g$ interchanges V_0 and V_1. This implies from (137) that

$$\psi^{(0)}(q) = -i(\partial_q + g)\psi^{(1)}(q). \tag{140}$$

Alternatively, a different sequence of canonical transformations can be used which give an integral operator relating $\psi^{(0)}$ to $\psi^{(1)}$ which becomes a differential operator upon inversion. Beginning from $H^{(0)}$ (126), the one-variable shift $p \mapsto p + ig(q)$ gives the Hamiltonian

$$H^{(a)} = p^2 + 2ipg - \lambda \tag{141}$$

where V_0 satisfies (128). Note that p has been ordered on the left of g. This is to facilitate the transformation

$$q \mapsto \frac{1}{q} qp = q + \frac{i}{p}.$$

This leads to the transformed Hamiltonian

$$H^{(b)} = p^2 + 2ipg - 2g_{,q} - \lambda. \tag{142}$$

A similarity transformation $p \mapsto p - ig(q)$ cancels the linear momentum term, leaving the final Hamiltonian

$$H^{(1)} = p^2 + V_1, \tag{143}$$

where V_1 is given by (135). The final wavefunction in terms of the original is

$$\psi^{(1)}(q) = (e^{-\int g dq} p^{-1} e^{\int g dq})^{\check{}} \psi^{(0)}(q). \tag{144}$$

Inverting this gives the expected differential relation (140).

The operator in (140) annihilates the wavefunction $e^{-\int g dq}$. If this wavefunction is in the Hilbert space of $H^{(1)}$, the transformation is not an isomorphism, and the operator is non-unitary. There is a solution of $H^{(0)}$ corresponding to this wavefunction. To obtain it, one applies the canonical transformation (139) to $e^{-\int g dq}$. This gives a familiar integral expression[27] for the solution complementary to $e^{\int q dq}$, which can be checked to be the other solution of $\check{H}^{(0)}$ with zero eigenvalue.

The method of intertwining has been realized in terms of canonical transformations. This means that all of the problems which can be solved by intertwining can be solved with canonical transformations. This includes all problems which are essentially hypergeometric, confluent hypergeometric, or one of their generalizations. Furthermore, the Rodrigues' and differential recursion formulae for the special functions may all be obtained from canonical transformations of this kind.

3.7 Classical vs. Quantum Transformations

The distinct behaviors classically and quantum mechanically of a sequence of elementary canonical transformations were discussed in Section 2.5. A different perspective on this will given by considering the classical and quantum transformations between two Hamiltonians whose classical forms are the same as their quantum forms in a natural ordering. The point will be to show that a different sequence of elementary transformations is needed to implement the transformation classically and quantum mechanically. Furthermore, it will be shown that the accumulated transformation is a highly non-trivial factor ordering of the classical transformation. This indicates that attempts to solve a quantum problem by factor ordering the classical canonical transformation will generally be in vain. Only in very special cases will the quantum ordering be sufficiently simple, e.g., polynomial, that one could hope to find it by hand. Constructing the sequence of elementary transformations which solve the problem quantum mechanically is a more fruitful course.

The example is the transformation between the Hamiltonians

$$H^{(0)} = p^2 + e^{2q} \mapsto H^{(1)} = p^2. \tag{145}$$

These Hamiltonians have the same form classically and quantum mechanically if they are ordered as written. Quantum mechanically, the solutions of $\check{H}^{(0)}$ are Bessel functions. The transformation to $H^{(1)}$ would give their construction in terms of plane waves. This will not be the emphasis here. Rather, the focus will be on the difference between the sequence of elementary transformations which implement the transformation classically and quantum mechanically.

Consider the problem classically. The transformation

$$q \mapsto \ln q, \qquad p \mapsto qp, \tag{146}$$

simplifies the potential

$$H_{cl}^{(a)} = q^2 p^2 + q^2. \tag{147}$$

An interchange

$$(q, p) \mapsto (p, -q) \tag{148}$$

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gives

$$H_{cl}^{(b)} = (1 + q^2)p^2. \tag{149}$$

Finally, the change of variables

$$q \mapsto \sinh q, \qquad p \mapsto \frac{1}{\cosh q}p, \tag{150}$$

gives

$$H_{cl}^{(1)} = p^2. \tag{151}$$

Denoting the phase space variables in the final equation by (q', p'), the full accumulated transformation in terms of the initial variables is

$$q' = \operatorname{arcsinh}(-e^{-q}p), \qquad p' = (p^2 + e^{2q})^{1/2}. \tag{152}$$

Now consider the problem quantum mechanically. The first two transformations are the same and give

$$H_{qu}^{(a)} = q^2 p^2 - iqp + q^2, \tag{153}$$

and

$$H_{qu}^{(b)} = p^2(1 + q^2) + ipq. \tag{154}$$

The transformation

$$q \mapsto \frac{1}{p}qp = q + \frac{i}{p} \tag{155}$$

leads to

$$H_{qu}^{(c)} = (1 + q^2)p^2 - iqp. \tag{156}$$

Again, the point canonical transformation (150) ends the process

$$H_{qu}^{(1)} = p^2. \tag{157}$$

Note that the sequences of elementary transformations which perform the full transformation classically and quantum mechanically are similar, but different. An extra transformation is needed quantum mechanically to cancel a term that arose from ordering. The full quantum transformation is

$$\begin{aligned} q' &= \operatorname{arcsinh}(-e^{-q}p) - \frac{i}{(1 + (e^{-q}p)^2)^{1/2}}e^{-q}, \\ p' &= e^q(1 + (e^{-q}p)^2)^{1/2}. \end{aligned} \tag{158}$$

The functions appearing in these expressions are defined in terms of their power series expansions. Clearly, the ordering is non-trivial, and while the correspondence with (152) is evident, it would have been difficult to discover by hand.

This emphasizes the point that classical and quantum canonical transformations are not simply related. It is more fruitful to construct the quantum canonical transformation directly than to attempt to factor order a classical transformation.

3.8   Particle on $2n+1$-sphere

As a final example, consider the radial Hamiltonian for a particle propagating on an $2n+1$-dimensional sphere

$$H^{(0)} = p^2 - 2ni\cot q\,p. \tag{159}$$

Its solution by canonical transformations illustrates the use of the intertwining canonical transformation. First make the point canonical transformation

$$\frac{-1}{\sin q}p \mapsto p, \qquad \cos q \mapsto q.$$

This is stated in inverse form, contrary to the convention followed above. This is often useful with point canonical transformations because it is more intuitive when looking for changes of variable to simplify an equation. The transformed Hamiltonian is found to be

$$H^{(a)} = (1-q^2)p^2 + (2n+1)iqp. \tag{160}$$

This is recognized as corresponding with the equation for the Gegenbauer polynomials.

The intertwining transformation p^{-n} taking

$$q \mapsto q + \frac{ni}{p}$$

can now be used to cancel the n-dependence of the Hamiltonian. Noting that

$$q^2 \mapsto (\frac{1}{p^n}qp^n)^2 = q^2 + 2niq\frac{1}{p} - \frac{n^2+n}{p^2}, \tag{161}$$

one finds

$$H^{(b)} = (1-q^2)p^2 + iqp - n^2. \tag{162}$$

Clearly, it would have been possible to shift n by any amount: this gives the relation between Gegenbauer polynomials of different n.

Finally, undoing the original point canonical transformation

$$p \mapsto \frac{-1}{\sin q}p, \qquad q \mapsto \cos q,$$

gives the free-particle Hamiltonian

$$H^{(1)} = p^2 - n^2. \tag{163}$$

Because the physical problem was that of a free-particle on a sphere, this is the free-particle on a circle. The spectrum of $H^{(1)}$ is discrete, and the constant shift produces

a time-dependent phase factor $e^{in^2 q_0}$ relative to the usual free-particle eigenfunctions on the circle

$$\psi_m^{(1)} = \cos mq \, e^{-im^2 q_0}. \tag{164}$$

(The other independent solution is found by using $\sin mq$.) The original wavefunctions are given in terms of the free-particle eigenfunctions by

$$\psi_m^{(0)} = (P_{\cos q} p^n P_{\arccos q}) \check{\psi}_{m+n}^{(1)}(q) = \left(\frac{i}{\sin q} \partial_q \right)^n \cos(m+n)q \, e^{-i(m^2 + 2mn)q_0}. \tag{165}$$

The indexing is determined by the condition that $m = 0$ corresponds to the normalizable solution with lowest energy. This agrees with the result obtained by the intertwining method[13] and is recognized as a formula for the Gegenbauer polynomials $c_m^{(n)}(\cos q)$.

In principle, this result is valid for real n. For n non-integer, one requires an integral representation of the fractional differential operator. It is likely that this can be constructed by manipulating the definition of the composite similarity transformation in terms of the Fourier transform of an ordinary similarity transformation. This would be analogous to the discussion of the origin of the Rodrigues' formula for the Hermite polynomials. There are subtleties involving endpoints of the integrals which are beyond the scope of this paper. I hope to return to this in a later work.

4   Conclusion

It has been shown how, using a few elementary canonical transformations which have quantum mechanical implementations, a Schrödinger function can be trivialized and, thereby, its solutions found. The fact that the infinitesimal versions of these elementary transformations classically generate the full canonical algebra is argued to imply that in principle any canonical transformation can be implemented quantum mechanically. Issues of operator ordering break the parallel structure between classical and quantum canonical transformations, so that in general different transformations are needed to reach the trivial Schrödinger function in each case. This raises the interesting possibility of the inequivalence of classical and quantum integrability.

By defining quantum canonical transformations algebraically in terms of a topological transformation group consisting of ordered expressions in the quantum variables q and p, consistent with the canonical commutation relations, it was possible to work outside of a specific Hilbert space. This allowed the use of transformations that are non-unitary when represented on a particular Hilbert space, either because they change the measure in the inner product or because they do not define an isomorphism. While not of importance for evolution, such transformations are important tools for constructing the solutions to the wave equation. Raising and lowering operators[11], intertwining operators[13, 14] and

differential realizations of Lie algebras[15] provide well-known examples of undeniable importance. As a by-product of the fact that the quantum canonical transformations are defined outside of the Hilbert space, they enable the construction of the general solution of the wave equation, including the non-normalizable solutions. This may be important in contexts outside of quantum mechanics where normalizability of solutions is less important.

This approach also gives new tools for proving the physical equivalence of quantum theories. Rather than attempting to factor order a classical canonical transformation between two theories, one can construct the quantum transformation in a more systematic fashion. This enables one to construct quantum transformations that are non-polynomial factor orderings of the classical transformation. A non-trivial example illustrating this is the proof of the equivalence of the Moncrief and Witten/Carlip formulations of 2+1-quantum gravity on the torus[28].

Further work is necessary to elaborate the collection of tools for using the quantum canonical transformations, especially in the many-variable context. A fruitful direction for future work is the extension of this approach to field theory where it may perhaps shed new light on integrable systems or renormalizability.

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$$\begin{array}{rcl} p & \mapsto & -q \\ q & \mapsto & p \end{array} \qquad\qquad \check{I}\psi(q) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} dq'\, e^{iqq'}\psi(q')$$

$$\begin{array}{rcl} p & \mapsto & q \\ q & \mapsto & -p \end{array} \qquad\qquad (I^{-1})\check{}\,\psi(q) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} dq'\, e^{-iqq'}\psi(q')$$

$$\begin{array}{rcl} p & \mapsto & p - if(q)_{,q} \\ q & \mapsto & q \end{array} \qquad\qquad (e^{-f(q)})\check{}\,\psi(q)$$

$$\begin{array}{rcl} p & \mapsto & p \\ q & \mapsto & q + ig(p)_{,p} \end{array} \qquad\qquad (e^{-g(p)})\check{}\,\psi(q)$$

$$\begin{array}{rcl} p & \mapsto & \dfrac{1}{f(q)_{,q}}p \\[2mm] q & \mapsto & f(q) \end{array} \qquad\qquad \check{P}_{f(q)}\psi(q) = \psi^{(0)}(f(q))$$

$$\begin{array}{rcl} p & \mapsto & g(p) \\[2mm] q & \mapsto & \dfrac{1}{g(p)_{,p}}q \end{array} \qquad \check{P}_{g(p)}\psi(q) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\bar{q}\, e^{i\bar{q}q} \int_{-\infty}^{\infty} dq'\, e^{-ig(\bar{q})q'}\psi(q')$$

Figure 1: Elementary and composite elementary canonical transformations