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Canonical transformations and non-unitary evolution

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Abstract
We test the idea that transformations which, at the classical level, can be interpreted as evolutions are represented within quantum mechanics by unitary operators. To this end, we consider non-trivial canonical transformations which leave invariant the form of the Hamilton function of a system. We demonstrate that infinite families of such transformations exist for a variety of familiar conservative systems of one degree of freedom. We show how the precise form of integral equations for the stationary state wavefunctions implied by the existence of these canonical transformations can be pinned down by exploiting the algebra of the transformations and a symmetry of their generating functions. We recover several integral equations found in the literature on standard special functions of mathematical physics. We find that when one of the classical canonical transformations we consider is non-linear, its quantum implementation is non-unitary. We end with some comments on the implications of our findings for semiclassical studies and a brief discussion relevant to string theory of the generalization to scalar field theories in 1 + 1 dimensions.

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1. Introduction

Given the formal similarities between quantum mechanics and the Hamiltonian formulation of classical mechanics, it is not surprising that there have been several attempts to define, within quantum mechanics, transformations analogous to the canonical transformations underpinning the powerful Hamilton–Jacobi method. The founding fathers of quantum mechanics were content to identify the quantum analogues of canonical transformations as unitary transformations of the position and momentum operators which preserve the canonical commutation relations [1, 2]. However, to enhance the scope of applications, various operator-based extensions of this notion of a quantum canonical transformation have been proposed [3, 4]. The path-integral formulation of quantum mechanics (and quantum field theory) with its c-number representation of coordinates and momenta has also prompted more ambitious constructions [5], but these are not without their complications [6] (because of the ambiguous interrelationships between the momenta p_i and coordinates q_i introduced in the discretization of the path integrals [7]). Finally, there are treatments [8, 9] of canonical transformations within the quantum theory which focus on their consequences for wavefunctions (or, within the field theory, wavefunctionals [10, 11]).

In his pioneering work on changes of representation effected by *unitary* operators $\widehat{U}$, Dirac observed [12] that matrix elements of $\widehat{U}$ could be related to a quantum generating function F which reduces to the generating function $\mathcal{F}$ (of the first kind) in the limit $\hbar \to 0$ for a classical canonical transformation: specifically, if $\widehat{U}$ transforms the coordinate operator $\widehat{q}$ (with eigenkets $|q_1\rangle$) into the coordinate operator $\widehat{Q} = \widehat{U}\widehat{q}\widehat{U}^\dagger$ (with eigenkets $|Q_1\rangle = \widehat{U}|q_1\rangle$), then $F = F(q_1, Q_2)$ is defined so that

$$\mathrm{e}^{(\mathrm{i}/\hbar)F(q_1,Q_2)} = \langle q_1|Q_2\rangle = \langle q_1|\widehat{U}|q_2\rangle. \tag{1.1}$$

In terms of F, the transformation between the wavefunctions $\phi_\alpha(q) = \langle q|\alpha\rangle$ and $\Phi_\alpha(Q) = \langle Q|\alpha\rangle$ of a stationary state $|\alpha\rangle$ in the two representations reads

$$\phi_\alpha(q) = \int \mathrm{e}^{(\mathrm{i}/\hbar)F(q,Q)}\Phi_\alpha(Q)\,\mathrm{d}Q. \tag{1.2}$$

Equations (1.1) and (1.2) have been exploited very successfully at the semiclassical level [13–15]. In [9], a generalization of (1.2) has been postulated, namely

$$\phi_\alpha(q) = n_\alpha \int \mathrm{e}^{(\mathrm{i}/\hbar)F(q,Q)}\Phi_\alpha(Q)\,\mathrm{d}Q \tag{1.3}$$

where the novel element, the normalization factor n_α, is assumed to be independent of q, but, as the notation suggests, is permitted to depend on the choice of state $|\alpha\rangle$ in a non-trivial way. In effect, when $|n_\alpha| \neq 1$, the state dependence of n_α in (1.3) accommodates the possibility (raised earlier in [16, 17]) that the quantum counterparts of canonical transformations may not be represented by unitary operators. (In our work, unless stated otherwise, we deal with systems of one degree of freedom but use of the quantum canonical transform in (1.3) is not limited to such systems [18–20].)

In [9], there is no analysis of the mechanism for non-unitarity. The introduction of the state-dependent normalization factor n_α in [9] was prompted by the explicit construction of normalized stationary-state wavefunctions of a specific model (the Liouville model) using the canonical transform in (1.3). However, it has been observed [3] that the natural definition of quantum canonical transformations as changes of the non-commuting phase-space variables which preserve the canonical commutation relations is purely algebraic in character (without any reference to an underlying Hilbert space and its inner product), and hence, such transformations are not intrinsically unitary (or non-unitary for that matter). Although it does not seem to be widely appreciated, several of the familiar tools for obtaining closed-form solutions in quantum mechanics can be construed as quantum canonical transformations and few of these are unitary [3, 21].

In this paper, we are interested in those quantum canonical transformations which have a counterpart within classical mechanics. Our aim is to refine our understanding of the circumstances under which such transformations can be non-unitary. Specifically, we discuss a class of quantum canonical transformations which relate equivalent quantum systems. In this context, it is natural to expect that if these transformations act within a single Hilbert space, they should be unitary [3]. Although this property is definitely a sufficient requirement for establishing the equivalence of two quantum theories, we identify examples of quantum canonical transformations of this kind which are non-unitary. The distinguishing feature of these transformations is that their classical counterparts are non-linear.

The classical counterparts of the transformations we consider have the property that the transformed Hamiltonian function (or Kamiltonian) $\mathcal{K}(Q, P) \equiv \mathcal{H}(q(Q, P), p(Q, P))$ is the same as the original Hamiltonian function $\mathcal{H}$, i.e. $\mathcal{K}(Q, P) = \mathcal{H}(Q, P)$. For systems of one degree of freedom, these transformations map trajectories of such systems (level curves of $\mathcal{H}$) onto themselves and, thus, amount to evolutions. At the quantum level, the new wavefunctions $\Phi_\alpha(Q)$ and the old wavefunctions $\phi_\alpha(q)$ coincide, i.e. $\Phi_\alpha(Q) = \phi_\alpha(Q)$ (because the Hamiltonian operators for q and Q are identical in form), and the integral transform in (1.3) reduces to an integral equation for stationary state eigenfunctions. To facilitate the derivation of these integral equations, we restrict ourselves to form-preserving canonical transformations for which the quantum generating function $F(q, Q)$ reduces to its classical counterpart $\mathcal{F}(q, Q)$. We also limit ourselves to Hamiltonians describing a particle of mass m in the potential $\mathcal{V}(q)$.

In section 3, we demonstrate that, in addition to the free theory ($\mathcal{V} \equiv 0$), there are six distinct choices of potential $\mathcal{V}(q)$ for which infinite families $\{\mathcal{F}_\mu(q, Q)\}$ of non-trivial form-preserving and quantum correction-free generating functions exist (μ is a continuous label of the members of these families). These potentials include some of the most ubiquitous (notably the linear and quadratic) potentials, and the integral equations

$$\psi_\alpha(q) = \mathcal{N}_\alpha(\mu) \int \mathrm{e}^{(\mathrm{i}/\hbar)\mathcal{F}_\mu(q,Q)} \psi_\alpha(Q)\, \mathrm{d}Q \tag{1.4}$$

apply to several standard special functions of mathematical physics (in the notation of [22], the parabolic cylinder functions D_n (integer order), the Airy function Ai, the modified Bessel functions K_σ (imaginary order), the Mathieu functions ce_r and se_r and the modified Mathieu functions $Mc_r^{(1)}$ and $Ms_r^{(1)}$). None of these integral equations is novel but our interpretation of their origin is.

The major preoccupation of this paper is not with the kernels $\mathrm{e}^{(\mathrm{i}/\hbar)\mathcal{F}_\mu(q,Q)}$ in these integral equations, but with the reciprocals $\mathcal{N}_\alpha(\mu)$ of their eigenvalues. We show that these reciprocals can also be obtained (modulo, in some cases, a phase) by exploiting the algebra and symmetries of the pertinent canonical transformations. Two distinct and complementary methods apply. For those potentials for which the canonical transformations form an Abelian group (the linear and quadratic potentials), the composition of canonical transformations implies a functional relation for $\mathcal{N}_\alpha(\mu)$ which determines it up to a phase (see section 4). For the other potentials, we can take advantage of a remarkable symmetry in the dependence of the corresponding generating functions $\mathcal{F}_\mu(q, Q)$ on μ, q and Q (described in section 5).

In section 6, we close by discussing the significance of our findings apropos the issue of unitarity. We also remark on lines of investigation suggested by this work. To make the paper self-contained, we begin in section 2 with a brief summary of the use of the quantum canonical transform focusing on the relation between the quantum generating function $F(q, Q)$ and its classical counterpart $\mathcal{F}(q, Q)$. We demonstrate that this relation respects the algebra of the composition of canonical transformations (a fact we use extensively in section 4) and spell out the conditions under which the quantum corrections to $\mathcal{F}(q, Q)$ vanish. Some of the results in sections 3 and 5 have been reported in [23].

2. The quantum canonical transform

Let $\{\phi_\alpha(q)\}$ denote the complete set of stationary wavefunctions of a quantum system with the Hamiltonian operator $\widehat{h}\big(q, \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial q}\big)$ and let $\widehat{H}\big(Q, \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial Q}\big)$ be the realization of the Hamiltonian of the system for another choice of generalized coordinate Q and $\{\Phi_\alpha(Q)\}$, the corresponding complete set of stationary wavefunctions. The quantum canonical transform relates the $\phi_\alpha(q)$

to the $\Phi_\alpha(Q)$ via an integral relationship of the form in (1.3). The quantum generating function $F(q, Q)$ is fixed by the requirement that $\phi_\alpha(q)$ and $\Phi_\alpha(Q)$ are eigenfunctions of the same complete set of commuting observables with exactly the same set of quantum numbers α. The state-dependent relative normalization n_α is chosen so that the normalizations of $\phi_\alpha(q)$ and $\Phi_\alpha(Q)$ are compatible.

For a system with a non-degenerate energy spectrum (such as those considered in sections 4 and 5), the restriction on $F(q, Q)$ reduces to the condition that $\phi_\alpha(q)$ and $\Phi_\alpha(Q)$ are eigenfunctions of $\widehat{h}$ and $\widehat{H}$, respectively, with the same energy E_α. Substituting for ϕ_α in $\widehat{h}\phi_\alpha = E_\alpha\phi_\alpha$ using (1.3) and then replacing the product $E_\alpha\Phi_\alpha$ by $\widehat{H}\Phi_\alpha$, we find that, after the requisite number of integrations by parts and appealing to the completeness of the Φ_α, this condition implies that $F(q, Q)$ should satisfy

$$\widehat{h}\left(q, \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial q}\right)\mathrm{e}^{(\mathrm{i}/\hbar)F(q,Q)} = \widehat{H}\left(Q, -\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial Q}\right)\mathrm{e}^{(\mathrm{i}/\hbar)F(q,Q)} \tag{2.1}$$

provided the endpoint terms generated in the integrations by parts vanish. These terms take the form of the bilinear combination

$$P\left(\Phi_\alpha, \mathrm{e}^{(\mathrm{i}/\hbar)F(q,Q)}\right) = \mathrm{e}^{(\mathrm{i}/\hbar)F(q,Q)}\frac{\partial}{\partial Q}\Phi_\alpha - \Phi_\alpha\frac{\partial}{\partial Q}\mathrm{e}^{(\mathrm{i}/\hbar)F(q,Q)} \tag{2.2}$$

for the Hamiltonian

$$\widehat{H}\left(Q, \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial Q}\right) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial Q^2} + V(Q) \tag{2.3}$$

considered below. For bound states, the vanishing of the wavefunction and its first derivative at infinity guarantees that the bilinear concomitant in (2.2) is zero.

The relation of the quantum generating function to a generating function $f_{\mathrm{cl}}(q, Q)$ of a canonical transformation within the Hamiltonian formulation of classical mechanics can be brought out by adopting for $F(q, Q)$ an expansion in powers of $\mathrm{i}\hbar$:

$$F(q, Q) = \sum_{n=0}^{\infty}\mathcal{F}_n(q, Q)(\mathrm{i}\hbar)^n.$$

If we take $\widehat{H}\left(Q, \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial Q}\right)$ to be given by (2.3) and $\widehat{h}\left(q, \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial q}\right)$ to be given by

$$\widehat{h}\left(q, \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial q}\right) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + v(q)$$

then substitution of this expansion into (2.1) yields for $\mathcal{F}_0$

$$\frac{1}{2m}\left(\frac{\partial\mathcal{F}_0}{\partial q}\right)^2 + v(q) = \frac{1}{2m}\left(-\frac{\partial\mathcal{F}_0}{\partial Q}\right)^2 + V(Q) \tag{2.4}$$

and for the other $\mathcal{F}_n$ $(n > 0)$

$$\sum_{k=0}^{n}\left(\frac{\partial\mathcal{F}_k}{\partial q}\frac{\partial\mathcal{F}_{n-k}}{\partial q} - \frac{\partial\mathcal{F}_k}{\partial Q}\frac{\partial\mathcal{F}_{n-k}}{\partial Q}\right) = \frac{\partial^2\mathcal{F}_{n-1}}{\partial q^2} - \frac{\partial^2\mathcal{F}_{n-1}}{\partial Q^2}. \tag{2.5}$$

Equation (2.4) is automatically satisfied if we identify $\mathcal{F}_0(q, Q)$ as the classical generating function of a canonical transformation $(q, p) \longrightarrow (Q, P)$ for which the original Hamiltonian function $\mathcal{H}(q, p) = p^2/(2m) + v(q)$ and the transformed Hamiltonian function (or Kamiltonian) $\mathcal{K}(Q, P) = P^2/(2m) + V(Q)$. If $\partial^2\mathcal{F}_0/\partial q^2 = \partial^2\mathcal{F}_0/\partial Q^2$, i.e. $\mathcal{F}_0$ is of the form

$$\mathcal{F}_0(q, Q) = \mathcal{F}_+(q_+) + \mathcal{F}_-(q_-) \tag{2.6}$$

where $q_\pm \equiv (q \pm Q)/2$ and $\mathcal{F}_+$ and $\mathcal{F}_-$ are arbitrary functions, then (2.5) implies that the quantum corrections $\mathcal{F}_n$ ($n \geqslant 1$) can be taken to be zero.

The parallel between quantum and classical generating functions also extends to the composition of transformations. Let $F_1(q, q_i)$ and $F_2(q_i, Q)$ denote the quantum generating functions for the canonical transformations $(q, p) \longrightarrow (q_i, p_i)$ and $(q_i, p_i) \longrightarrow (Q, P)$, respectively. The exact relation among these generating functions and the quantum generating function $F_c(q, Q)$ for the composition $(q, p) \longrightarrow (Q, P)$ reads

$$n_\alpha^{(1)} n_\alpha^{(2)} \int \mathrm{e}^{(\mathrm{i}/\hbar)[F_1(q,q_i)+F_2(q_i,Q)]}\,\mathrm{d}q_i = n_\alpha^{(c)}\,\mathrm{e}^{(\mathrm{i}/\hbar)F_c(q,Q)}. \tag{2.7}$$

To identify the relation between the classical contribution f_c to F_c and the classical contributions to F_1 and F_2 (assumed to be f_1 and f_2, respectively), we can evaluate the integration over q_i in (2.7) in the stationary phase approximation. Retaining only the terms most singular in $\hbar$, we obtain

$$n_\alpha^{(c)}\,\mathrm{e}^{(\mathrm{i}/\hbar)f_c(q,Q)} = \sqrt{\frac{2\pi\hbar\mathrm{i}}{\kappa}}\, n_\alpha^{(1)} n_\alpha^{(2)}\,\mathrm{e}^{(\mathrm{i}/\hbar)f_s(q,Q)} \tag{2.8}$$

where

$$f_s(q, Q) \equiv f_1(q, \overline{q_i}) + f_2(\overline{q_i}, Q) \tag{2.9}$$

with $\overline{q_i}$ chosen such that

$$\frac{\partial}{\partial q_i}\left(f_1(q, q_i) + f_2(q_i, Q)\right)\bigg|_{q_i=\overline{q_i}} = 0 \tag{2.10}$$

and we have made the generically valid assumption that

$$\kappa \equiv \left(\frac{\partial^2 f_1}{\partial q_i^2} + \frac{\partial^2 f_2}{\partial q_i^2}\right)\bigg|_{q_i=\overline{q_i}}$$

is non-zero. (For simplicity, we have also assumed that there is only one stationary point.) Interpretation of (2.8) is complicated by the unknown, but, in general, singular dependence of the relative normalizations $n_\alpha^{(1)}$, $n_\alpha^{(2)}$ and $n_\alpha^{(c)}$ on $\hbar$. Nevertheless, the essential singularities in $\hbar$ in (2.8) can only match if the dependence on q and Q cancels—i.e. f_c and f_s differ at most by a constant. Exactly the same relation between f_c and f_s is implied by the canonical formalism of classical mechanics. We have that

$$\frac{\partial f_s}{\partial q} = \frac{\partial f_1}{\partial q} + \left(\frac{\partial f_1}{\partial q_i} + \frac{\partial f_2}{\partial q_i}\right)\bigg|_{q_i=\overline{q_i}} \frac{\partial \overline{q_i}}{\partial q} = \frac{\partial f_1}{\partial q} = +p$$

$$\frac{\partial f_s}{\partial Q} = \frac{\partial f_2}{\partial Q} + \left(\frac{\partial f_1}{\partial q_i} + \frac{\partial f_2}{\partial q_i}\right)\bigg|_{q_i=\overline{q_i}} \frac{\partial \overline{q_i}}{\partial Q} = \frac{\partial f_2}{\partial Q} = -P$$

i.e. the partial derivatives of f_s coincide with those of f_c. As far as the composition of transformations is concerned, the relation between classical and quantum generating functions found in semiclassical work based on (1.2) is not destroyed by the insertion of the state-dependent normalization factor n_α in (1.3).

3. Invariant Hamiltonian functions

Quantum generating functions $F(q, Q)$ which give rise to integral equations can be obtained by determining *classical* generating functions $\mathcal{F}_0(q, Q)$ of the form in (2.6) which induce canonical transformations $q, p \longrightarrow Q, P$ such that the Kamiltonian function $\mathcal{K}(Q, P) \equiv \mathcal{H}(q(Q, P), p(Q, P))$ is the same as the original Hamiltonian function $\mathcal{H}$, i.e. $\mathcal{K}(Q, P) = \mathcal{H}(Q, P)$. (Below, we drop the subscript 0, denoting $\mathcal{F}_0$ by $\mathcal{F}$.)

We consider a canonically conjugate pair of variables q and p for which the Hamiltonian function is

$$\mathcal{H}(q, p) = \frac{p^2}{2m} + \mathcal{V}(q).$$

Inspection of the relations for the momenta in terms of a classical generating function $\mathcal{F}(q, Q)$,

$$p = \frac{\partial \mathcal{F}}{\partial q} = \frac{1}{2}[\mathcal{F}'_-(q_-) + \mathcal{F}'_+(q_+)] \qquad P = -\frac{\partial \mathcal{F}}{\partial Q} = \frac{1}{2}[\mathcal{F}'_-(q_-) - \mathcal{F}'_+(q_+)] \tag{3.1}$$

shows that at least for the case of the free theory ($V \equiv 0$) there are non-trivial canonical transformations under which the form of the Hamiltonian is unchanged: for the generating functions $\mathcal{F}^+_{\text{free}} = \mathcal{F}_-(q_-)$ and $\mathcal{F}^-_{\text{free}} = \mathcal{F}_+(q_+)$, where $\mathcal{F}_+$ and $\mathcal{F}_-$ are arbitrary, the transformed generalized momentum $P = +p$ and $P = -p$, respectively, from which the form invariance of the free Hamiltonian $\mathcal{H}_{\text{free}} = p^2/(2m)$ is obvious.

More generally, substituting for the momenta in

$$\frac{p^2}{2m} + \mathcal{V}(q) = \frac{P^2}{2m} + \mathcal{V}(Q)$$

using (3.1), we deduce that the following relation must hold between $\mathcal{V}$ and $\mathcal{F}_\pm$:

$$\frac{1}{2m}\mathcal{F}'_+(q_+)\mathcal{F}'_-(q_-) = \mathcal{V}(q_+ - q_-) - \mathcal{V}(q_+ + q_-). \tag{3.2}$$

To proceed, we assume that $\mathcal{F}'_-$ and $\mathcal{V}$ are analytic and expand both sides of (3.2) in powers of q_- to obtain ($k = 0, 1, 2, \ldots$)

$$\frac{1}{2m}\mathcal{F}'_+(x)\mathcal{F}^{(k+1)}_-(0) = [(-1)^k - 1]\mathcal{V}^{(k)}(x) \tag{3.3}$$

where we have set $q_+ = x$. If we ignore the possibility that $\mathcal{V}'(x) \equiv 0$ (in which case we recover the results given above for the free theory), then (3.3) for $k = 1$ implies that $\mu \equiv \mathcal{F}^{(2)}_-(0) \neq 0$ and

$$\mathcal{F}'_+(x) = -\frac{4m}{\mu}\mathcal{V}'(x). \tag{3.4}$$

Substituting (3.4) into (3.3), it reduces to the simultaneous requirements that *odd* derivatives of $\mathcal{V}$ are given by

$$\mathcal{V}^{(k)}(x) = \frac{\mathcal{F}^{(k+1)}_-(0)}{\mathcal{F}^{(2)}_-(0)}\mathcal{V}'(x) \tag{3.5}$$

and that $\mathcal{F}_-$ is even (so that the derivatives $\mathcal{F}^{(n)}_-(0) = 0$ for n odd).

From (3.4), we immediately have that

$$\mathcal{F}_+(x) = -\frac{4m}{\mu}\mathcal{V}(x)$$

where we have dropped an irrelevant constant of integration. The implications of (3.5) for $\mathcal{V}$ and $\mathcal{F}_-$ depend on whether or not the third derivative $\mathcal{V}^{(3)}$ vanishes.

If $\mathcal{V}^{(3)}(x) \neq 0$, then (3.5) implies that $\rho \equiv \mathcal{F}^{(4)}_-(0)/\mathcal{F}^{(2)}_-(0) \neq 0$, $\mathcal{V}^{(3)}(x) = \rho V^{(1)}(x)$ and $\mathcal{F}^{(2k)}_-(0) = \rho^{k-1}\mu$ for $k > 1$. Thus, since ρ may be of either sign, the potential can be either the combination of hyperbolic functions ($\rho = +\beta^2 > 0$),

$$\mathcal{V}_+(x) = A\cosh\beta x + B\sinh\beta x$$

Table 1. Standard forms of potentials $\mathcal{V}$ and the corresponding (classical) generating functions $\mathcal{F}_\mu$.

	$\mathcal{V}(q)$	$\mathcal{F}_\mu(q, Q)$
Quadratic	$\frac{1}{2}\lambda q^2$	$-\frac{m\lambda}{2\mu}(q+Q)^2 + \frac{\mu}{8}(q-Q)^2$
Sinusoidal	$\frac{\lambda}{4a^2}\cos 2aq$	$-\frac{m\lambda}{\mu a^2}\cos a(q+Q) - \frac{\mu}{4a^2}\cos a(q-Q)$
Even hyperbolic	$\frac{\lambda}{4a^2}\cosh 2aq$	$-\frac{m\lambda}{\mu a^2}\cosh a(q+Q) + \frac{\mu}{4a^2}\cosh a(q-Q)$
Linear	λq	$-\frac{2m\lambda}{\mu}(q+Q) + \frac{\mu}{8}(q-Q)^2$
Exponential	$\frac{\lambda}{2a}\,\mathrm{e}^{2aq}$	$-\frac{2m\lambda}{\mu a}\,\mathrm{e}^{a(q+Q)} + \frac{\mu}{4a^2}\cosh a(q-Q)$
Odd hyperbolic	$\frac{\lambda}{2a}\sinh 2aq$	$-\frac{2m\lambda}{\mu a}\sinh a(q+Q) + \frac{\mu}{4a^2}\cosh a(q-Q)$

or the combination of sinusoidal functions ($\rho = -\beta^2 < 0$),

$$\mathcal{V}_-(x) = A\cos\beta x + B\sin\beta x$$

where β, A and B are arbitrary constants. The corresponding forms of $\mathcal{F}_-$ are (up to arbitrary additive constants)

$$\mathcal{F}_-^+(x) = \frac{\mu}{\beta^2}\cosh\beta x$$

and

$$\mathcal{F}_-^-(x) = -\frac{\mu}{\beta^2}\cos\beta x$$

respectively. If we assume that $\mathcal{V}^{(3)}(x) \equiv 0$, then (3.5) implies that, with the exception of $\mathcal{F}_-^{(2)}(0)$, all the even derivatives $\mathcal{F}_-^{(2n)}(0) = 0$. Discarding arbitrary additive constants, the potential is of the quadratic form $\mathcal{V}(x) = Ax^2 + Bx$, where, as above, A and B are arbitrary constants, and $\mathcal{F}_-$ is the quadratic $\mathcal{F}_-(x) = \mu x^2/2$.

Not only are there several classes of potential $\mathcal{V}(q)$ compatible with (3.2), but also, for each class of potentials, there is an infinite family of canonical transformations distinguished by different values of the parameter μ which is not fixed by the considerations above. By translation of the origin or the inversion $q \longrightarrow -q$ or translation followed by inversion, all members of the classes of non-trivial potentials identified above can be reduced to one of those in table 1. We also include the families of generating functions $\mathcal{F}_\mu$ of canonical transformations which leave the corresponding Hamiltonians unchanged. In what follows, we take $\lambda > 0$, a choice which embraces the physically more interesting scenarios.

Below (in section 5), we shall have cause to invoke the limit $\mu \to \infty$. From (3.1) and (3.4), the difference in momenta

$$P - p = \frac{4m}{\mu}\mathcal{V}'(q_+). \tag{3.6}$$

The difference in the coordinates $Q - q$ $(= -2q_-)$ in terms of $p + P$ can be obtained by inversion of the relation

$$P + p = \mathcal{F}_-'(q_-) \tag{3.7}$$

implied by (3.1). Together, (3.6) and (3.7) imply that, for our choices of $\mathcal{F}_-$, both $P - p$ and $Q - q$ are of order $1/\mu$ for large μ. (In the case of the sinusoidal potential, use of the principal value of arcsin in the inversion of (3.7) is understood.) Hence, in the limit $\mu \to \infty$, all the canonical transformations of interest reduce to the identity transformation.

4. Integral equations for the quadratic and linear potentials

It is natural to ask whether any of the families of canonical transformations we have identified are groups. At the level of generating functions, this question translates into whether when two generating functions $\mathcal{F}_{\mu_1}$ and $\mathcal{F}_{\mu_2}$ of a particular family in table 1 are combined according to (2.9), the resulting generating function $\mathcal{F}_{\mu_1\mu_2}$ is also a member of that family (to within an additive constant). This is not automatic since these families of generating functions have been constructed by restricting their members to be of the special form in (2.6) and this constraint cannot, in general, be respected by the prescription in (2.9). However, it turns out that, because of the simple geometrical operations in phase space effected by members of the families of canonical transformations corresponding to the quadratic and linear potentials, these two families do form groups. We are able to exploit the Abelian character of these groups to convert (2.7) into a functional relationship for the reciprocals $\mathcal{N}_\alpha(\mu)$ of eigenvalues and so fix them up to a phase factor (see (4.4) and (4.8)).

4.1. The quadratic potential

The canonical transformations which leave the Hamiltonian function associated with this potential unchanged are linear transformations of the phase plane and so must be either a rotation, an area-preserving shear or an area-preserving squeeze [24]. The observation that, for the rescaled canonical variables $q_s \equiv (m\lambda)^{1/4}q$ and $p_s \equiv p/(m\lambda)^{1/4}$, the Hamiltonian function

$$\mathcal{H} = \frac{1}{2}\sqrt{\frac{\lambda}{m}}\left(p_s^2 + q_s^2\right)$$

suggests that it should be possible to decompose these transformations in terms of a rotation as

$$\begin{bmatrix} Q \\ P \end{bmatrix} = \begin{pmatrix} (m\lambda)^{-1/4} & 0 \\ 0 & (m\lambda)^{1/4} \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} (m\lambda)^{1/4} & 0 \\ 0 & (m\lambda)^{-1/4} \end{pmatrix} \begin{bmatrix} q \\ p \end{bmatrix}$$

where the angle of rotation θ is dependent on the choice μ. In fact, this does prove to be the case with the free parameter μ uniquely related to the angle of rotation θ by

$$\mu = -2\sqrt{\lambda m}\cot\frac{\theta}{2}.$$

The totality of these linear transformations thus constitutes a faithful matrix representation of the rotation group $SO(2)$.

It is convenient to work with generating functions parametrized by θ instead of μ, namely

$$F(q, Q|\theta) = \tfrac{1}{2}m\omega[2\,\mathrm{cosec}\,\theta\, qQ - \cot\theta(q^2 + Q^2)] \tag{4.1}$$

where $\omega \equiv \sqrt{\lambda/m}$. We write the corresponding integral equation for eigenfunctions $\{\psi_n(q)\}$ (n a non-negative integer) of the harmonic oscillator Hamiltonian

$$\widehat{h}_{\mathrm{ho}} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + \frac{1}{2}m\omega^2 q^2$$

as

$$\psi_n(q) = N_n(\theta)\int \mathrm{e}^{(\mathrm{i}/\hbar)F(q,\,Q|\theta)}\psi_n(Q)\,\mathrm{d}Q. \tag{4.2}$$

Since $\widehat{h}_{\mathrm{ho}}$ commutes with the parity operator $\widehat{P}$ and has a non-degenerate spectrum, its eigenfunctions are automatically either even or odd. Although the generating function $F(q, Q|\theta)$ has been constructed only with a view to ensure that the integral on the right-hand side of (4.2) is an eigenfunction of $\widehat{h}_{\mathrm{ho}}$ with the same eigenenergy as $\psi_n(q)$, the dependence of $F(q, Q|\theta)$ on q and Q guarantees that this integral also has the same parity as $\psi_n(q)$. The generating function pertinent to the sinusoidal potential shares this property.

Use of θ in (4.2) simplifies the treatment of the composition of transformations. We can immediately identify the quantum generating function $F_c(q, Q)$ for the composition of two transformations with generating functions $F_1 = F(q, q_i|\theta_1)$ and $F_2 = F(q_i, Q|\theta_2)$, respectively, as $F_c(q, Q) = F(q, Q|\theta_1 + \theta_2)$. Accordingly, in this context, (2.7) reads

$$N_n(\theta_1)N_n(\theta_2) \int \mathrm{e}^{(\mathrm{i}/\hbar)[F(q,q_i|\theta_1)+F(q_i,Q|\theta_2)]}\,\mathrm{d}q_i = N_n(\theta_1+\theta_2)\,\mathrm{e}^{(\mathrm{i}/\hbar)F(q,Q|\theta_1+\theta_2)}$$

which, on evaluation of the Gaussian integral over q_i, becomes

$$N_n(\theta_1+\theta_2) = \sqrt{\frac{2\pi\hbar}{m\omega\mathrm{i}}}\sqrt{\frac{\sin\theta_1\sin\theta_2}{\sin(\theta_1+\theta_2)}}N_n(\theta_1)N_n(\theta_2). \tag{4.3}$$

The functional relation in (4.3) has the solution

$$N_n(\theta) = \sqrt{\frac{m\omega\mathrm{i}}{2\pi\hbar}}\frac{\mathrm{e}^{c_n\theta}}{\sqrt{\sin\theta}} \tag{4.4}$$

where the coefficient c_n is arbitrary.

The coefficient c_n can be fixed by appealing to the fact that, under the inversion $q, p \longrightarrow -q, -p$ (corresponding to the choice of $\theta = \pi$ in $F(q, Q|\theta)$), the eigenfunctions $\psi_n(q)$ transform in a well-defined manner: $\psi_n(-q) = (-1)^n\psi_n(q)$. From (4.1) and (4.4),

$$\lim_{\theta\to\pi} N_n(\theta)\,\mathrm{e}^{(\mathrm{i}/\hbar)F(q,Q|\theta)} = \mathrm{i}\,\mathrm{e}^{c_n\pi}\,\delta(q+Q)$$

which, on substitution in (4.2), implies $\psi_n(q) = \mathrm{i}\,\mathrm{e}^{c_n\pi}\,\psi_n(-q)$. Consistency with the parity properties of the $\psi_n(q)$ is achieved by taking $c_n = -(n+1/2)\mathrm{i}$.

In its final form, our integral equation for the eigenfunctions $\psi_n(q)$ of the harmonic oscillator reads

$$\psi_n(q) = \sqrt{\frac{m\omega\mathrm{i}}{2\pi\hbar}}\frac{\mathrm{e}^{-\mathrm{i}(n+1/2)\theta}}{\sqrt{\sin\theta}}\int \exp(\mathrm{i}[m\omega/(2\hbar)][2\,\mathrm{cosec}\,\theta\,qQ - \cot\theta(q^2+Q^2)])\psi_n(Q)\,\mathrm{d}Q. \tag{4.5}$$

To make the connection with known results, we note that we may read off from (4.5) that the expansion coefficients of $N_0(\theta)\,\mathrm{e}^{(\mathrm{i}/\hbar)F(q,Q|\theta)}$ in the orthonormal basis $\{\psi_n(Q)\}$ are $\mathrm{e}^{\mathrm{i}n\theta}\psi_n(q)$ and, hence, construct the identity

$$\exp(\mathrm{i}[m\omega/(2\hbar)][2\,\mathrm{cosec}\,\theta\,qQ - \cot\theta(q^2+Q^2)]) = \sqrt{\frac{2\pi\hbar}{m\omega\mathrm{i}}}\sqrt{\sin\theta}\sum_n \mathrm{e}^{+\mathrm{i}(n+1/2)\theta}\psi_n(q)\psi_n(Q).$$

Invoking the relation of the $\psi_n(q)$ to the parabolic cylinder function $D_n(x)$ [22], namely

$$\psi_n(q) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{n!}}D_n(\sqrt{2m\omega/\hbar}q)$$

we recover one of the addition theorems for the D_n given in chapter 11 of [25]. (To obtain this addition theorem in the precise form given in [25], we must set $\mathrm{e}^{\mathrm{i}\theta} = \mathrm{i}\tan\phi$, $\sqrt{m\omega/\hbar}q = \mathrm{e}^{\mathrm{i}\pi/4}\lambda$ and $\sqrt{m\omega/\hbar}Q = \mathrm{e}^{\mathrm{i}3\pi/4}\mu$.)

4.2. The linear potential

The relevant canonical transformations involve an area-preserving shear of the phase plane coupled with a shift of the origin:

$$\begin{bmatrix} Q \\ P \end{bmatrix} = \begin{pmatrix} 1 & -2\nu \\ 0 & 1 \end{pmatrix} \begin{bmatrix} q \\ p \end{bmatrix} + 2m\lambda\nu \begin{bmatrix} -\nu \\ 1 \end{bmatrix} \equiv \mathcal{T}_\nu \begin{bmatrix} q \\ p \end{bmatrix}$$

where we have introduced the parameter $\nu \equiv 2/\mu$ which makes the algebra of these transformations more transparent. (The factor of 2 in the definition of ν is a matter of convenience.) Because of the shift in origin, it is perhaps not obvious that this class of geometrical operations should form a group, but, in fact, the composition

$$\mathcal{T}_{\nu_1}\mathcal{T}_{\nu_2} = \mathcal{T}_{\nu_1+\nu_2} \tag{4.6}$$

so that the transformations $\mathcal{T}_\nu$ are a representation of an Abelian affine group.

Let $F_\nu(q, Q)$ denote the generating function of these canonical transformations when ν and not μ is adopted as the free parameter, i.e.

$$F_\nu(q, Q) = -m\lambda\nu(q + Q) + \frac{1}{4\nu}(q - Q)^2$$

and let $\psi_E(q)$ (E real) denote the eigenfunction of

$$\widehat{h}_{\text{linear}} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + \lambda q$$

with eigenenergy E. Identifying F_1, F_2 and F_c in (2.7) with F_{ν_1}, F_{ν_2} and $F_{\nu_1+\nu_2}$, respectively, we find that the reciprocals $N_E(\nu)$ of the eigenvalues in the integral equation involving the eigenfunction $\psi_E(q)$ must satisfy

$$N_E(\nu_1 + \nu_2) = \sqrt{4\pi\hbar \mathrm{i}}\sqrt{\frac{\nu_1\nu_2}{\nu_1 + \nu_2}}\, \mathrm{e}^{-(\mathrm{i}m^2\lambda^2/\hbar)\nu_1\nu_2(\nu_1+\nu_2)} N_E(\nu_1)N_E(\nu_2). \tag{4.7}$$

Equation (4.7) determines $N_E(\nu)$ to be of the form

$$N_E(\nu) = \frac{1}{\sqrt{4\pi\hbar \mathrm{i}\nu}}\, \mathrm{e}^{(\mathrm{i}/\hbar)\left(c_E\nu - m^2\lambda^2\nu^3/3\right)}. \tag{4.8}$$

The E dependence of the coefficient c_E can be pinned down by using the relation of eigenfunctions of non-zero energy $\psi_E(q)$ to the zero energy eigenfunction $\psi_0(q)$:

$$\psi_E(q) = \eta_E\psi_0(q - E/\lambda) \tag{4.9}$$

where η_E is a constant of modulus unity which we assume below is absorbed into the definition of $\psi_E(q)$ with an appropriate choice of the phase.

Using (4.9) to substitute for $\psi_E(Q)$ and $\psi_E(q)$ in the integral equation

$$\psi_E(q) = N_E(\nu)\int \mathrm{e}^{(\mathrm{i}/\hbar)F_\nu(q,Q)}\psi_E(Q)\,\mathrm{d}Q \tag{4.10}$$

we find, after the change of variable $Q \to Q' = Q - E/\lambda$,

$$\begin{aligned}\psi_0(q - E/\lambda) &= N_E(\nu)\,\mathrm{e}^{-\mathrm{i}2mE\nu/\hbar}\int \mathrm{e}^{(\mathrm{i}/\hbar)F_\nu(q-E/\lambda,Q')}\psi_0(Q')\,\mathrm{d}Q' \\ &= \frac{N_E(\nu)}{N_0(\nu)}\,\mathrm{e}^{-\mathrm{i}2mE\nu/\hbar}\psi_0(q - E/\lambda)\end{aligned}$$

where to obtain the last equality we have invoked (4.10) again. The choice $c_E = 2mE$ is indicated.

An independent check of these results is given by working with the momentum space equivalent of (4.10):

$$\widetilde{\psi}_E(p) = N_E(\nu)\int K(p,P)\widetilde{\psi}_E(P)\,\mathrm{d}P \tag{4.11}$$

where the kernel

$$\begin{aligned} K(p,P) &\equiv \int \mathrm{e}^{-\mathrm{i}pq/\hbar}\,\mathrm{e}^{(\mathrm{i}/\hbar)F_\nu(q,Q)}\,\mathrm{e}^{+\mathrm{i}PQ/\hbar}\frac{\mathrm{d}Q\,\mathrm{d}q}{2\pi\hbar} \\ &= \sqrt{4\pi\hbar\mathrm{i}\nu}\,\mathrm{e}^{-\mathrm{i}[\nu/(4\hbar)](p+P)^2}\delta(P-p-2m\lambda\nu) \end{aligned}$$

and the Fourier transform

$$\widetilde{\psi}_E(p) \equiv \frac{1}{\sqrt{2\pi\hbar}}\int \mathrm{e}^{-\mathrm{i}pq/\hbar}\psi_E(q)\,\mathrm{d}q = \mathrm{e}^{-\mathrm{i}Ep/(\hbar\lambda)}\widetilde{\psi}_0(p).$$

The delta function in $K(p,P)$ enforces the relation between the momenta in the canonical transformation generated by $F_\nu(q,Q)$ and reduces (4.11) to the algebraic equation

$$\widetilde{\psi}_0(p)\,\mathrm{e}^{-\mathrm{i}p^3/(6m\lambda\hbar)} = N_E(\nu)\sqrt{4\pi\hbar\mathrm{i}\nu}\,\mathrm{e}^{-(\mathrm{i}/\hbar)(2mE\nu-m^2\lambda^2\nu^3/3)}\widetilde{\psi}_0(p+2m\lambda\nu)\,\mathrm{e}^{-\mathrm{i}(p+2m\lambda\nu)^3/(6m\lambda\hbar)}.$$

Since $\widetilde{\psi}_0(p) = C\,\mathrm{e}^{+\mathrm{i}p^3/(6m\lambda\hbar)}$, where C is a normalization constant, we recover the above results for $N_E(\nu)$.

The zero energy eigenfunction $\psi_0(q)$ (and hence all the other eigenfunctions $\psi_E(q)$) is related to the Airy function $\mathrm{Ai}(x)$ [22]:

$$\psi_0(q) = \frac{\gamma}{\sqrt{\lambda}}\mathrm{Ai}(\gamma q)$$

where $\gamma \equiv (2m\lambda/\hbar^2)^{1/3}$. (For the sake of definiteness, the normalization is fixed so that $\langle\psi_E|\psi'_E\rangle = \delta(E-E')$.) Thus, in terms of the Airy function $\mathrm{Ai}(x)$, our integral equation (4.10) amounts to the relation

$$\mathrm{Ai}(x) = \frac{1}{\sqrt{4\pi\mathrm{i}s}}\,\mathrm{e}^{-\mathrm{i}s^3/12}\int \mathrm{e}^{\mathrm{i}[-s(x+X)/2+(x-X)^2/(4s)]}\mathrm{Ai}(X)\,\mathrm{d}X$$

where we have set $x = \gamma q$, $X = \gamma Q$ and $s = \hbar\gamma^2\nu$.

5. Integral equations for the other potentials

In section 3, we found that, for potentials $\mathcal{V}(x)$ for which $\mathcal{V}^{(3)} \neq 0$, non-trivial form-preserving correction-free generating functions $\mathcal{F}_\mu(q,Q)$ exist only if $\mathcal{V}''(x) = \rho\mathcal{V}(x)$ (ρ is a constant). A related implication is that the dependence of these generating functions on q and Q must be such that

$$\frac{\partial^2\mathcal{F}_\mu}{\partial q^2} = \frac{\rho}{4}\mathcal{F}_\mu = \frac{\partial^2\mathcal{F}_\mu}{\partial Q^2}. \tag{5.1}$$

The dependence on μ is such that

$$\left(\mu\frac{\partial}{\partial\mu}\right)^2\mathcal{F}_\mu = \mathcal{F}_\mu$$

which, setting $\mu = \mu(z) \equiv \mu_0\,\mathrm{e}^{\sqrt{\rho}z/2}$, becomes

$$\frac{\partial^2}{\partial z^2}\mathcal{F}_{\mu(z)} = \frac{\rho}{4}\mathcal{F}_{\mu(z)}. \tag{5.2}$$

Table 2. Parameters of the transformation $z(\mu) = 2\rho^{-1/2}\ln(\mu/\mu_0)$.

$\mathcal{V}(q)$	μ_0	$\sqrt{\rho}/2$
Sinusoidal	$2\sqrt{m\lambda}$	ia
Even hyperbolic	$2\sqrt{m\lambda}$i	a
Exponential	$4\sqrt{m\lambda a}$i	a
Odd hyperbolic	$2\sqrt{2m\lambda a}$i	a

The similarity of (5.1) and (5.2) suggests that it should be possible to treat z in $\mathcal{F}_{\mu(z)}(q, Q)$ in formally the same way as the generalized coordinates q and Q. In fact, we find that, with appropriate choices of μ_0 (which are listed in table 2),

$$\mathcal{F}_{\mu(z)}(q, Q) = \mathcal{F}_{\mu(q)}(z, Q) = \mathcal{F}_{\mu(Q)}(q, z) \tag{5.3}$$

confirming that the roles of z and q (or z and Q) may be interchanged.

Used in conjunction with the integral equation (1.4), (5.3) implies that

$$\frac{\psi_\alpha(q)}{\mathcal{N}_\alpha(\mu(z))} = \int \mathrm{e}^{(\mathrm{i}/\hbar)\mathcal{F}_{\mu(z)}(q,Q)}\psi_\alpha(Q)\,\mathrm{d}Q = \int \mathrm{e}^{(\mathrm{i}/\hbar)\mathcal{F}_{\mu(q)}(z,Q)}\psi_\alpha(Q)\,\mathrm{d}Q = \frac{\psi_\alpha(z)}{\mathcal{N}_\alpha(\mu(q))}.$$

Thus, the reciprocals $\mathcal{N}_\alpha(\mu)$ of eigenvalues are given, to within a constant C_α, by

$$\mathcal{N}_\alpha(\mu) = \frac{C_\alpha}{\psi_\alpha(z)} \tag{5.4}$$

where $z = z(\mu) \equiv \ln(\mu/\mu_0)^{2/\sqrt{\rho}}$. The constant C_α can be fixed by the requirement that

$$\lim_{\mu\to\infty} \mathcal{N}_\alpha(\mu)\,\mathrm{e}^{(\mathrm{i}/\hbar)\mathcal{F}_\mu(q,Q)} = \delta(q - Q) \tag{5.5}$$

reflecting the fact that, in the limit $\mu \longrightarrow \infty$, we recover the identity transformation from $\mathcal{F}_\mu(q, Q)$ (cf the end of section 3). The determination of C_α is inessential to the conclusions we draw in section 6 about unitarity as these rest on the fact that the μ-dependent factor in (5.4) is state-dependent.

To establish the limit on the left-hand side of (5.5), we consider the integral

$$\int \mathrm{e}^{(\mathrm{i}/\hbar)\mathcal{F}_\mu(q,Q)}\Phi(Q)\,\mathrm{d}Q \tag{5.6}$$

where $\Phi(Q)$ is a suitable test function and $\mu \gg 1$, and apply the method of stationary phase to extract the leading term in an asymptotic series (in $1/\mu$) for the integral. Only this leading term is needed for the exact evaluation of the limit in (5.5). Since $\hbar$ is kept fixed, this usage of the method of stationary phase is not equivalent to a semiclassical approximation. In the limit under consideration ($\mu \to \infty, \hbar$ fixed), it is stationary points of the term in $\mathcal{F}_\mu$ which is a function of $q - Q$ that contribute, whereas in the limit $\hbar \to 0$ (μ fixed), it would be stationary points of the *whole* of $\mathcal{F}_\mu$.

By way of illustration, we now discuss the cases of the exponential and sinusoidal potentials in more detail.

5.1. The exponential potential

The Hamiltonian

$$\widehat{h}_{\text{exponential}} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + \frac{\lambda}{2a}\,\mathrm{e}^{2aq}$$

has eigenfunctions of energy $E_k = \hbar^2 k^2/(2m)$ given up to a normalization constant by

$$\psi_k(q) \propto K_{i(k/a)}(\sqrt{m\lambda a}\, \mathrm{e}^{aq}/[\hbar a^2]) \tag{5.7}$$

where K_σ denotes a modified Bessel function of order σ (section 9.6 in [22]). Substitution of (5.7) in (5.4) yields, for the reciprocals of eigenvalues,

$$\mathcal{N}_k(\mu) = C_k / K_{i(k/a)}(\mu/[4\mathrm{i}\hbar a^2]), \tag{5.8}$$

where the constant C_k has still to be determined by consideration of the $\mu \longrightarrow \infty$ limit.

Asymptotic analysis for $\mu \gg 1$ via the method of stationary phase implies that, to leading order, the integral

$$\int \mathrm{e}^{(\mathrm{i}/\hbar)\mathcal{F}_\mu(q,Q)} \Phi(Q)\, \mathrm{d}Q \sim \sqrt{2\pi} \sqrt{\frac{4\hbar \mathrm{i}}{\mu}}\, \mathrm{e}^{-\mu/(4\hbar \mathrm{i} a^2)} \Phi(q).$$

Thus, (5.5) is satisfied provided

$$\lim_{\mu \to \infty} \sqrt{\frac{4\hbar \mathrm{i} a^2}{\mu}}\, \mathrm{e}^{-\mu/(4\hbar \mathrm{i} a^2)} \mathcal{N}_k(\mu) = \frac{a}{\sqrt{2\pi}} \tag{5.9}$$

which, on the substitution of (5.8) and use of the leading term in the asymptotic expansion of $K_\sigma(x)$ for $x \gg 1$, reduces to the requirement that $C_k = a/2$.

In terms of the variables $y \equiv \sqrt{m\lambda a}\, \mathrm{e}^{aq}/(\hbar a^2)$, $Y \equiv \sqrt{m\lambda a}\, \mathrm{e}^{aQ}/(\hbar a^2)$, $p = \mathrm{i}k/a$ and $w \equiv \mu/(4\hbar \mathrm{i} a^2)$, our integral equation reads

$$2K_p(w)K_p(y) = \int_0^\infty \mathrm{e}^{-[yY/w + w(y/Y + Y/y)]/2} K_p(Y) \frac{\mathrm{d}Y}{Y}$$

which coincides formally with equation (6.653.2) in [26] (after the change of integration variable $Y \longrightarrow x \equiv wy/Y$).

5.2. The sinusoidal potential

We confine our attention to the denumerable set of eigenfunctions $\psi_s(q)$ ($s = 0, \pm 1, \pm 2, \ldots$) of

$$\widehat{h}_{\text{sinusoidal}} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + \frac{\lambda}{4a^2}\cos 2aq$$

which are related to the Mathieu functions ce_r and se_r:

$$\psi_s(q) = \begin{cases} \mathcal{C}_s ce_s(aq, \delta) & s = 0, 1, 2, \ldots \\ \mathcal{C}_s se_{|s|}(aq, \delta) & s = -1, -2, \ldots \end{cases} \tag{5.10}$$

where the dimensionless rescaled strength of the potential $\delta \equiv m\lambda/(4\hbar^2 a^4)$ and $\mathcal{C}_s$ denotes a normalization constant.

The choice of the range of integration in the integral equation for the ψ_s,

$$\psi_s(q) = N_s(\mu) \int \mathrm{e}^{(\mathrm{i}/\hbar)\mathcal{F}_\mu(q,Q)} \psi_s(Q)\, \mathrm{d}Q$$

is dictated by the consideration that the bilinear concomitant $P(\psi_s, \mathrm{e}^{(\mathrm{i}/\hbar)\mathcal{F}_\mu(q,Q)})$ (defined in (2.2)) vanishes. This can be achieved by exploiting the periodicity of the generating function $\mathcal{F}_\mu(q, Q)$ (period $2\pi/a$ in q or Q) and the eigenfunctions $\psi_s(q)$ (period π/a for s even and $2\pi/a$ for s odd). Thus, we take the range of integration to be over one period of the generating function from 0 to $+2\pi/a$. (Use of these non-symmetric limits facilitates the comparison with the integral equations tabulated in chapter 20 of [22].)

Substituting for the wavefunction in (5.4) using (5.10) and invoking the proportionality of $ce_r(-\mathrm{i}x, \eta)$ and $se_r(-\mathrm{i}x, \eta)$ to the modified Mathieu functions $Mc_r^{(1)}(x, \eta)$ and $Ms_r^{(1)}(x, \eta)$, respectively, we find that

$$N_s(\mu) = \frac{C_s}{M_s^{(1)}(\ln[\mu/\sqrt{4m\lambda}], \delta)} \tag{5.11}$$

where C_s is independent of μ and $M_s^{(1)}(x, \eta)$ denotes the modified Mathieu function $Mc_s^{(1)}(x, \eta)$ for $s \geqslant 0$ and the modified Mathieu function $Ms_{|s|}^{(1)}(x, \eta)$ for $s < 0$.

In the asymptotic analysis of the integral in (5.6) for large μ, we encounter in the present case two points of stationary phase: $Q = Q_1 = q + O(\mu^{-2})$ and $Q = Q_2 = q - \sigma_q \pi/a + O(\mu^{-2})$, where $\sigma_q \equiv 2H(q - \pi/a) - 1$ in which $H(x)$ denotes the Heaviside step function (defined, for example, in section 1.1 of [27]). To leading order, the asymptotic expansion reads

$$\int_0^{2\pi/a} \mathrm{e}^{(\mathrm{i}/\hbar)\mathcal{F}_\mu(q,Q)} \Phi(Q)\,\mathrm{d}Q \sim \sqrt{\frac{8\pi\hbar}{\mu}} \left[\mathrm{e}^{-\mathrm{i}\mu/(4\hbar a^2)+\mathrm{i}\pi/4}\Phi(q) + \mathrm{e}^{+\mathrm{i}\mu/(4\hbar a^2)-\mathrm{i}\pi/4}\Phi(q - \sigma_q\pi/a)\right]. \tag{5.12}$$

To proceed, it is necessary to recognize that the choice of the appropriate space of test functions $\Phi(q)$ depends on the properties of the eigenfunctions $\{\psi_s(q)\}$ under consideration. Accordingly, $\Phi(q)$ is drawn from either of two spaces $\mathcal{S}_p$ $(p = 0, 1)$: a space $\mathcal{S}_0$ of periodic functions of period π/a appropriate to the eigenfunctions ψ_s for even s, and a space $\mathcal{S}_1$ of periodic functions of period $2\pi/a$ appropriate to the eigenfunctions ψ_s for odd s. Furthermore, parallelling the property that $\psi_s(q - \sigma_q\pi/a) = (-1)^s\psi_s(q)$, we must require that test functions drawn from $\mathcal{S}_1$ are such that $\Phi(q - \sigma_q\pi/a) = -\Phi(q)$. Thus, for test functions drawn from $\mathcal{S}_p$, (5.12) becomes

$$\int_0^{2\pi/a} \mathrm{e}^{(\mathrm{i}/\hbar)\mathcal{F}_\mu(q,Q)} \Phi(Q)\,\mathrm{d}Q \sim 2\,\mathrm{i}^{-p}\sqrt{\frac{8\pi\hbar}{\mu}} \cos[\mu/(4\hbar a^2) - (p + 1/2)\pi/2]\Phi(q) \tag{5.13}$$

so that, for a suitable choice of $N_s(\mu)$, $\lim_{\mu\longrightarrow\infty} N_s(\mu)\,\mathrm{e}^{(\mathrm{i}/\hbar)\mathcal{F}_\mu(q,Q)}$ can have the sifting (or reproducing) property expected of a delta function (see, for example, section 1.2 of [27]).

To leading order, the asymptotic expansion of $M_s^{(1)}(\ln[\mu/\sqrt{4m\lambda}], \delta)$ in the limit of large μ (>0) is (from the real part of equation (20.9.1) in [22])

$$M_s^{(1)}(\ln[\mu/\sqrt{4m\lambda}], \delta) \sim \frac{\mathrm{i}^{|s|-p}}{\sqrt{\pi}} \sqrt{\frac{8\hbar a^2}{\mu}} \cos[\mu/(4\hbar a^2) - (p + 1/2)\pi/2] \tag{5.14}$$

where $p = 0$ (1) for s even (odd). (Despite appearances, the right-hand side of (5.14) is real-valued consistent with the reality of $M_s^{(1)}(x, \eta)$ for real-valued arguments x and η.) Combining (5.11), (5.13) and (5.14) in (5.5), we conclude that $C_s = \mathrm{i}^{|s|}a/(2\pi)$.

Introducing $\zeta \equiv \ln[\mu/\sqrt{4m\lambda}]$ and the variables $u \equiv aq$ and $U \equiv aQ$, the integral equation for the ψ_s reads

$$\psi_s(u/a) = \frac{\mathrm{i}^{|s|}}{2\pi} \frac{1}{M_s^{(1)}(\zeta, \delta)} \int_0^{2\pi} \exp(-2\mathrm{i}\sqrt{\delta}(\cosh\zeta \cos u \cos U + \sinh\zeta \sin u \sin U))\psi_s(U/a)\,\mathrm{d}U$$

which for ζ real is tantamount to the complex conjugate of equations (20.7.34) and (20.7.35) in [22].

6. Discussion

In this paper, we have shown that linear homogeneous integral equations for the stationary state wavefunctions of some quantum systems can be interpreted as arising from a dynamical symmetry at the classical level, namely a non-trivial canonical transformation of the full phase space which leaves invariant the form of the Hamilton function of the corresponding classical system. As we remarked in the introduction, for the systems of one degree of freedom under consideration, such canonical transformations amount to evolutions. The question thus arises whether or not the integral equations we have identified cannot be more simply understood as specializations to states of definite energy of the standard integral equation

$$\Psi_\alpha(q,t) = \int K(q,t;q',t')\Psi_\alpha(q',t')\,\mathrm{d}q' \tag{6.1}$$

for the time evolution of a wavefunction $\Psi_\alpha(q,t)$ in terms of the propagator $K(q,t;q',t') = \langle q,t|q',t'\rangle$.

For a state of definite energy (with wavefunction $\Psi_\alpha(q,t) = \mathrm{e}^{-(\mathrm{i}/\hbar)E_\alpha t}\psi_\alpha(q)$), (6.1) reduces to

$$\psi_\alpha(q) = \mathrm{e}^{(\mathrm{i}/\hbar)E_\alpha(t-t')}\int K(q,q'|t-t')\psi_\alpha(q')\,\mathrm{d}q' \tag{6.2}$$

where use has been made of the fact that for conservative systems (for which stationary states exist), the propagator $K(q,t;q',t')$ must be a function of the time difference $t-t'$—i.e. $K(q,t;q',t') = K(q,q'|t-t')$. Equation (6.2) can be cast into the form of (1.4) (with the continuous parameter μ related to the time difference $t-t'$), but there is a difference in the nature of the kernels: the kernel $K(q,q'|t-t')$ in (6.2) is *perforce* unitary, whereas the kernel $\mathrm{e}^{(\mathrm{i}/\hbar)\mathcal{F}_\mu(q,Q)}$ in (1.4) does *not* have to be.

This distinction is visible in the nature of the reciprocals $\mathcal{N}_\alpha(\mu)$ of the kernel's eigenvalues: when the kernel associated with $\mathrm{e}^{(\mathrm{i}/\hbar)\mathcal{F}_\mu(q,Q)}$ is unitary, then, as in (6.2), the dependence of $\mathcal{N}_\alpha(\mu)$ on the choice of state $|\alpha\rangle$ must reside in a multiplicative factor which is a complex number of magnitude unity (and vice versa). The reciprocals of eigenvalues found for the exponential and sinusoidal potentials considered in this paper do not possess this property (see (5.8) and (5.11)). Thus, the corresponding integral equations cannot be viewed as special cases of (6.1). By contrast, the integral equations derived for the linear and quadratic potentials can be recognized (with the identifications $\theta \to \omega(t-t')$ and $\nu \to (t-t')/2m$ in (4.5) and (4.10), respectively) as specializations of (6.1) to states of definite energy. (Expressions for the propagator K for these two potentials can be found, for example, in [28].)

The observation that not all canonical transformations which effect evolutions at the classical level are unitary is the primary result of this paper. The fact that the quantum equivalents of the canonical transformations discussed in connection with the linear and quadratic potentials are unitary is a consequence of their linearity [29, 30]. Our results in section 4 provide an independent confirmation of this connection between linearity and unitarity.

In semiclassical studies involving two different sets of canonical variables (q,p) and (Q,P), it is customary to assume unitarity from the outset. Then, the transformation matrix element $\langle q|Q\rangle$ exists ($|q\rangle$ and $|Q\rangle$ denote eigenkets of the coordinate operators $\widehat{q}$ and $\widehat{Q}$, respectively) and, invoking the stationary phase approximation, is given by

$$\langle q|Q\rangle = A(q,Q)\,\mathrm{e}^{(\mathrm{i}/\hbar)\mathcal{F}(q,Q)}$$

where $\mathcal{F}(q, Q)$ is the classical generating function (of the first kind) for the canonical transformation $(q, p) \longrightarrow (Q, P)$ and the pre-exponential factor [31]

$$A(q, Q) = \left[-\frac{1}{2\pi i\hbar} \frac{\partial^2 \mathcal{F}}{\partial q \partial Q} \right]^{1/2}. \tag{6.3}$$

The relation to our work is brought out by an alternative characterization of these results, namely that the transformation between wavefunctions is taken to be (1.2) with the (approximate) quantum generating function

$$F(q, Q) = \mathcal{F}(q, Q) - i\hbar \ln A(q, Q). \tag{6.4}$$

In the more typical case where unitarity does not apply (and so the transformation matrix element $\langle q|Q\rangle$ does *not* exist), our work suggests that one can proceed by replacing (1.2) by (1.3) with its state-dependent relative normalization n_α. In addition, $A(q, Q)$ in (6.4) should be obtained *not* from (6.3) but by demanding (as we have done in our work) that (2.1) is satisfied up to and including terms of order $\hbar$. For the Hamiltonian operators of section 2, this requirement implies the following linear homogenous first-order partial differential equation for A:

$$\frac{\partial \mathcal{F}}{\partial q} \frac{\partial A}{\partial q} - \frac{\partial \mathcal{F}}{\partial Q} \frac{\partial A}{\partial Q} = -\frac{1}{2} \left(\frac{\partial^2 \mathcal{F}}{\partial q^2} - \frac{\partial^2 \mathcal{F}}{\partial Q^2} \right) A$$

We have not exhausted the full range of integral equations which can be constructed by invoking the quantum canonical transform. For the families of canonical transformations that we have considered, which do not constitute Abelian groups, there is a (possibly infinite) sequence of integral equations corresponding to the repeated composition of these transformations. Consideration of the composition of a transformation to angle-action variables with its inverse could give rise to still more integral equations. However, the most interesting line of further investigation in our opinion is the extension of the work in this paper to quantum field theory.

There are some almost immediate parallels of our results for theories of a scalar field $\varphi(\sigma, \tau)$ in 1 + 1 dimensions (σ denotes the spatial dimension and τ the time in natural units such that $\hbar = 1 = c$). This is in part a consequence of the fact that the (first quantized) Hamiltonian functionals $H[\varphi, \pi]$ for these theories are not too dissimilar in form from the Hamilton functions $\mathcal{H}$ we have considered:

$$H[\varphi, \pi] = \frac{1}{2} \int [\pi^2 + (\partial\varphi/\partial\sigma)^2] \, d\sigma + \int V(\varphi) \, d\sigma$$

where π is the field momentum conjugate to φ and the 'potential density' V describes the self-coupling of φ. If we consider canonical transformations $\varphi, \pi \longrightarrow \Phi, \Pi$ induced by generating functionals of the form ($\varphi_\pm \equiv (\varphi \pm \Phi)/2$)

$$F[\varphi, \Phi] = \int \varphi \frac{\partial \Phi}{\partial \sigma} \, d\sigma + \int [F_+(\varphi_+) + F_-(\varphi_-)] \, d\sigma$$

then we find that a sufficient condition for the transformed Hamilton functional to be of the same form as the original Hamilton functional is that

$$\frac{1}{2} \frac{\partial F_+}{\partial \varphi_+} \frac{\partial F_-}{\partial \varphi_-} = V(\varphi_+ - \varphi_-) - V(\varphi_+ + \varphi_-) \tag{6.5}$$

provided the $F_\pm$ either vanish or are periodic at the endpoints of the integration over σ. Apart from an inessential factor of m, (6.5) is formally identical to the condition established in section 3 for the invariance of Hamilton functions under canonical transformations (equation (3.2)) with $V(\varphi)$ replacing the potential $\mathcal{V}(q)$ and $\varphi_\pm(\sigma, \tau)$ the combinations

$q_{\pm} = (q \pm Q)/2$. In the Schrödinger representation [32] of the corresponding second quantized field theories, we have, putting aside the issue of renormalization, a class of integral equations for the wavefunctionals Ψ_α of the form

$$\Psi_\alpha[\varphi] = \mathcal{N}_\alpha[\mu] \int e^{iF_\mu[\varphi,\Phi]} \Psi_\alpha[\Phi] \mathcal{D}\Phi$$

where, in terms of the generating functions $\mathcal{F}_\mu$ listed in table 1,

$$F_\mu[\varphi, \Phi] = \int \varphi \frac{\partial \Phi}{\partial \sigma} \, d\sigma + \int \mathcal{F}_\mu(\varphi, \Phi) \, d\sigma$$

and $\mathcal{N}_\alpha$ is a functional of μ (which is now a function of σ and τ).

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