Integration of the Schrödinger equation by canonical transformations

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Owing to the operator nature of the quantum dynamical variables, classical canonical transformations for integrating the equations of motion cannot be extended to the quantum domain. In this paper, a general procedure is developed to construct the sequences of quantum canonical transformations for integrating the Schrödinger equations. The sequence is made of three elementary canonical transformations that constitute a much larger class than the unitary transformations. In conjunction with the procedure, we also developed a factorization technique that is analogous to the method of integration factor in classical integration. For demonstration, with the same procedure we integrate nine nontrivial models, including the centripetal barrier potential, the Kratzer's molecular potential, the Morse potential, the Pöschl-Teller potential, the Hulthén potential, etc.

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I. INTRODUCTION

In classical mechanics, there are two approaches for integrating the equations of motion, one is by solving the second-order differential equations directly, the other is by eliminating one of the conjugate variables with canonical transformations [1]. In the latter case, the equation of motion becomes trivial. For one-dimensional periodic systems or multidimensional separable systems, a general scheme is to transform the Hamiltonian $H(p,q)$ into $H(J)$ by

$$J=\frac{1}{2\pi}\oint p(E,q)dq, \quad \theta=\frac{\partial}{\partial J}\int^{q} p(J,q)dq, \tag{1.1}$$

where J is the action variable and θ is the conjugate angle variable. Under weak perturbations, even when the system is not integrable, Eq. (1.1) still helps identify the quasiaction variables that change slowly with time from the angle variables that are nearly periodic in time. In addition, if $H=H(p,q;\lambda)$ where the parameter λ varies slowly (adiabatically) with time as the result of some external influence, it can be shown that the action variable in Eq. (1.1) remains invariant when averaged over the period of motion (adiabatic invariance theorem) [2].

In quantum mechanics, the situation is different. Because of the noncommutative nature of the quantum variables, there is no obvious way to extend the canonical transformation to the quantum level. For example, the action and angle variables for the harmonic oscillator are $J=1/2(p^2+q^2)$ and $\theta=\arctan(q/p)$, respectively. These expressions, in particular, the one for the angle variable, are not well defined in noncommutative operator algebra. Equation (1.1) cannot be used because there is not a known way to extend the Riemann integration to operators. It is therefore interesting to ask: Is there a scheme to "integrate" a quantum system by canonical transformations, as an alternative to the method of solving the Schrödinger equation directly?

In classical mechanics, canonical transformations are those that preserve the Poisson bracket $\{p,q\}=-1$. In quantum mechanics, the natural extension is those that preserve the commutation relations $[p,q]=-i$ [3]. Although unitary transformations have such a property and have been used synonymously as quantum canonical transformations, they do not represent the full class of canonical transformation. There are simple and important canonical transformations, such as transformations to the polar or spherical coordinates, that do not have corresponding unitary transformations [4]. In the past decade, a broader class of canonical transformation, called isometric transformation, has been studied thoroughly [5,6]. The class is defined by transformation of the type $(p,q)\rightarrow(CpC^{-1},CqC^{-1})$, where C is not necessarily unitary, nevertheless, the transformation preserves the commutation relation $[p,q]=-i$. In the class of isometric transformation, three elementary types have been shown to be particularly interesting. They are the interchange transformation, the similarity transformation, and the point transformation [5,6]. It was conjectured that every quantum canonical transformation may be decomposed into a finite sequence of these three elementary transformations [6,7], although whether or not every classical integrable system may be integrated in the quantum level by canonical transformations is still an open question.

Although canonical transformation has not yet become a popular technique for solving quantum models, much progress has been made in the past three decades. For example, Moshinsky, Seligmen, and Wolf have converted the radial Coulomb potential to the harmonic oscillator with canonical transformations [8]. Leyvraz and Seligmen have reduced the Hamiltonians to $H(J)$ with canonical transformations for the harmonic oscillator, the repulsive oscillator, and the free-falling particle [7]. Anderson showed that the three elementary transformations mentioned above are closely related to known techniques for solving differential equations, and pointed out all systems that may be solved by the intertwining method may also be solved by canonical transformations [6,9].

In this paper, we present a procedure for finding the sequence of canonical transformations that may be used to integrate quantum systems. As demonstrations, we use the procedure to solve nine known models. All of them may be found in Ref. [10], where they are integrated by the conventional method of solving the Schrödinger equation. The

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model Hamiltonians are $H(p,q)=1/2p^2+V(q)$ with the following different types of $V(q)$:

(1) U/q^2,
(2) $U(q-1/q)^2$, the centripetal barrier potential [10–12],
(3) $U(1/q^2-2/q)$, the Kratzer's molecular potential [10,12],
(4) $-Ue^{-q}$, the central-force model of deuteron [10],
(5) $U(e^{-2q}-2e^{-q})$, the Morse potential [10,12],
(6) $U\csc^2 q$, the Pöschl-Teller potential [10,13],
(7) $-U\mathrm{sech}^2 q$, the modified Pöschl-Teller potential [10,12],
(8) $1/2U(1-\coth 1/2q)$, the Hulthén potential [10],
(9) $1/2U(1+\tanh 1/2q)$, the step potential [10],

where U are arbitrary positive constants. Model (3) has been solved in Ref. [8] by first embedding it into a higher-dimensional configuration space, then converting to the problem of harmonic oscillator. As we shall see, our method is straightforward and much simpler. A special case of model (7) with $U=1$ has also been solved previously using a different procedure that corresponds to the intertwining method [6,9]. With the procedure presented in this paper, the case with arbitrary U may be solved. Except for these special cases, all the models are, to the best of our knowledge, solved by canonical transformations for the first time. Similar to factorizing algebraic expressions, the procedure is not meant to work for arbitrary potential functions. Yet for solvable models, it offers a general and logical approach.

For each model, the solution consists of three parts: (i) the sequence of elementary transformations that reduces $H(p,q)$ to J, (ii) the reverse sequence that brings the eigenfunction of J to the eigenfunction of $H(p,q)$, and (iii) the boundary conditions that determines the allowed energy levels. Because the transformation from J to any $H(J)$ is canonical (point transformation, Sec. II), there is not *a priori* preference of $H(J)$ over J. This is different from classical integrable cases where $H(J)$ is determined by Eq. (1.1). In models (3)–(9), we factorize the Hamiltonian into two parts and integrate only the part that has the same null space as $H-E$. It is the introduction of this technique that makes our integration procedure applicable to a broad collection of models in systematic way.

II. INTEGRATION BY CANONICAL TRANSFORMATIONS

In this section, we show step by step the procedure that leads to the integration of the nine models. After the integration, $H(p,q)$ is transformed to J, the Heisenberg equation $\dot{J}=i[H,J]=0$ becomes trivial. J becomes a constant of motion, and the wave function of stationary states is simply the eigenfunction of J, i.e., $\Psi(\theta)=e^{ik\theta}$, where k is an eigenvalue of J. The eigenfunctions of $H(p,q)$ may be obtained from $\Psi(\theta)$ by the same sequence of canonical transformations that reduces $H(p,q)$ to J. Before we introduce the procedure, let us briefly discuss the three elementary canonical transformations that are used to perform the integration. The following table shows their definitions and the corresponding transformations of the eigenfunctions [6]:

$$\text{interchange } \mathbf{I}: \quad (p,q)\rightarrow(q,-p)$$

$$\psi_{\mathrm{I}}(q)=\int e^{iqu}\Psi(u)du, \tag{2.1}$$

$$\text{similarity } \mathbf{S}: \quad (p,q)\rightarrow(p+f'(q),q)$$

$$\psi_{\mathrm{S}}(q)=e^{if(q)}\Psi(q), \tag{2.2}$$

$$\text{point } \mathbf{P}: \quad (p,q)\rightarrow\left(\frac{1}{g'(q)}p,g(q)\right)$$

$$\psi_{\mathrm{P}}(q)=\Psi[g^{-1}(q)], \tag{2.3}$$

where f' means df/dq and g^{-1} means the inverse function of g. $\psi_{\mathrm{I}}(q)$ in Eq. (2.1) is the eigenfunction before the interchange transformation if and only if $\Psi(q)$ is the eigenfunction after the transformation. In other words, $H(p,q)\psi_{\mathrm{I}}(q)=E\psi_{\mathrm{I}}(q)\Leftrightarrow H(q,-p)\Psi(q)=E\Psi(q)$, with the same eigenvalue E. Similarly, $\psi_{\mathrm{S}}(q)$ and $\psi_{\mathrm{P}}(q)$ in Eqs. (2.2) and (2.3) are the eigenfunctions before the similarity transformation and the point transformation, respectively. Namely, $H(p,q)\psi_{\mathrm{S}}(q)=E\psi_{\mathrm{S}}(q)\Leftrightarrow H(p+f',q)\Psi(q)=E\Psi(q)$ and $H(p,q)\psi_{\mathrm{P}}(q)=E\psi_{\mathrm{P}}(q)\Leftrightarrow H(1/g'p,g)\Psi(q)=E\Psi(q)$. Note that the eigenvalues E are preserved under these transformations. These eigenfunction transformations may be verified readily. For example, $p\psi_{\mathrm{I}}=-id\psi_{\mathrm{I}}/dq$ leads to $p\psi_{\mathrm{I}}(q)=\int e^{iqu}[u\Psi(u)]du$ and integration by parts leads to $q\psi_{\mathrm{I}}(q)=\int e^{iqu}[-p\Psi(u)]du$. To simplify the decomposing, we also use the following two composite transformations frequently:

$$\tilde{\mathbf{S}}: \quad (p,q)\rightarrow(p,q-f'(p)) \quad \psi_{\tilde{\mathrm{S}}}(q)=e^{if(p)}\Psi(q), \tag{2.4}$$

$$\mathbf{L}_p: \quad \left(\frac{1}{g'(q)}[p+f'(q)],g(q)\right)\rightarrow(J,\theta)$$

$$\psi_{\mathrm{L}_p}(q)=e^{-if(q)}\Psi[g(q)]. \tag{2.5}$$

$\tilde{\mathbf{S}}$ is the composite transformation of $\mathbf{I}$, $\mathbf{S}$, and $\mathbf{I}^{-1}$, where $\mathbf{I}^{-1}$: $(q,-p)\rightarrow(p,q)$ is the inverse of $\mathbf{I}$. $\psi_{\tilde{\mathrm{S}}}(q)$ may also be written as $\int e^{iqv}e^{if(v)}\int e^{-ivu}\Psi(u)du\,dv$, which is equivalent to $e^{if(p)}\Psi(q)$. $\mathbf{L}_p$ is the composite transformation of $\mathbf{S}^{-1}$ and $\mathbf{P}^{-1}$, where $\mathbf{S}^{-1}$: $(p+f',q)\rightarrow(p,q)$ is the inverse of $\mathbf{S}$ and $\mathbf{P}^{-1}$: $(1/g'p,g)\rightarrow(p,q)$ is the inverse of $\mathbf{P}$. In the process of reducing the Hamiltonian, three important kinds of linear forms are used. They are called the p-linear form, the q-linear form, and the $\tilde{p}$-linear form. Hamiltonians of the p-linear form, $G(q)[p+F(q)]$, may be transformed to J by $\mathbf{L}_p$ with $1/g'(q)=G(q)$ and $f'(q)=F(q)$. The q-linear form, $G(p)[q+F(p)]$, may be transformed first to the p-linear form by the interchange $\mathbf{I}$ transformation. The $\tilde{p}$-linear form, $G(p+F)$, where $G=G[q+h(p)]$ and $F=F[q+h(p)]$, may also be transformed first to the p-linear form by $\tilde{\mathbf{S}}$ with $q\rightarrow q-h(p)$.

Now we are ready to describe the procedure for reducing the Hamiltonians from $H(p,q)$ to J. First, we use a point $\mathbf{P}$

transformation with $q \to g(q)$ to simplify the potential $V(q)$. Then, we use a similarity **S** transformation with $p \to p + f'(q)$ to bring in additional terms from $1/2p^2$ for eliminating the simplified $V(q)$. As will be explained in model (1), there are always two choices of the similarity transformation. They lead to two different solutions for reducing the Hamiltonian to J and correspondingly two independent wave functions. This is in accordance with the fact that a second-order differential equation has two independent solutions. If one makes the right choice of $g(q)$ and $f(q)$, after these transformations the Hamiltonian may become much simpler. For example, it may become a q-linear form and the rest steps to J are just an interchange **I** transformation followed by an $\mathbf{L}_p$ transformation. A technique introduced in this paper is the factorization of $H-E$ and integrating only one of its factors that has the same null space. For simpler models such as models (1) and (2), whether the integration is for $H-E$ or H makes no difference, but for models (3)–(9) the factorization of $H-E$ is crucial. This technique is analogous to the use of integration factors in classical integration, where a differential form is integrated by factorizing out or multiplying an integration factor first.

In the solution of the following models, four positive constants α, β, γ, and ϵ will be used in the transformations. Their definitions are

$$\alpha \equiv \frac{1}{2}(1+\sqrt{1+8U}), \quad \beta \equiv \sqrt{2U}, \quad \gamma \equiv \sqrt{|2U-2E|},$$

$$\epsilon \equiv \sqrt{2|E|}. \tag{2.6}$$

$E=1/2\epsilon^2>0$ for cases (1), (2), (6), (9), and $E=-1/2\epsilon^2<0$ for cases (3), (4), (5), (7), (8).

(1) $V(q)=U/q^2$, where q is from 0 to ∞. For this example, we first use the point transformation

$$\mathbf{P}: \quad (p,q) \to (2\sqrt{q}p, \sqrt{q}),$$

such that $V \to U/q$ and $1/2p^2 \to 2(\sqrt{q}p)^2$. Then, we use a similarity transformation

$$\mathbf{S}: \quad (p,q) \to \left(p - \frac{i\alpha}{2q}, q\right),$$

such that $1/2p^2$ may be further transformed to $2(\sqrt{q}p)^2 - 2i\alpha p - 1/2\alpha(\alpha-1)/q$. The last term cancels the simplified potential U/q, if $1/2\alpha(\alpha-1)=U$, namely, $\alpha = 1/2(1 \pm \sqrt{1+8U})$. For the time being, we choose the positive root $\alpha = 1/2(1+\sqrt{1+8U})$ as defined in Eq. (2.6). The negative root will lead to the second independent eigenfunction and be discussed momentarily. After these transformations, $H - E \to 2(\sqrt{q}p)^2 - 2i\alpha p - E$. This is a q-linear form. By the interchange **I** transformation, it will be transformed to the p-linear form $-2q^2[p + i(\alpha-3/2)/q + E/(2q^2)]$, which may be reduced to J by $\mathbf{L}_p$ in Eq. (2.5) with $1/g' = -2q^2$ and $f' = i(\alpha - 3/2)/q + E/(2q^2)$. The eigenspace of $H(p,q)$ with eigenvalue E, equivalent to the null space of $H-E$, may be obtained through the corresponding eigenfunction transformations from the null space of J. Namely, from $\Psi(\theta)=c$ (constant) and Eq. (2.5), one obtains the eigenfunction before transformation $\mathbf{L}_p$,

$$\psi_{\mathrm{L}_p}(q) = c q^{\alpha-3/2} e^{iE/(2q)}.$$

From Eq. (2.1), one obtains the eigenfunction before transformation **I**,

$$\psi_{\mathrm{I}}(q) = \int e^{iqu} \psi_{\mathrm{L}_p}(u) du = c \int e^{iqu} u^{\alpha-3/2} e^{iE/(2u)} du.$$

From Eq. (2.2), one obtains the eigenfunction before transformation **S**,

$$\psi_{\mathrm{S}}(q) = q^{\alpha/2} \psi_{\mathrm{I}}(q) = c q^{\alpha/2} \int e^{iqu} u^{\alpha-3/2} e^{iE/(2u)} du.$$

Finally, from Eq. (2.3), one obtains the eigenfunction before transformation **P**, or the eigenfunction of $H(p,q)$ with eigenvalue E,

$$\psi(q) = \psi_{\mathrm{S}}(q^2) = c q^{\alpha} \int e^{iq^2 u} u^{\alpha-3/2} e^{iE/(2u)} du.$$

That is,

$$\psi(q) = c q^{1/2} J_{\alpha-1/2}(\epsilon q),$$

where

$$J_\nu(x) = 1/(-2\pi i)(x/2)^\nu \int e^{-x^2 t/4} t^{\nu-1} e^{1/t} dt$$

is the Bessel function. $\psi(q)$ remains finite as $q \to 0$ and ∞, for all U and E. Note that we denote all the normalization constants by c, although they may represent different values in different places. Changing α to $1-\alpha$, which is the negative root $1/2(1-\sqrt{1+8U})$, the transformations may also reduce $H-E$ to J. The corresponding wave function

$$\psi(q) = c q^{1/2} J_{-\alpha+1/2}(\epsilon q)$$

is independent of the first one, but diverges as $q \to 0$, hence, is excluded.

(2) The centripetal barrier potential $V(q) = U(q-1/q)^2$, where q is from 0 to ∞. This corresponds to the problem of three-dimensional harmonic oscillator with nonzero angular momentum, namely $[1/2(p^2+r^2) + l(l+1)/(2r^2) - E]R(r) = 0$. For this example, we first use the point transformation

$$\mathbf{P}: \quad (p,q) \to (2\sqrt{q}p, \sqrt{q}),$$

such that $V \to U(q+1/q-2)$ and $H - E \to 2qp^2 - ip + U(q + 1/q - 2) - E$. The terms Uq and U/q may be eliminated by the similarity transformation

$$\mathbf{S}: \quad (p,q) \to \left(p + \frac{i\beta}{2} - \frac{i\alpha}{2q}, q\right).$$

Then, $H-E$ is reduced to the q-linear form $2p(p+i\beta)[q-a/p-b/(p+i\beta)]$, where $a=i[\alpha/2-3/4-\beta/2-E/(2\beta)]$ and $b=i[\alpha/2-3/4+\beta/2+E/(2\beta)]$. It can be transformed by **I** to the p-linear form $-2q(q+i\beta)[p+a/q+b/(q+i\beta)]$, which is reduced to J by $\mathbf{L}_p$ in Eq. (2.5) with $1/g'=-2q(q+i\beta)$ and $f'=a/q+b/(q+i\beta)$. As in model (1), we start from the null space of J. $\Psi(\theta)=c$ is transformed, through the corresponding eigenfunction transformations, to

$$\psi(q)=c\left[e^{-\beta v/2}v^{\alpha/2}\int e^{iuv}u^{\alpha/2-3/4-\beta/2-E/(2\beta)}\times(u+i\beta)^{\alpha/2-3/4+\beta/2+E/(2\beta)}du\right]_{v=q^2}.$$

That is,

$$\psi(q)=c[e^{-v/2}v^{\alpha/2}{}_1F_1(\alpha/2+1/4-\beta/2-E/(2\beta),\alpha+1/2;v)]_{v=\beta q^2},$$

where

$${}_1F_1(a,c;x)=\Gamma(1-a)\Gamma(c)/[-2\pi i\Gamma(c-a)]\times\int e^{tx}(-t)^{a-1}(1-t)^{c-a-1}dt$$

is the confluent hypergeometric function. If $\psi(q)$ remains finite for $q\to 0$ and ∞, one must have $\alpha/2+1/4-\beta/2-E/(2\beta)=-n$, hence, $E=2\beta(n+\alpha/2+1/4-\beta/2)$, where n is a nonnegative integer. Changing α to $1-\alpha$ in the transformations, one obtains the second solution for reducing $H-E$ to J and the second independent wave function

$$\psi(q)=c[e^{-v/2}v^{1/2-\alpha/2}{}_1F_1(-\alpha/2+3/4-\beta/2-E/(2\beta),-\alpha+3/2;v)]_{v=\beta q^2}.$$

However, it diverges as $q\to 0$ and may be excluded.

In the following examples, we shall factorize $H-E$ into two parts. For instance, in model (3), $H-E=1/(2q)G$, where $G=qp^2-2Eq+2U/q-4U$. As in models (1) and (2), after the terms $-2Eq$ and $2U/q$ are eliminated by an **S** transformation, G will be reduced to a q-linear form. Since the null space of G is equivalent to the null space of $H-E$, the transformation from G to J is equally good for solving the wave functions and the energy levels.

(3) Kratzer's molecular potential $V(q)=U(1/q^2-2/q)$, where q is from 0 to ∞. This corresponds to the three-dimensional problem for the Coulomb potential with nonzero angular momentum. For this example, $H-E=1/(2q)G$, where $G=qp^2-2Eq+2U/q-4U$. After $-2Eq$ and $2U/q$ are eliminated by the similarity transformation

$$\mathbf{S}:\quad (p,q)\to\left(p+i\epsilon-\frac{i\alpha}{q},q\right),$$

G is reduced to the q-linear form $p(p+2i\epsilon)[q-a/p-b/(p+2i\epsilon)]$, where $a=i(\alpha-1-2U/\epsilon)$ and $b=i(\alpha-1+2U/\epsilon)$. It may be further transformed to J through **I** and $\mathbf{L}_p$ in Eq. (2.5) with $1/g'=-q(q+2i\epsilon)$ and $f'=a/q+b/(q+2i\epsilon)$. As explained in model (1), for the transformation of eigenfunctions, the starting point is the null space of J, i.e., $\Psi(\theta)=c$. Going through the corresponding eigenfunction transformations, one obtains

$$\psi(q)=c[e^{-v/2}v^{\alpha}{}_1F_1(\alpha-2U/\epsilon,2\alpha;v)]_{v=2\epsilon q}.$$

If $\psi(q)$ remains finite for $q\to 0$ and ∞, we must have $\alpha-2U/\epsilon=-n$, hence, $E=-1/2\epsilon^2=-2U^2(n+\alpha)^{-2}$, where n is a nonnegative integer. Changing α to $1-\alpha$ for the transformations, one obtains the second solution for reducing $H-E$ to J and the second independent wave function

$$\psi(q)=c[e^{-v/2}v^{1-\alpha}{}_1F_1(1-\alpha-2U/\epsilon,2-2\alpha;v)]_{v=2\epsilon q}.$$

However, it diverges as $q\to 0$ and may be excluded.

(4) The central-force model of deuteron $V(q)=-Ue^{-q}$, where q is from 0 to ∞. For this example, we first use the point transformation

$$\mathbf{P}:\quad (p,q)\to(-qp,-\ln q),$$

such that $V\to -Uq$ and $H-E\to 1/2qG$, where $G=qp^2-ip-2E/q-2U$. After $-2E/q$ is eliminated by the similarity transformation

$$\mathbf{S}:\quad (p,q)\to\left(p-\frac{i\epsilon}{q},q\right),$$

G is reduced to the q-linear form $p^2[q-i(2\epsilon-1)/p-\beta^2/p^2]$. It may be further transformed to J through **I** and $\mathbf{L}_p$ in Eq. (2.5) with $1/g'=-q^2$ and $f'=i(2\epsilon-1)/q+\beta^2/q^2$. From the corresponding eigenfunction transformations, one obtains

$$\psi(q)=cJ_{2\epsilon}(2\beta e^{-q/2}).$$

$\psi(q)$ remains finite as $q\to 0$ and ∞, for all U and E. Changing ϵ to $-\epsilon$ for the transformations, one obtains the second solution for reducing $H-E$ to J and the second independent wave function

$$\psi(q)=cJ_{-2\epsilon}(2\beta e^{-q/2}).$$

However, it diverges as $q\to\infty$ and may be excluded.

(5) The Morse potential $V(q)=U(e^{-2q}-2e^{-q})$, where q is from $-\infty$ to ∞. This potential describes the vibration of a diatomic molecule. It goes to zero when the two atoms are far away from each other, and increases very fast when they are close to each other. For this example, we first use the point transformation

$$\mathbf{P}:\quad (p,q)\to(-qp,-\ln q),$$

such that $V\to U(q^2-2q)$ and $H-E\to 1/2qG$, where $G=qp^2-ip+2Uq-2E/q-4U$. After $2Uq$ and $-2E/q$ are eliminated by the similarity transformation

$$\mathbf{S}: \quad (p,q) \to \left(p+i\beta-\frac{i\epsilon}{q},q\right),$$

G is reduced to the q-linear form $p(p+2i\beta)[q-a/p-b/(p+2i\beta)]$, where $a=i(\epsilon-1/2-\beta)$ and $b=i(\epsilon-1/2+\beta)$. It may be further transformed to J through $\mathbf{I}$ and $\mathbf{L}_p$ in Eq. (2.5) with $1/g'=-q(q+2i\beta)$ and $f'=a/q+b/(q+2i\beta)$. From the corresponding eigenfunction transformations, one obtains

$$\psi(q)=c[e^{-v/2}v^{\epsilon}{}_1F_1(\epsilon-\beta+1/2,2\epsilon+1;v)]_{v=2\beta e^{-q}}.$$

If $\psi(q)$ remains finite for $q\to\pm\infty$, we must have $\epsilon-\beta+1/2=-n$, hence, $E=-1/2\epsilon^2=-1/2(n-\beta+1/2)^2$, where n is a nonnegative integer. Changing ϵ to $-\epsilon$ for the transformations, one obtains the second solution for reducing $H-E$ to J and the second independent wave function

$$\psi(q)=c[e^{-v/2}v^{-\epsilon}{}_1F_1(-\epsilon-\beta+1/2,-2\epsilon+1;v)]_{v=2\beta e^{-q}}.$$

However, it diverges as $q\to\infty$ and may be excluded.

For models (3)–(5), we have made the factorization $H-E=F(q)G$ and reduced only G to J. But F can also be a function of p. This is the case for models (6)–(9), where the following factorization is used:

$$p(1-q^2)p+p(dq+c)+e = p\left\{\left[1-\left(q+\frac{a}{p}\right)^2\right]p+b\left(q+\frac{a}{p}\right)+c\right\}. \tag{2.7}$$

What is in the braces is the so-called $\tilde{p}$-linear form and may be transformed to the p-linear form $(1-q^2)p+bq+c$ by

$$\tilde{\mathbf{S}}:(p,q)\to\left(p,q-\frac{a}{p}\right). \tag{2.8}$$

The constants a,b are determined from the constants d,e. For given d,e, there are two sets of a,b satisfying Eq. (2.7). As will be explained in model (6), the two sets will lead to the same eigenfunction, hence, only one set of them will be discussed.

(6) The Pöschl-Teller potential $V(q)=U\csc^2 q$, where q is from 0 to π. For this example, we first use the point transformation

$$\mathbf{P}: \quad (p,q)\to\left(-2\sqrt{1-q^2}p,\frac{1}{2}\cos^{-1}q\right),$$

such that $V\to 2U/(1-q)$ and $H-E\to 2p(1-q^2)p-2ipq+2U/(1-q)+2-E$. After $2U/(1-q)$ is eliminated by the similarity transformation

$$\mathbf{S}: \quad (p,q)\to\left(p+\frac{i\alpha}{2(1-q)},q\right),$$

$H-E$ is reduced to

$$2p(1-q^2)p+2ip[(\alpha-1)q+\alpha]+\frac{1}{2}(\alpha^2-\epsilon^2)-2\alpha+2.$$

This can be factorized by Eq. (2.7) into

$$2p\left\{\left[1-\left(q+\frac{a}{p}\right)^2\right]p+b\left(q+\frac{a}{p}\right)+i\alpha\right\},$$

where $a=-i[(\alpha\pm\epsilon)/2-1]$, $b=i(\mp\epsilon+1)$. The $\tilde{p}$-linear form in the braces may be further transformed to J through $\tilde{\mathbf{S}}$ in Eq. (2.8) and $\mathbf{L}_p$ in Eq. (2.5) with $1/g'=1-q^2$ and $f'=(bq+i\alpha)/(1-q^2)$. From the corresponding eigenfunction transformations, one obtains

$$\begin{aligned}\psi(q)&=c\{(1-u)^{\alpha/2}p^{(\alpha\pm\epsilon)/2-1}[(1-u)^{-(\alpha\mp\epsilon+1)/2}\\&\quad\times(1+u)^{(\alpha\pm\epsilon-1)/2}]\}_{u=\cos 2q}\\&=c\left[(1-v)^{\alpha/2}\oint(u-v)^{-(\alpha\pm\epsilon)/2}\right.\\&\quad\left.\times(1-u)^{-(\alpha\mp\epsilon+1)/2}(1+u)^{(\alpha\pm\epsilon-1)/2}du\right]_{v=\cos 2q}.\end{aligned}$$

That is,

$$\psi(q)=c[(1-v)^{\alpha/2}{}_2F_1((\alpha\mp\epsilon)/2,(\alpha\pm\epsilon)/2,\alpha+1/2;(1-v)/2)]_{v=\cos 2q},$$

where

$${}_2F_1(a,b,c;x)=\Gamma(1-a)\Gamma(c)/[2\pi i\Gamma(c-a)]\times\oint(-t)^{b-c}(1-t)^{c-a-1}(x-t)^{-b}dt$$

is the hypergeometric function. Since ${}_2F_1(a,b,c;x)={}_2F_1(b,a,c;x)$, the solutions for $\pm\epsilon$ lead to the same eigenfunction. If $\psi(q)$ remains finite for $q\to 0$ and π, we must have $1/2(\alpha\mp\epsilon)=-n$, hence $E=1/2\epsilon^2=1/2(2n+\alpha)^2$, where n is a nonnegative integer. Changing α to $1-\alpha$ for the transformations, one obtains the second solution for reducing $H-E$ to J and the second independent wave function

$$\psi(q)=c[(1-v)^{1/2-\alpha/2}{}_2F_1((1-\alpha-\epsilon)/2,(1-\alpha+\epsilon)/2,-\alpha+3/2;(1-v)/2)]_{v=\cos 2q}.$$

However, it diverges as $q\to 0$ and π, hence may be excluded.

(7) The modified Pöschl-Teller potential $V(q)=-U\,\mathrm{sech}^2 q$, where q is from $-\infty$ to ∞. One may simplify the potential by the point transformation

$$\mathbf{P}: \quad (p,q)\to((1-q^2)p,\tanh^{-1}q).$$

Then, $V\to -U(1-q^2)$ and $H-E\to 1/2(1-q^2)G$, where $G=p(1-q^2)p-2E/(1-q^2)-2U$. After $-2E/(1-q^2)$ is eliminated by the similarity transformation

$$\mathbf{S}: \quad (p,q)\to\left(p+\frac{i\epsilon}{2(1-q)}-\frac{i\epsilon}{2(1+q)},q\right),$$

G is reduced to

$$p(1-q^2)p+2i\epsilon pq+\epsilon^2-\epsilon-2U.$$

This may be factorized by Eq. (2.7) into

$$p\left\{\left[1-\left(q+\frac{a}{p}\right)^2\right]p-2i(\alpha-1)\left(q+\frac{a}{p}\right)\right\},$$

where $a=-i(\alpha+\epsilon-1)$. The $\tilde{p}$-linear form in the braces may be further transformed to J through $\tilde{\mathbf{S}}$ in Eq. (2.8) and $\mathbf{L}_p$ in Eq. (2.5) with $1/g'=1-q^2$ and $f'=-2i(\alpha-1)q/(1-q^2)$. From the corresponding eigenfunction transformations, one obtains

$$\psi(q)=c[(1-v^2)^{\epsilon/2}{}_2F_1(-\alpha+\epsilon+1,\alpha+\epsilon,\epsilon+1;(1-v)/2)]_{v=\tanh q}.$$

If $\psi(q)$ remains finite for $q\to\pm\infty$, we must have $-\alpha+\epsilon+1=-n$, hence $E=-1/2\epsilon^2=-1/2(n-\alpha+1)^2$, where n is a nonnegative integer. To obtain the second independent solution, we replace the similarity transformation by

$$\mathbf{S}:\quad (p,q)\to\left(p-\frac{i\epsilon}{2(1-q)}-\frac{i\epsilon}{2(1+q)},q\right).$$

The corresponding steps for reducing $H-E$ to J are $\tilde{\mathbf{S}}$ in Eq. (2.8) with $a=i\alpha$ and $\mathbf{L}_p$ in Eq. (2.5) with $1/g'=1-q^2$ and $f'=2i(\alpha q-\epsilon)/(1-q^2)$. The second independent wave function is then

$$\psi(q)=c[(1+v)^{\epsilon/2}(1-v)^{-\epsilon/2}\times{}_2F_1(\alpha,1-\alpha,1-\epsilon;(1-v)/2)]_{v=\tanh q}.$$

However, it diverges as $q\to\infty$ and may be excluded.

(8) The Hulthén potential $V(q)=1/2U(1-\coth 1/2\,q)$, where q is from 0 to ∞. For this example, we first use the point transformation

$$\mathbf{P}:\quad (p,q)\to\left(\frac{1}{2}(1-q^2)p,2\coth^{-1}q\right),$$

such that $V\to 1/2U(1-q)$ and $H-E\to 1/8(1-q^2)G$, where $G=p(1-q^2)p+4(U-E)/(1+q)-4E/(1-q)$. After $4(U-E)/(1+q)$ and $-4E/(1-q)$ are eliminated by the similarity transformation

$$\mathbf{S}:\quad (p,q)\to\left(p+\frac{i\gamma}{1+q}+\frac{i\epsilon}{1-q},q\right),$$

G is reduced to

$$p(1-q^2)p+2ip[\epsilon(1+q)+\gamma(1-q)]+(\epsilon-\gamma)^2-(\epsilon-\gamma).$$

This may be factorized by Eq. (2.7) into

$$p\left\{\left[1-\left(q+\frac{a}{p}\right)^2\right]p+2i(\epsilon+\gamma)\right\},$$

where $a=-i(\epsilon-\gamma)$. The $\tilde{p}$-linear form in the braces may be further transformed to J through $\tilde{\mathbf{S}}$ in Eq. (2.8) and $\mathbf{L}_p$ in Eq. (2.5) with $1/g'=1-q^2$ and $f'=2i(\epsilon+\gamma)/(1-q^2)$. From the corresponding eigenfunction transformations, one obtains

$$\psi(q)=c[(1+v)^{-\gamma}(1-v)^{\epsilon}{}_2F_1(\epsilon-\gamma,\epsilon-\gamma+1,2\epsilon+1;(1-v)/2)]_{v=\coth(q/2)}.$$

If $\psi(q)$ remains finite for $q\to 0$ and ∞, we must have $\epsilon-\gamma=-n$, hence, $E=-1/2(2U-n^2)^2/(2n)^2$, where n is a positive integer. Changing ϵ to $-\epsilon$ for the transformations, one obtains the second solution for reducing $H-E$ to J and the second independent wave function

$$\psi(q)=c[(1+v)^{-\gamma}(1-v)^{-\epsilon}{}_2F_1(-\epsilon-\gamma,-\epsilon-\gamma+1,-2\epsilon+1;(1-v)/2)]_{v=\coth(q/2)}.$$

However, it diverges as $q\to\infty$ and may be excluded.

(9) The step potential $V(q)=1/2U(1+\tanh 1/2q)$, where q is from $-\infty$ to ∞. For this example, we first use the point transformation

$$\mathbf{P}:\quad (p,q)\to\left(\frac{1}{2}(1-q^2)p,2\tanh^{-1}q\right),$$

such that $V\to 1/2U(1+q)$ and $H-E\to 1/8(1-q^2)G$, where $G=p(1-q^2)p+4(U-E)/(1-q)-4E/(1+q)$. Comparing this with the factor G in model (8), we obtain the rest of the transformations. (i) For $E<U$, the rest of the transformations are the same as in model (8) with the replacement $\gamma\to\pm i\epsilon$ and $\epsilon\to\pm\gamma$. Therefore, the first and second wave functions are

$$\psi(q)=c[(1+v)^{\pm i\epsilon}(1-v)^{\pm\gamma}{}_2F_1(\pm\gamma\pm i\epsilon,\pm\gamma\pm i\epsilon+1,\pm 2\gamma+1;(1-v)/2)]_{v=\tanh(q/2)}.$$

Since ${}_2F_1(a,b,c;x)=(1-x)^{c-a-b}{}_2F_1(c-b,c-a,c;x)$, the solutions for $\pm i\epsilon$ lead to the same eigenfunction. The solution for $+\gamma$ remains finite as $q\to\pm\infty$ and the solution for $-\gamma$ diverges as $q\to\infty$. (ii) For $E>U$, the rest of the transformations are the same as in model (8) with the replacement $\gamma\to\pm i\epsilon$ and $\epsilon\to\pm i\gamma$. Therefore, the first and second wave functions are

$$\psi(q)=c[(1+v)^{\pm i\epsilon}(1-v)^{\pm i\gamma}{}_2F_1(\pm i\gamma\pm i\epsilon,\pm i\gamma\pm i\epsilon+1,\pm 2i\gamma+1;(1-v)/2)]_{v=\tanh(q/2)}.$$

For the same reason as above, the solutions for $\pm i\epsilon$ lead to the same eigenfunction. The solutions for $\pm i\gamma$ remain finite as $q\to\pm\infty$.

III. DISCUSSIONS

In the last section, we have shown step by step how to integrate Hamiltonians in the quantum level by canonical transformations. In the nine demonstrated models, it is seen that the procedure presented in this paper may be used in a consistent and systematic way. In the process leading to the middle step, namely, the p-linear, q-linear, and $\tilde{p}$-linear forms, two ways of reduction emerge naturally, each corresponds to one of the two independent solutions. The factorization of $H-E$ corresponds to the integration factor in classical integration. Yet, as we have mentioned in the beginning, the procedure does not work for arbitrary potentials. Now we shall see where the obstacles are.

The first step in the procedure is to choose a suitable function $g(q)$ for the point transformations to simplify the potentials. However, the point transformations also change $1/2p^2$ to a more complicated form $1/2(1/g'p)^2$. If the form is no more complicated than polynomials of p and q, it may be possible to factorize the form into one of the linear forms. In the examples we worked out, the choice of g and subsequent factorization is not particularly difficult. This is because the original potential functions may be simplified by $g=\sqrt{q}$, $\ln q$, $\cos^{-1}q$, $\tanh^{-1}q$, or $\coth^{-1}q$. These functions do not introduce additional complicated terms into $1/2p^2$ because their derivatives are simple roots of rational functions. If it is not apparent in the first place, the factorization is also more difficult than the classical counter part because of the noncommutative nature of the operator algebra.

It may be interesting to compare our procedure with the intertwining procedure outlined in Ref. [6]. In the intertwining procedure, three transformations are used: (1) the similarity transformation $\mathbf{S}$: $p\rightarrow p+ig(q)$, (2) the transformation $\tilde{\mathbf{S}}$: $q\rightarrow q+i/p$, and (3) the transformation $\mathbf{S}^{-1}$: $p\rightarrow p-ig(q)$. The first similarity transformation, $1/2p^2 \rightarrow 1/2p^2+ipg-1/2(g'+g^2)$, is used to cancel the potential V. That is, one sets

$$\frac{1}{2}(g'+g^2)=V+\lambda. \tag{3.1}$$

If, in addition, one sets

$$g'=V-V_0, \tag{3.2}$$

after the three transformations, the original Hamiltonian $H=1/2p^2+V^2$ will be reduced to another, hopefully easier Hamiltonian $H_0=1/2p^2+V_0^2$. The availability of an appropriate g and a solvable V_0 that satisfy Eqs. (3.1) and (3.2) may limit the generality of the intertwining procedure. When $V_0=0$, H_0 contains only one variable and is trivial to solve. For this case, Eqs. (3.1) and (3.2) are equivalent to

$$g'=g^2-2\lambda, \quad g'=V. \tag{3.3}$$

If $\lambda=0$, the solutions of Eq. (3.3) are $g=-1/(q+c)$ and $V=1/(q+c)^2$. By changing the variable, it is equivalent to the problem with $V=1/q^2$, namely, model (1) with $U=1$. If $\lambda<0$, set $2\lambda=-k^2$, the solutions of Eq. (3.3) are $g=k\tan(kq+c)$ and $V=k^2\sec^2(kq+c)$. By changing the variable, it is equivalent to the problem with $V=\csc^2 q$, namely, model (6) with $U=1$. If $\lambda>0$, set $2\lambda=k^2$, the solutions of Eq. (3.3) are $g=-k\tanh(kq+c)$ and $V=-k^2\,\mathrm{sech}^2(kq+c)$. By changing the variable, it is equivalent to the problem with $V=-\mathrm{sech}^2 q$, namely, model (7) with $U=1$. For an arbitrary V, one may solve g by Eq. (3.1) with λ as an undetermined parameter, and use the solution g and Eq. (3.2) to determine V_0. But there is no guarantee that $H_0=1/2p^2+V_0^2$ will be easier to solve than $H=1/2p^2+V^2$. For this reason, we were not able to find the solutions by the intertwining procedure except for models (1), (6), and (7).

It is clear now neither our procedure nor the intertwining procedure are set to work for arbitrary potentials. Nevertheless, the relations between canonical transformation and some standard techniques for solving differential equations, as pointed out in Ref. [6], seem to give some warrant to the method of canonical transformation, at least for models solvable by conventional techniques of differential equations. In this light, it may be advantageous to try canonical transformations first. But the point we wish to make in this paper is not just the technical viability of the method of canonical transformation. In classical mechanics, canonical transformations play more important roles in the analysis of dynamical systems than solving equations of motion. A famous example is the Kolmogorov-Arnold-Moser theorem, in which sequences of canonical transformations are used to prove the existence of the invariant trajectories [14–16]. The powerful techniques used in the proof of the Kolmogorov-Arnold-Moser theorem cannot be extended to quantum mechanics because they all involve Riemann integrals of dynamical variables. It may be possible to show that the three elementary canonical transformations, together with their large variety of combinations, may serve as an equally powerful set of tools for the analysis of quantum dynamical systems. This will be the direction of our future work.

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