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Non-Hermitian techniques of canonical transformations in quantum mechanics

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The quantum-mechanical version of the four kinds of classical canonical transformations is investigated by using non-Hermitian operator techniques. To help understand the usefulness of this approach, the eigenvalue problem of a harmonic oscillator is solved in two different types of canonical transformations. The quantum form of the classical Hamilton-Jacobi theory is also employed to solve time-dependent Schrödinger wave equations, showing that when one uses the classical action as a generating function of the quantum canonical transformation of time evolutions of state vectors, the corresponding propagator can easily be obtained.

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I. INTRODUCTION

The idea of canonical transformations is one of the highlights of classical mechanics [1]. It is not only theoretically but also practically important, and provides some clue to the quantization of classical systems. But the interesting point is that, even though the canonical transformations and the Hamilton-Jacobi theory are very helpful for solving classical equations of motions, there have appeared until now no serious attempts to use these ideas while solving quantum-mechanical problems. One of the reasons may be that as long as one restricts oneself to the unitary forms of canonical transformations there is no room for nontrivial transformations.

It was Anderson who seriously began to doubt the usual usage of the unitary canonical transformations, and he initiated a nonunitary technique of canonical transformations [2]. His idea is that the commutation relations $[q_r, p_s] = i\delta_{rs}$, $[q_r, q_s] = [p_r, p_s] = 0$ are preserved not only under unitary transformations but also following similarity transformations

$$Q_r = Cq_rC^{-1}, \;\; P_s = Cp_sC^{-1}. \tag{1}$$

Observing the fact that any canonical transformation can be decomposed into three basic canonical transformations, he computed the eigenvalue equation of harmonic oscillators and also calculated propagators for some model cases. Even though his idea is quite general it lacks clear classical counterparts.

In this paper we follow the traditional "mixed matrix element technique" of canonical transformations [3]. But the difference is that our mixed matrix elements are not unitary, thus allowing us to incorporate Anderson's idea of nonunitary canonical transformations. In fact, it is shown that quantum versions of canonical transformations exist and are formally similar to the classical ones. Using the full classical properties of canonical transformations we are able to solve the eigenvalue equation of a harmonic oscillator in a canonically transformed new space. Even the time-dependent Schrödinger equations of free particles and harmonic oscillators can be solved by using the quantum version of the Hamilton-Jacobi theory.

This paper is organized in the following way. Nonunitary quantum canonical transformations which have classical analogies are introduced in Sec. II. In Sec. III, the quantum version of a classical canonical transformation is used to solve the energy eigenstates of harmonic oscillators. The time evolutions of the Schrödinger wave equations of free particles and harmonic oscillators are also solved by using the quantum version of the Hamilton-Jacobi theory. Conclusions and further discussions are given in Sec. IV.

II. QUANTUM CANONICAL TRANSFORMATIONS

In classical mechanics there are four different types of canonical transformations, depending on the forms of generating functions $F_1(q_r, Q_s, t)$, $F_2(q_r, P_s, t)$, $F_3(p_r, Q_s, t)$, and $F_4(p_r, P_s, t)$. Even though some of them are related there are transformations which cannot be described by any other type of transformation. In this paper the quantum versions of the first and second types of canonical transformations are presented. The other two remaining ones can be inferred from these.

A. Canonical transformations of the first kind

Suppose $|q'\rangle = |q'_1, \ldots, q'_f\rangle$ is a simultaneous eigenket of observables q_r, $r = 1, \ldots, f$, such that

$$q_r|q'\rangle = q'_r|q'\rangle, \tag{2}$$
$$\langle q'|q''\rangle = \frac{1}{\rho(q')}\delta(q' - q''),$$
$$\int d^f q'\, |q'\rangle\rho(q')\langle q'| = 1.$$

From now on we use the convention that various eigenvalues of an observable q_r are denoted by attaching primes

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such as q_r', q_r'', etc. Schrödinger equations are sometimes readily solvable in different basis kets $|Q't\rangle = |Q_1', \ldots, Q_f', t\rangle$ which are defined with respect to $|q'\rangle$ by

$$\langle q'|Q't\rangle = e^{iF(q_r', Q_s', t)}, \quad (3)$$

where F is a function of real numbers q_r' and Q_s' and time t. Transformations of these kinds were investigated from the early days of quantum mechanics [3]. One should note that for an arbitrary function F the completeness condition of $|Q't\rangle$ is not guaranteed. Transformations which do not satisfy the completeness condition lose some information. Here we consider only the generating functions which meet the completeness condition. The general case will be considered in Appendix B. Suppose that for some density function $\rho(Q', t)$ they are complete, that is,

$$\langle Q't|Q''t\rangle = \frac{1}{\rho(Q', t)}\delta(Q' - Q''), \quad (4)$$

$$\int d^f Q'\, |Q't\rangle\rho(Q', t)\langle Q't| = 1. \quad (5)$$

In this case we are able to define other observables Q_r, $r = 1, \ldots, f$, such that

$$Q_r|Q't\rangle = Q_r'|Q't\rangle. \quad (6)$$

If all the vectors $|Q't\rangle$ do not form a complete set, the right hand side of Eq. (5) is no longer an identity operator but some projection operator. But as long as this projection operator commutes with the Hamiltonian operator, one may restrict one's interest to the invariant subspace of the projection operator without causing any internal contradiction. In this subspace completeness equation (5) is satisfied, and all of our techniques can be applied even to this case. An example of this kind is presented in Sec. III.

To get the quantum analogy of classical canonical transformations let us assume that $F(q_r, Q_s, t)$ is a "well-ordered" operator in the sense that it is a sum of q functions multiplied by Q functions on the right. In that case we have

$$\langle q'|F(q_r, Q_s, t)|Q't\rangle = F(q_r', Q_s', t)\langle q'|Q't\rangle. \quad (7)$$

In this case "the non-Hermitian canonical momentum operators" p_r and P_r, which are defined by

$$\langle q'|p_r|Q't\rangle = -i\frac{\partial}{\partial q_r'}\langle q'|Q't\rangle, \quad (8)$$

$$\langle Q't|P_r|q'\rangle = -i\frac{\partial}{\partial Q_r'}\langle Q't|q'\rangle, \quad (9)$$

can be recast in the familiar forms of classical mechanics

$$p_r = \frac{\partial F}{\partial q_r}, \quad P_r = -\frac{\partial F^\dagger}{\partial Q_r}. \quad (10)$$

Note that even if q_r and Q_s are observables the corresponding canonical momentum operators may not be Hermitian. In fact, their Hermitian conjugations are

$$p_r^\dagger = \rho(q)^{-1}p_r\rho(q), \quad P_r^\dagger = \rho(Q, t)^{-1}P_r\rho(Q, t). \quad (11)$$

These non-Hermitian properties are essential for our investigation and will be discussed more carefully in the last part of this section.

We now proceed to get the Schrödinger equation of motion in the canonically transformed Q space. Let $|t\rangle$ be a Schrödinger ket whose motion is given by $i\frac{d}{dt}|t\rangle = H(q_r, p_s, t)|t\rangle$. The Q-space wave function $\phi(Q_r', t) = \langle Q't|t\rangle$ in terms of q-space wave function $\psi(q_r', t) = \langle q'|t\rangle$ is given by

$$\phi(Q_r', t) = \int e^{-iF^*(q_r', Q_s', t)}\psi(q_r', t)\rho(q_r')d^f q'. \quad (12)$$

Applying the usual wave equation to $\psi(q_r', t)$ one obtains

$$i\frac{\partial}{\partial t}\phi(Q_r', t) = K\left(Q_r', -i\frac{\partial}{\partial Q_s'}, t\right)\phi(Q_r', t), \quad (13)$$

where the Q space Hamiltonian $K(Q_r, P_s, t)$ is

$$K(Q_r, P_s, t) = H(q_r, p_s, t) + \frac{\partial F^\dagger}{\partial t}. \quad (14)$$

After solving (13) the true wave function in q space is constructed by

$$\psi(q_r', t) = \int e^{iF(q_r', Q_s', t)}\phi(Q_r', t)\rho(Q_r', t)d^f Q'. \quad (15)$$

At this point we would like to emphasize that to get the completeness condition (B1), oftentimes one is forced to use "wrong" density functions in the original q space. For example, in a one-dimensional case the proper density function $\rho(x)$ of the Cartesian coordinate x is constant. But when one uses a generating function of the form $F(x, Q) = x^3 Q$, one is obliged to employ the wrong density function $\widetilde{\rho}(x) = 2x^3$. Even more, because of (11), the Hamiltonian becomes non-Hermitian. These two problems cancel each other out to resolve the dilemma. This can be seen in the following way. First rescale the original basis kets such that

$$\widetilde{|q'\rangle} = |q'\rangle S(q')^{-1}, \quad (16)$$

where

$$S(q) = \left(\frac{\widetilde{\rho}(q)}{\rho(q)}\right)^{\frac{1}{2}}, \quad (17)$$

and $\widetilde{\rho}(q)$ is a new density function. These rescaled kets satisfy the following completeness conditions:

$$\widetilde{\langle q'}|\widetilde{q''\rangle} = \frac{1}{\widetilde{\rho}(q')}\delta(q' - q''), \quad (18)$$

$$\int d^f q' \widetilde{|q'\rangle}\widetilde{\rho}(q')\widetilde{\langle q'|} = 1.$$

The corresponding conjugate momentum operator $\widetilde{p}_r$ defined by

$$\widetilde{\langle q'}|\widetilde{p}_r|\widetilde{q''\rangle} = -i\frac{\partial}{\partial q_r'}\widetilde{\langle q'}|\widetilde{q''\rangle} \quad (19)$$

is related to p_r by a similarity transformation

$$\widetilde{p}_r = Sp_rS^{-1}. \quad (20)$$

To investigate how the Schrödinger wave equation changes under this similarity transformation we make use of the standard ket $\rangle$ which is introduced by Dirac in his famous book on quantum mechanics [4]. For a given set of basis kets $|q'\rangle$ it, by definition, satisfies

$$\langle q'|\rangle = 1. \tag{21}$$

The reason why one introduces the standard ket is that any state $|1\rangle$ such as $\langle q'|1\rangle = \psi(q')$ can be written as $\psi(q)\rangle$, that is, a function $\psi(q)$ of an observable q operating on the standard ket $\rangle$. When one chooses another set of basis kets $|\widetilde{q'}\rangle$ one may use another standard ket $\widetilde{\rangle}$ such as $\widetilde{\langle q'|}\widetilde{\rangle} = 1$. From (16) it is clear that

$$\widetilde{\rangle} = S(q)\,\rangle. \tag{22}$$

Applying this similarity transformation to the original Schrödinger equation

$$H(q_r, p_s, t)\,\psi(q_r, t)\,\rangle = i\frac{\partial\psi}{\partial t}\,\rangle \tag{23}$$

the following similar non-Hermitian Schrödinger equation is produced:

$$H(q_r, \widetilde{p}_s, t)\,\psi(q_r, t)\,\widetilde{\rangle} = i\frac{\partial\psi}{\partial t}\,\widetilde{\rangle}. \tag{24}$$

It means that as long as one uses a $p_r = -i\frac{\partial}{\partial q_r}$ representation one may freely choose different density functions while the wave function and the Schrödinger equation remain intact. The sole requirement is that one should use a non-Hermitian Hamiltonian, which is tolerable as far as the wave function is concerned. But the physically meaningful transition probabilities should be constructed by using the original density function at which the Hamiltonian is Hermitian, and so also for the wave function normalization. This fact will be explained when the quantization of the harmonic oscillator is treated.

B. Canonical transformations of the second type

Consider two observables q_r and P_s with corresponding eigenkets $|q'\rangle$ and $|P't\rangle$ which are related by

$$\langle q'|P't\rangle = e^{iF(q'_r, P'_s, t)}\ , \tag{25}$$

where the generating function $F(q'_r, P'_s, t)$ is a function of real variables q'_r, P'_s, and t. Since P'_s is a continuous number, the corresponding ket is normalized by

$$\langle P't|P''t\rangle = \frac{1}{\rho(P', t)}\delta(P' - P''). \tag{26}$$

Consider a "well-ordered operator" $F(q, P, t)$ such that

$$\langle q'|F(q_r, P_s, t)|P't\rangle = F(q'_r, P'_s, t)\langle q'|P't\rangle. \tag{27}$$

The operators defined by

$$\langle q'|p_r|P't\rangle = -i\frac{\partial}{\partial q'_r}\langle q'|P't\rangle,$$
$$\langle P't|Q_r|q'\rangle = i\frac{\partial}{\partial P'_r}\langle P't|q'\rangle \tag{28}$$

can be written as

$$p_r = \frac{\partial F}{\partial q_r}, \quad Q_r = \frac{\partial F^\dagger}{\partial P_r}. \tag{29}$$

The wave equation in P space is

$$i\frac{\partial}{\partial t}\phi(P'_r, t) = K\left(i\frac{\partial}{\partial P'_r}, P'_s, t\right)\phi(P'_r, t), \tag{30}$$

where $\phi(P'_r, t) = \langle P't|t\rangle$ and $K = H + \frac{\partial F^\dagger}{\partial t}$ is a Hamiltonian in P space.

III. APPLICATIONS OF QUANTUM CANONICAL TRANSFORMATIONS

As much as the concept of classical canonical transformations is practically helpful for solving equations of motion, so also is the technique of quantum canonical transformations. It can be used not only for eigenvalue problems, but also for the time evolutions of state vectors including time-dependent perturbations. In this paper only some ideal physical systems are treated to clarify this concept.

A. Energy eigenfunctions of a harmonic oscillator

As an application of type 1 canonical transformations, consider the following Hamiltonian of a harmonic oscillator:

$$H(q,p) = \tfrac{1}{2}\left(q^2 + p^2\right)\ . \tag{31}$$

To solve the energy eigenvalue equation one may choose a generating function $F(q, Q) = \frac{1}{2}q^2 \cot Q$ which is well known from classical mechanics. In this case $|Q'\rangle$ is defined by

$$\langle q'|Q'\rangle = e^{i\frac{1}{2}q'^2 \cot Q'}. \tag{32}$$

Since F is an even function of q, any wave function in Q space becomes an even function in q space whenever Q space is transformed to q space by using the transition amplitude (32). In fact one may prove that

$$\int_0^\pi dQ'|Q'\rangle\rho(Q')\langle Q'| = \mathbf{1}_+, \tag{33}$$

where $\rho(Q) = \mathrm{cosec}^2 Q$, and $\mathbf{1}_+$ is the even-parity projection operator in q space. Since the Hamiltonian operator (31) commutes with $\mathbf{1}_+$ one may push along this line but only to obtain even-parity wave functions. The quantization of energy is very intuitive when a generating function of this type is used. (See Appendix A for more details.)

To get the complete wave functions the following definition of Q is employed:

$$Q = p + iq. \tag{34}$$

Assuming that it is a type 1 canonical transformation one can write p as $p = \frac{\partial F(q,Q)}{\partial q}$. Substituting this into (34), $F(q,Q)$ can be solved to give

$$F(q,Q) = -\frac{i}{2}q^2 + qQ. \tag{35}$$

Since this generating function contains a bilinear term in q and Q, there will be no such problem as the one which we encountered previously. By direct calculations it can be shown that basis kets $|Q'\rangle$ are in fact complete, and the corresponding density functions are

$$\rho(q) = \frac{1}{2\pi}e^{-q^2}, \quad \rho(Q) = 1. \tag{36}$$

The transformed operator P which can be read off from (10) and (35) is

$$P = -q. \tag{37}$$

The Hamiltonian K in Q space is

$$K = iQP + \frac{1}{2}Q^2 + \frac{1}{2}. \tag{38}$$

This Hamiltonian is non-Hermitian. Even worse, since $p = Q - iq$ is non-Hermitian, the original Hamiltonian (31) is non-Hermitian. All these unusual facts are reflected in the "wrong density functions" given by (36). As we already pointed out in the preceding section, there would be no problem at all as far as the wave function is concerned. One may convince oneself by checking the final wave function (44).

By (38) the time-independent Schrödinger wave equation in Q space is

$$\left(Q\frac{\partial}{\partial Q} + \frac{1}{2}Q^2 + \frac{1}{2}\right)\phi(Q) = E\,\phi(Q)\ . \tag{39}$$

This first order differential equation can easily be solved, giving the following wave function:

$$\phi(Q) = N\,Q^\nu\,e^{-\frac{1}{4}Q^2}, \tag{40}$$

where $\nu = E - \frac{1}{2}$, and N is a normalization constant which must be determined after the wave function in q space

$$\psi(q) = Ne^{\frac{1}{2}q^2}\int_{-\infty}^{\infty} e^{iqQ-\frac{1}{4}Q^2}Q^\nu dQ \tag{41}$$

is evaluated. It is not difficult to show that this is proportional to $D_\nu(\sqrt{2}q)$, where $D_\nu(z)$ is the *parabolic cylindrical function* defined by [5]

$$D_\nu(z) = \sqrt{\frac{2}{\pi}}2^\nu e^{-\frac{\pi}{2}\nu i}e^{\frac{z^2}{4}}\int_{-\infty}^{\infty} x^\nu e^{-2x^2+2ixz}dx, \qquad \mathrm{Re}\,\nu > -1. \tag{42}$$

For noninteger ν, it is known that $D_\nu(z)$ diverges as z goes to $-\infty$ [6]. That means the energy of the harmonic oscillator should be

$$E = n + \frac{1}{2}, \quad n = 0, 1, \dots\ . \tag{43}$$

The corresponding wave function is

$$\psi_n(q) = Ne^{\frac{1}{2}q^2}\left(\frac{1}{i}\frac{d}{dq}\right)^n\int_{-\infty}^{\infty} e^{iqQ-\frac{1}{4}Q^2}dQ$$
$$= N'(-1)^n e^{\frac{1}{2}q^2}\left(\frac{d}{dq}\right)^n e^{-q^2}. \tag{44}$$

This wave function coincides with the usual form constructed directly in the cartesian coordinate system.

B. Propagators

Our technique can also be used to solve the time-dependent Schrödinger wave equations. In classical mechanics there is an elegant way of solving equations of motion known as the Hamilton-Jacobi theory, which uses the classical action as the generating function. In that case the transformed Hamiltonian vanishes. Since the transformed quantum Hamiltonian (14) looks like the classical one, one may expect similar results for quantum mechanics. But, because of the noncommutative properties of quantum canonical variables, there may arise terms which are proportional to $\hbar$ which we simply put equal to 1.

To convince ourselves of the advantage of our quantum Hamilton-Jacobi theory for solving the time-dependent Schrödinger equations, we first consider one-dimensional free particles. The corresponding Hamiltonian is

$$H = \frac{1}{2}p^2. \tag{45}$$

The classical action for Q to q time evolution during t is

$$S(q,Q,t) = \frac{(q-Q)^2}{2t}. \tag{46}$$

That means the best well-ordered quantum generator for this time evolution is

$$F(q,Q,t) = \frac{1}{2t}(q^2 - 2qQ + Q^2). \tag{47}$$

Using this generating function the transformed ket $|Q't\rangle$ is defined by

$$\langle q'|Q't\rangle = e^{iF(q',Q',t)}. \tag{48}$$

Note that we are using the Schrödinger picture. That is the reason why the original basis ket $|q'\rangle$ is time independent. By direct calculation we obtain the following density functions:

$$\rho(q) = 1, \quad \rho(Q,t) = \frac{1}{2\pi t}\ . \tag{49}$$

The canonical momentum p, P, and the Q-space Hamiltonian K are given by

$$p = \frac{q-Q}{t}, \quad P = p, \quad K = \frac{i}{2t}. \tag{50}$$

The classical Hamiltonian in Q space vanishes, but in quantum physics it is propotional to $\hbar$. The equation of motion in Q space is

$$i\frac{\partial\phi}{\partial t} = \frac{i}{2t}\phi, \tag{51}$$

and the solution with a convenient normalization constant is

$$\phi(Q,t) = \sqrt{\frac{2\pi t}{i}}\phi(Q). \tag{52}$$

The true wave equation in q space is therefore

$$\psi(q,t) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi i t}} e^{i\frac{(q-Q)^2}{2t}} \phi(Q)dQ. \tag{53}$$

To understand the physical meaning of this propagation equation we investigate the $t \to 0$ limit. With the help of

$$\lim_{t\to 0} \frac{e^{i\frac{(x'-x'')^2}{2t}}}{\sqrt{2\pi i t}} = \delta(x' - x'') \tag{54}$$

it is clear that $\phi(q)$ is nothing but $\psi(q,0)$. This means that the free particle propagator is, by (53),

$$G(q',t|q'',0) = \frac{1}{\sqrt{2\pi i t}} e^{i\frac{(q'-q'')^2}{2t}}. \tag{55}$$

At this point we would like to emphasize that by a direct path integral it is known that the general form of a propagator is [7]

$$G(q',t|q'',0) = f(t)e^{iS_{\rm cl}}, \tag{56}$$

where $S_{\rm cl}$ is the classical action and $f(t)$ is an undetermined function of time. In our approach $f(t)$ is related to the "wrong" density function $\rho(Q,t)$ and the $\hbar$ proportional "non-Hermitian" Hamiltonian K in Q space.

Using a similar technique one can solve the time-dependent Schrödinger equation for harmonic osillators. The well-ordered generating function would be

$$F(q,Q,t) = \frac{1}{2}(q^2 + Q^2)\cot t - qQ\,\text{cosect}\ , \tag{57}$$

which is just the classical action for Q to q time evolution during t [1]. One can prove the completeness condition for $|Q',t\rangle$, obtaining simultaneously the following density functions:

$$\rho(q) = 1, \ \ \rho(Q,t) = \frac{1}{2\pi \sin t}. \tag{58}$$

If q and Q commute, the tranformed Hamiltonian K vanishes. But for quantum theory it does not but is proportional to $\hbar$, that is,

$$K(Q,P,t) = \frac{i}{2}\cot t. \tag{59}$$

Using this Hamiltonian the Schrödinger equation in Q space can be solved, giving the following time-dependent wave function:

$$\phi(Q,t) = \sqrt{\frac{2\pi \sin t}{i}}\phi(Q). \tag{60}$$

With the help of (58) and (54) one obtains the following propagator of a harmonic oscillator:

$$G(q',t|q'',0) = \frac{1}{\sqrt{2\pi i \sin t}} e^{iF(q',q'',t)}, \tag{61}$$

where $F(q',q'',t)$ is the classical action given by (57).

To see why the quantum generating function which has the classical analogy is so successful, consider the following classical generating function for infinitesmal time evolution:

$$F(q_r,P_s) = \sum_r q_r P_r - \delta t H(q_r,P_s), \tag{62}$$

where $H = \frac{1}{2}\sum_r P_r^2 + V(q_s)$ is the usual Hamiltonian. Using this we define a state $|P'\rangle$ by $\langle q'|P'\rangle = e^{iF(q',P')}$. Then the density functions in both q and P spaces are trivial and Q_r, which is defined by $\frac{\partial F^\dagger}{\partial P_r}$, is Hermitian. This means that all the eigenkets $|Q'\rangle$ form a complete set. To get the physical meaning of $|Q'\rangle$ consider $\langle q'|Q'\rangle$. Using the completeness of eigenkets $|P'\rangle$ one has

$$\langle q'|Q'\rangle = \int_{-\infty}^{\infty} \frac{dP'}{2\pi} \langle q'|P'\rangle\langle P'|Q'\rangle$$
$$= \int_{-\infty}^{\infty} \frac{dP'}{2\pi} e^{i\sum q'_r P'_r - i\delta t H(q'_r,P'_s)} \langle P'|Q'\rangle. \tag{63}$$

Now the term $e^{i\sum q'_r P'_r}$ in the last part of this equation can be written as $\langle Q' \leftarrow q'|P'\rangle$, where $|Q' \leftarrow q'\rangle$ is an eigenket of Q_r whose eigenvalue is q'_r. Using this fact (63) can be simplified as

$$\langle q'|Q'\rangle = \langle Q' \leftarrow q'|e^{-i\delta t H(Q_r,P_s)}|Q'\rangle, \tag{64}$$

that is, $|Q' \leftarrow q'\rangle = e^{-i\delta t H}|q'\rangle$. This means that (62) is a both classically and quantum mechanically correct generating function of the infinitesimal time evolutions.

IV. CONCLUSION AND DISCUSSION

We would like to emphasize that when the quantum analogies of classical canonical transformations are seriously employed, one obtains useful quantum canonical transformations which can be used to solve either time-independent or time-dependent Schrödinger equations. Furthermore, the generating operators of quantum canonical transformations can be inferred from the classical generating functions. In this way the classical canonical transformations have some part in quantum mechanics. This classical analogy is our strong point which becomes rather obscure when one uses abstract similarity transformation formalism. (See Appendix B for more details.) We expect that our idea will produce more fruitful results when applied to the perturbation theory of quantum mechanics.

Note added. After submission of this paper we received papers from Professor T. Curtright which show similar interests in the quantum canonical transformations [8].

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APPENDIX A: ENERGY QUANTIZATIONS OF HARMONIC OSCILLATORS

Consider a harmonic oscillator whose Hamiltonian is given by

$$H(q,p)=\frac{1}{2}(q^2+p^2). \tag{A1}$$

To get some insight into the energy quantization of a harmonic oscillator we introduce the transformation

$$\langle q'|Q'\rangle = e^{i\frac{1}{2}q'^2\cot Q'}. \tag{A2}$$

Because of (33) this transformation is complete only for the even-parity subspace of $\psi(q)$. The corresponding non-Hermitian operators p and P are given by

$$p=\frac{\partial F}{\partial q}=q\cot Q\ , \tag{A3}$$

$$P=-\frac{\partial F^\dagger}{\partial Q}=\frac{1}{2}\text{cosec}^2 Q q^2\ .$$

From the commutation relation $[q,p]=i$ we have the equation

$$[q,\cot Q]=iq^{-1}. \tag{A4}$$

Using this relation the Q-space Hamiltonian $K(Q,P)=H(q,p)$ can be shown to be

$$K(Q,P)=P+\frac{3}{2}i\cot Q. \tag{A5}$$

The eigenvalue equation $K(Q,P)\varphi=E\varphi$ in Q space is therefore

$$-i\left(\frac{\partial}{\partial Q}-\frac{3}{2}\cot Q\right)\varphi=E\varphi. \tag{A6}$$

It can immediately be solved, giving

$$\varphi(Q)=N\sin^{\frac{3}{2}}Q e^{iEQ}, \tag{A7}$$

where N is a normalization constant. Since $|Q'\rangle$ is defined by (A2) the wave function in Q space should satisfy $\varphi(Q'+\pi)=\varphi(Q')$. This means that

$$e^{i(\frac{3}{2}+E)\pi}=1. \tag{A8}$$

This together with the positive energy condition yields

$$E=(2n+\tfrac{1}{2}),\ n=0,1,2,\dots\ . \tag{A9}$$

The wave function $\psi(q')$ in q space is given by

$$\begin{aligned}\psi_{2n}(q') &= N'\int_0^\pi dQ'\rho(Q')\langle q'|Q'\rangle\varphi(Q') \\ &= N''\int_0^\pi dQ'\frac{1}{\sin^{\frac{1}{2}}Q'} \\ &\quad\times\exp\left(\frac{i}{2}q'^2\cot Q'+i(2n+\tfrac{1}{2})Q'\right).\end{aligned} \tag{A10}$$

When we compare this equation with the well known result for a harmonic oscillator (61)

$$\sum_{n=0}^{\infty}\psi_{2n}(q')\psi_{2n}^*(0)e^{-i(2n+\frac{1}{2})T}=\left(\frac{1}{2\pi i}\right)^{\frac{1}{2}}\frac{e^{\frac{i}{2}q'^2\cot T}}{\sin^{\frac{1}{2}}T}, \tag{A11}$$

we obtain the correct even-parity wave functions.

APPENDIX B: GENERALIZATIONS AND RELATION TO SIMILARITY TRANSFORMATION APPROACH

In Appendix B we generalize some results obtained in Sec. II and investigate the relation between our method and the similarity transformation method given by (1). For simplicity we consider only a one-dimensional case.

Suppose $|q'\rangle$ is a set of ket vectors in a Hilbert space and $\widetilde{|q'\rangle}$ a new set of ket vectors in the same Hilbert space. In general, $\widetilde{|q'\rangle}$ may not form a complete orthogonal set. One can make $\widetilde{|q'\rangle}$ complete by introducing a new inner product in the same Hilbert space, which will be shown later in this Appendix. In this case the original $|q'\rangle$ and the new $\widetilde{|q'\rangle}$ will be complete with respect to two different inner products, that is, with respect to the old and to the new ones, respectively. Then the dual vector $\widetilde{\langle q'|}$ should be defined using the new inner product. Suppose that $|q'\rangle$ and $\widetilde{|q'\rangle}$ are complete with density functions $\rho(q')$ and $\widetilde{\rho}(q')$, respectively. Then one gets

$$\int dq'\,|q'\rangle\rho(q')\langle q'|=1, \tag{B1}$$

$$\int dq'\,\widetilde{|q'\rangle}\widetilde{\rho}(q')\widetilde{\langle q'|}=1.$$

For some cases $|q'\rangle$ or $\widetilde{|q'\rangle}$ may be incomplete. In that case the left hand side of (5) should be replaced by appropriate projection operators. The operators q and $\widetilde{q}$ which are defined by

$$q|q'\rangle=q'|q'\rangle,\ \ \widetilde{q}\widetilde{|q'\rangle}=q'\widetilde{|q'\rangle} \tag{B2}$$

will be Hermitian with respect to the old inner product and the new one, respectively. It can be shown that the two density functions together with $\widetilde{|q'\rangle}$ determine the new inner product uniquely. To clarify this point, let us consider the following.

Let us write $\widetilde{|q'\rangle}\equiv C(t)|q'\rangle$, where $C(t)$ can be regarded as a time-dependent similarity transformation. Then $\widetilde{q}=CqC^{-1}$. A new dual vector $\widetilde{\langle q'|}$ can be expressed in terms of the old one as

$$\widetilde{\langle q'|}=\langle q'|C^\dagger M, \tag{B3}$$

where M is an operator defining the new inner product. In other words, $(\alpha,\beta)=\langle\alpha|M|\beta\rangle$, where (,) denotes the new inner product. Using the completeness relation we can find

$$C^\dagger MC=\frac{\rho(q)}{\widetilde{\rho}(q)}, \tag{B4}$$

and conclude that ρ, $\widetilde{\rho}$, and C determine M completely. In Sec. II we restricted ourselves to the cases where both $|q'\rangle$ and $\widetilde{|q'\rangle}$ form complete orthogonal sets with respect to the same inner product. In this case, $M=1$ and C is "almost unitary" in the sense that $C\sqrt{\frac{\widetilde{\rho}}{\rho}}$ is unitary. This is not always true. As shown above, in general cases we are forced to introduce two different inner products.

Now we study how the momentum operators transform. Using (B4) and the fact that momentum operators are defined by

$$\langle q'|p = -i\frac{\partial}{\partial q'}\langle q'|, \quad \widetilde{\langle q'|}\widetilde{p} = -i\frac{\partial}{\partial q'}\widetilde{\langle q'|}, \tag{B5}$$

one can easily prove that

$$\widetilde{p} = \widetilde{C}p\widetilde{C}^{-1}, \quad \widetilde{q} = \widetilde{C}q\widetilde{C}^{-1}, \tag{B6}$$

with $\widetilde{C} = (C^{\dagger}M)^{-1}$. Next we consider the Schrödinger equation

$$H(q,p,t)|t\rangle = i\frac{d}{dt}|t\rangle. \tag{B7}$$

Multiplying both sides by $\widetilde{\langle q'|}$, we have

$$\widetilde{\langle q'|}H(q,p,t)|t\rangle = i\frac{\partial}{\partial t}\widetilde{\langle q'|}t\rangle - \widetilde{\langle q'|}\dot{G}|t\rangle, \tag{B8}$$

where $\dot{G}$ is defined by

$$\widetilde{\langle q'|}\dot{G} = i\frac{\partial}{\partial t}\widetilde{\langle q'|}. \tag{B9}$$

One can express $\dot{G}$ using the similarity tranformation

$$\dot{G} = i\widetilde{C}\frac{\partial}{\partial t}\widetilde{C}^{-1}. \tag{B10}$$

Denoting

$$K(\widetilde{q},\widetilde{p},t) \equiv H(q,p,t) + \dot{G}, \tag{B11}$$

one can write the Schrödinger equation in $\widetilde{q}$ space as

$$K\left(q', -i\frac{\partial}{\partial q'}, t\right)\widetilde{\langle q'|t\rangle} = i\frac{\partial}{\partial t}\widetilde{\langle q'|t\rangle}\ . \tag{B12}$$

To find $K(\widetilde{q},\widetilde{p},t)$ in terms of $\widetilde{q}$ and $\widetilde{p}$, (B6) may, in principle, be used. However as in Sec. II, some interesting results can be obtained if the transformation is expressed in the form

$$\langle q'\widetilde{|q''\rangle} = e^{iF(q',q'',t)}, \quad \widetilde{\langle q''|}q'\rangle = e^{-iG(q'',q',t)}, \tag{B13}$$

where F and G are some functions obeying the relation

$$\int dq'' e^{iF(q',q'',t)}\widetilde{\rho}(q'',t)e^{-iG(q'',q''',t)} = \frac{\delta(q'-q''')}{\rho(q')}. \tag{B14}$$

As in Sec. II we assume that $F(q,\widetilde{q},t)$ and $G(\widetilde{q},q,t)$ are "well-ordered" operators in the sense that in $F(q,\widetilde{q},t)$ all q's are on the left, and in $G(\widetilde{q},q,t)$ all q's are on the right. Then (10) corresponds to

$$p = \frac{\partial}{\partial q}F(q,\widetilde{q},t), \quad \widetilde{p} = -\frac{\partial}{\partial \widetilde{q}}G(\widetilde{q},q,t), \tag{B15}$$

and we also have

$$\dot{G} = \frac{\partial}{\partial t}G(\widetilde{q},q,t). \tag{B16}$$

Equation (B15) can be used to get $\widetilde{q}$ and $\widetilde{p}$ in terms of q and p. In "almost unitary" cases considered in Sec. II, we get

$$G(\widetilde{q},q,t) = F(q,\widetilde{q},t)^{\dagger}. \tag{B17}$$

The two density functions can be absorbed into F and G, which is obvious from (B14)–(B16). In this case we have $\rho = 1$ and $\widetilde{\rho} = 1$.

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