Canonical Transformations and the Hamilton-Jacobi Theory in Quantum Mechanics

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Canonical transformations using the idea of quantum generating functions are applied to construct a quantum Hamilton-Jacobi theory, based on the analogy with the classical case. An operator and a c-number forms of the time-dependent quantum Hamilton-Jacobi equation are derived and used to find dynamical solutions of quantum problems. The phase-space picture of quantum mechanics is discussed in connection with the present theory.

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I. INTRODUCTION

Various mechanical problems can be elegantly approached by the Hamiltonian formalism, which not only found well-established ground in classical theories [1], but also provided much physical insight in the early development of quantum theories [4-10]. It is curious though that the concept of canonical transformations, which plays a fundamental role in the Hamiltonian formulation of classical mechanics, has not attracted as much attention in the corresponding formulation of quantum mechanics. A relatively small quantity of literature is available as of now on this subject [4-10]. The main reason for this is probably that canonical variables in quantum mechanics are not c-numbers but noncommuting operators, manipulation of which is considerably involved. In spite of this difficulty, the great success of canonical transformations in classical mechanics makes it desirable to investigate the possibility of application of the concept of canonical transformations in quantum mechanics at least to the extent allowed in view of the analogy with the classical case.

The usefulness of the classical canonical transformations is most visible in the Hamilton-Jacobi theory where one seeks a generating function that makes the transformed Hamiltonian become identically zero [1]. A quantum analog of the Hamilton-Jacobi theory has previously been considered by Leacock and Padgett [8] with particular emphasis on the quantum Hamilton’s characteristic function and applied to the definition of the quantum action variable and the determination of the bound-state energy levels [11]. However, the dynamical aspect of the quantum Hamilton-Jacobi theory appears to remain untouched. In the present study, we concentrate on this aspect of the problem, and derive the time-dependent quantum Hamilton-Jacobi equation following closely the procedure that lead to the classical Hamilton-Jacobi equation.

The analogy between the classical and quantum Hamilton-Jacobi theories can be best exploited by employing the idea of the quantum generating function that was first introduced by Jordan [4] and Dirac [5], and recently reconsidered by Lee and l’Yi [10]. The “well-ordered” operator counterpart of the quantum generating function is used in constructing our quantum Hamilton-Jacobi equation, which resembles in form the classical Hamilton-Jacobi equation. By means of well-ordering, a unique operator is associated with a given c-number function, thereby the ambiguity in the ordering problem is removed. We identify the quantum generating function accompanying the quantum Hamilton-Jacobi theory as the quantum Hamilton’s principal function, and apply this theory to find the dynamical solutions of quantum problems.

The prevailing conventional belief that physical observables should be Hermitian operators invokes in our discussion the unitary transformation that transforms one Hermitian operator to another. This along with the fact that the unitary transformation preserves the fundamental quantum condition for the new canonical variables \([\hat{Q}, \hat{P}] = i\hbar\) if the old canonical variables satisfy \([q, p] = i\hbar\) provides a good reason why we call the unitary transformation the quantum canonical transformation. This definition of the quantum canonical transformation is analogous to the classical statement that the classical canonical transformation keeps the Poisson brackets invariant, i.e., \([Q, P]_{PB} = [q, p]_{PB} = 1\). In our current discussion of the quantum canonical transformation we will consider exclusively the case of the unitary transformation.

The paper is organized as follows. In Sec. II the quantum canonical transformation using the idea of the quantum generating function is briefly reviewed, and the transformation relation between the new Hamiltonian and the old Hamiltonian expressed in terms of the quantum generating function is derived. From this relation, and by analogy

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with the classical case, we arrive at the quantum Hamilton-Jacobi equation in Sec. III. It will be found that the
unitary transformation of the special type \( \hat{U}(t) = \hat{T}(t) \hat{A} \) where \( \hat{T}(t) \) is the time-evolution operator and \( \hat{A} \) is an
arbitrary time-independent unitary operator satisfies the quantum Hamilton-Jacobi equation. Sec. IV is devoted to
the discussion of the quantum phase-space distribution function under canonical transformations. The differences
between our approach and that of Ref. [12] are described. Boundary conditions and simple applications of the theory
are given in Sec. V, where to perceive the main idea easily most of the discussion is developed with the simple case
\( \hat{A} = \hat{I} \), the unit operator, while keeping in mind that the present formalism is not restricted to this case. Finally, Sec.
VI presents concluding remarks.

II. QUANTUM CANONICAL TRANSFORMATIONS

Let us begin our discussion by reviewing the theory of the quantum canonical transformations \[\hat{F}(\hat{q}, \hat{Q}, t)\]. A quantum
generating function that is analogous to a classical generating function is defined in terms of the matrix elements of
a unitary operator as follows \[\hat{F}(\hat{q}, \hat{Q}, t)\],

\[ e^{i\hat{F}(\hat{q}, \hat{Q}, t)/\hbar} \equiv \langle q_1|Q_2\rangle_t = \langle q_1|\hat{U}(t)|q_2\rangle, \tag{1} \]

where the unitary operator \( \hat{U}(t) \) transforms an eigenvector of \( \hat{q} \) into an eigenvector of \( \hat{Q} = \hat{U}\hat{q}\hat{U}^\dagger \), i.e., \(|Q_1\rangle_t = \langle q_1|\hat{U}(t)|q_1\rangle \)
and \(|P_1\rangle_t = \langle q_1|\hat{U}(t)|P_1\rangle \). Different types of the quantum generating function can be defined similarly \[\hat{F}(\hat{q}, \hat{P}, t)\], i.e.,

\[ e^{i\hat{F}(\hat{q}, \hat{P}, t)/\hbar} \equiv \langle q_1|P_2\rangle_t = \langle q_1|\hat{U}(t)|p_2\rangle, \]

\[ e^{i\hat{F}(\hat{P}, \hat{q}, t)/\hbar} \equiv \langle p_1|Q_2\rangle_t = \langle p_1|\hat{U}(t)|q_2\rangle, \]

\[ e^{i\hat{F}(\hat{P}, \hat{P}, t)/\hbar} \equiv \langle p_1|P_2\rangle_t = \langle p_1|\hat{U}(t)|p_2\rangle. \]

The quantum canonical transformation, or the unitary transformation, corresponds to a change of representation or
equivalently to a rotation of axes in the Hilbert space. The unitary transformation guarantees that the fundamental
quantum condition \[\hat{Q}, \hat{P} = [\hat{q}, \hat{p}] = i\hbar \] holds, the new canonical variables \( \hat{Q}, \hat{P} \) are Hermitian operators, and the
eigenvectors of \( \hat{Q} \) or \( \hat{P} \) form a complete basis. One should keep in mind that the eigenvalue \( Q_1 \) has the same numerical
value as the eigenvalue \( q_1 \) because the unitary transformation preserves the eigenvalue spectrum of an operator \[\hat{F}(\hat{q}, \hat{Q}, t)\]. In cases where it is convenient, one is free to interchange \( q_1 \) (or \( p_1 \)) with \( Q_1 \) (or \( P_1 \)).

Transformation relations between \( (\hat{q}, \hat{p}) \) and \( (\hat{Q}, \hat{P}) \) can be expressed in terms of the “well-ordered” generating
operator \( \hat{F}(\hat{q}, \hat{Q}, t) \) that is an operator counterpart of the quantum generating function \( \hat{F}(\hat{q}, \hat{Q}, t) \) as follows \[\hat{F}(\hat{q}, \hat{Q}, t)\],

\[ \hat{p} = \frac{\partial \hat{F}(\hat{q}, \hat{Q}, t)}{\partial \hat{q}}, \quad \hat{P} = -\frac{\partial \hat{F}(\hat{q}, \hat{Q}, t)}{\partial \hat{Q}}. \tag{2} \]

Similar expressions for other types of the generating operators can be immediately inferred by analogy with the
classical relations. For a later reference, we present the relations for \( \hat{F}(\hat{q}, \hat{P}, t) \) below,

\[ \hat{p} = \frac{\partial \hat{F}(\hat{q}, \hat{P}, t)}{\partial \hat{q}}, \quad \hat{Q} = -\frac{\partial \hat{F}(\hat{q}, \hat{P}, t)}{\partial \hat{P}}. \tag{3} \]

It is interesting to note that, whereas the four types of the generating functions in classical mechanics are related
with each other through the Legendre transformations \[\hat{F}(\hat{q}, \hat{Q}, t)\], the relations between the quantum generating functions of
different types can be expressed by means of the Fourier transformations. For example, the transition from \( \hat{F}(\hat{q}, \hat{Q}, t) \)
to \( \hat{F}(\hat{q}, \hat{P}, t) \) can be accomplished by

\[ e^{i\hat{F}(\hat{q}, \hat{P}, t)/\hbar} = \int dQ_2 \langle q_1|Q_2\rangle_t \langle Q_2|P_2\rangle_t, \]

\[ = \frac{1}{\sqrt{2\pi\hbar}} \int dQ_2 e^{i\hat{F}(\hat{q}, \hat{Q}, t)/\hbar} e^{i\hat{P}_2Q_2/\hbar}. \tag{4} \]

1 An eigenvalue \( X_1 \) and an eigenvector \( |X_1\rangle \) of an operator \( \hat{X} \) are defined by the equation, \( \hat{X} |X_1\rangle = X_1 |X_1\rangle \) \( (X = q, p, Q, \) and \( P) \). Different subindices are used to distinguish different eigenvalues or eigenvectors, e.g., \( X_2, |X_2\rangle \), etc.; The subscript \( t \) on a ket \( |\rangle_t \) (bra \( \langle \rangle_t \) expresses time dependence of the ket \( |\rangle_t \) (bra \( \langle \rangle_t \)).

2 A well-ordered operator \( \hat{G}(\hat{X}, \hat{Y}) \) is developed from a c-number function \( G(X_1, Y_2) \) such that \( \langle X_1|\hat{G}(\hat{X}, \hat{Y})|Y_2\rangle = G(X_1, Y_2) \langle X_1|Y_2\rangle \). For example, if \( G(X_1, Y_2) = X_1Y_2 + Y_2^2X_1^2 \), then \( \hat{G}(\hat{X}, \hat{Y}) = \hat{X}\hat{Y} + \hat{X}^2\hat{Y}^2 \).
The usefulness of the concept of the quantum generating function can be revealed, for example, by considering the unitary transformation $\hat{U} = e^{i g(\hat{q})/\hbar}$ where $g$ is an arbitrary real function. From the definition of the quantum generating function, we have

$$e^{i F_2(q_1, p_2)/\hbar} = (q_1 | e^{i g(\hat{q})/\hbar} | p_2),$$

$$= \frac{1}{\sqrt{2\pi\hbar}} e^{i g(q_1) + q_1 p_2}.$$  \hspace{1cm} (5)

The well-ordered generating operator is then given by

$$\bar{F}_2(\hat{q}, \hat{P}) = g(\hat{q}) + \hat{q} \hat{P} + \frac{i}{2} \ln 2\pi\hbar,$$  \hspace{1cm} (6)

and Eq. (3) yields the transformation relations

$$\hat{Q} = \hat{q},$$  \hspace{1cm} (7)

$$\hat{P} = \hat{p} - \frac{\partial g(\hat{q})}{\partial \hat{q}}.$$  \hspace{1cm} (8)

This shows that, in some cases, an introduction of the quantum generating function can provide an effective method of finding the transformation relations between $(\hat{q}, \hat{p})$ and $(\hat{Q}, \hat{P})$ without recourse to the equations $\hat{Q} = \hat{U} \hat{q} \hat{U}^\dagger$ and $\hat{P} = \hat{U} \hat{p} \hat{U}^\dagger$.

Now we consider the dynamical equations governing the time-evolution of quantum systems. The time-dependent Schrödinger equation for the system with the Hamiltonian $H(\hat{q}, \hat{p}, t)$ is given in terms of a time-dependent ket $|\psi_t\rangle$ by

$$i\hbar \frac{\partial}{\partial t} |\psi_t\rangle = H(\hat{q}, \hat{p}, t) |\psi_t\rangle.$$  \hspace{1cm} (9)

In $Q$-representation the time-dependent Schrödinger equation takes the form

$$i\hbar \frac{\partial}{\partial t} \psi^Q(Q_1, t) = K \left( Q_1, -i\hbar \frac{\partial}{\partial Q_1}, t \right) \psi^Q(Q_1, t),$$  \hspace{1cm} (10)

where $\psi^Q(Q_1, t) = \langle Q_1 | \psi_t \rangle$, and

$$K(\hat{Q}, \hat{P}, t) = H(\hat{q}, \hat{p}, t) + i\hbar \frac{\partial}{\partial t} \hat{U}^\dagger.$$  \hspace{1cm} (11)

The second term on the right hand side of Eq. (11) arises from the fact that we allow the time dependence of the unitary operator $\hat{U}(t)$, which indicates that, even though we adopt here the Schrödinger picture where the time dependence associated with the dynamical evolution of a system is attributed solely to the ket $|\psi_t\rangle$, $\hat{Q}$ and $|Q_1\rangle_t$ may depend on time also. In terms of the generating operator $\hat{F}_1(\hat{q}, \hat{Q}, t)$, Eq. (11) can be written as

$$K(\hat{Q}, \hat{P}, t) = H(\hat{q}, \hat{p}, t) + \frac{\partial}{\partial t} \hat{F}_1(\hat{q}, \hat{Q}, t).$$  \hspace{1cm} (12)

The equivalence of Eqs. (11) and (12) can be proved as shown in Appendix A. It is important to note that $K(\hat{Q}, \hat{P}, t)$ plays the role of the transformed Hamiltonian governing the time-evolution of the system in $Q$-representation. The analogy with the classical theory is remarkable.

**III. QUANTUM HAMILTON-JACOBI THEORY**

We are now ready to proceed to formulate the quantum Hamilton-Jacobi theory. One can immediately notice that, if $K(\hat{Q}, \hat{P}, t)$ of Eq. (12) vanishes, the time-dependent Schrödinger equation in $Q$-representation yields a simple solution, $\psi^Q = \text{const}$. This observation along with Eq. (2) naturally leads us to the following quantum Hamilton-Jacobi equation,

$$H \left( \hat{q}, \frac{\partial S_1(\hat{q}, \hat{Q}, t)}{\partial \hat{q}}, t \right) + \frac{\partial S_1(\hat{q}, \hat{Q}, t)}{\partial t} = 0,$$  \hspace{1cm} (13)
Differentiating this equation with respect to time, we obtain i.e., the canonical transformation mediated by a separable unitary operator is exactly the one that we seek. Assuming \( \langle \hat{q}, \hat{p}, t \rangle = 0 \), it seems desirable to search a corresponding c-number form of the quantum Hamilton-Jacobi equation. For this difficult to attain solutions of it due to its unfamiliar appearance as an operator partial differential equation. Thus it seems desirable to search a corresponding c-number form of the quantum Hamilton-Jacobi equation. Even though we arrive at the correct form of the quantum Hamilton-Jacobi equation, it seems at first sight quite difficult to attain solutions of it due to its unfamiliar appearance as an operator partial differential equation. Thus it seems desirable to search a corresponding c-number form of the quantum Hamilton-Jacobi equation. For this task, we note that, if the unitary operator \( \hat{U}(t) \) is assumed to be separable into \( \hat{U}(t) = \hat{T}(t) \hat{A} \), where \( \hat{T}(t) \) is the time-evolution operator and \( \hat{A} \) is an arbitrary time-independent unitary operator, then \( \psi Q(q, t) = \langle q, \hat{A}^\dagger \hat{T}(t) \rangle \psi(t = 0) = \langle q, \hat{A}^\dagger \rangle \psi(t = 0) \rangle = \text{const.} \). Thus this means that the left hand side of Eq. (10) becomes zero, i.e., the canonical transformation mediated by a separable unitary operator is exactly the one that we seek. Assuming \( \hat{U}(t) = \hat{T}(t) \hat{A} \), we rewrite Eq. (1) as

\[
\hat{A} \hat{q} \hat{t} = \langle q, \hat{A} \rangle \hat{q} \hat{t} = \psi(q, t) = \psi(q, t).
\]

Differentiating this equation with respect to time, we obtain

\[
\frac{i}{\hbar} \frac{\partial S_1}{\partial t} e^{iS_1/\hbar} = \langle q_1 | \hat{A} q_2 \rangle = \frac{1}{2} \langle q_1 | \hat{H} \hat{T} \hat{A} | q_2 \rangle,
\]

\[
\frac{1}{\hbar} H (q_1, -i \hbar \frac{\partial}{\partial q_1}, t) \langle q_1 | \hat{T} \hat{A} | q_2 \rangle = \frac{1}{\hbar} H (q_1, -i \hbar \frac{\partial}{\partial q_1}, t) e^{iS_1/\hbar}.
\]

Eq. (16) leads immediately to the desired c-number form of the quantum Hamilton-Jacobi equation

\[
\left[ H (q_1, -i \hbar \frac{\partial}{\partial q_1}, t) + \frac{\partial S_1(q_1, Q_2, t)}{\partial t} \right] e^{iS_1(q_1, Q_2, t)/\hbar} = 0.
\]

Substitution of \( S_2(q_1, P_2, t) \) for \( S_1(q_1, Q_2, t) \) generates another c-number form of the quantum Hamilton-Jacobi equation. The equations for the cases of \( S_3(p_1, Q_2, t) \) and \( S_4(p_1, P_2, t) \) can be derived through a similar process.

Consider a one-dimensional nonrelativistic quantum system whose Hamiltonian is given by

\[
H(q, \dot{q}, t) = \frac{\dot{q}^2}{2} + V(q, t).
\]

The c-number form of the quantum Hamilton-Jacobi equation (17) for this problem becomes

\[
\frac{1}{2} \left( \frac{\partial S_1}{\partial q_1} \right)^2 + \frac{\hbar^2}{2m} \frac{\partial^2 S_1}{\partial q_1^2} + V(q_1, t) + \frac{\partial S_1}{\partial t} = 0.
\]

We can see clearly that, in the limit \( \hbar \to 0 \), the above equation reduces to the classical Hamilton-Jacobi equation. The second term of Eq. (19) represents the quantum effect. We note that it has been known from the early days that substitution of \( \psi(q, t) = e^{iS(q, t)/\hbar} \) into the Schrödinger equation gives rise to the same Hamilton-Jacobi equation for
where $S(q,t)$ is interpreted merely as the complex-valued phase of the wave function (see, for example, Ref. [3]). The present approach more clearly shows the strong analogy between the classical and quantum Hamilton-Jacobi theories emphasizing that the quantum Hamilton’s principal function $S$ which is related with the wave function via Eq. (14) plays the role of the quantum counterpart of the classical generating function. Moreover, as discussed later in Sec. V, $e^{iS_1/\hbar}$ defined in Eq. (14) can be interpreted as a propagator under a certain choice of $\dot{A}$.

It may be viewed that the Hamilton-Jacobi equation in the form of Eq. (19) is no more tractable analytically than the Schrödinger equation for general potential problems. Nevertheless, it would be possible at least to obtain an approximate solution of it using a perturbative method as follows. Since the solution of Eq. (19) is given by the classical Hamilton’s principal function in the limit $\hbar \to 0$, we can expand the general solution in powers of $\hbar$:

$$S_1 = S_1^{(0)} + \hbar S_1^{(1)} + \hbar^2 S_1^{(2)} + \cdots,$$

(20)

where $S_1^{(0)}$ is the classical Hamilton’s principal function. Substituting Eq. (20) into Eq. (19) and collecting coefficients of the same orders in $\hbar$, we can obtain

$$1/2 \left( \frac{\partial S_1^{(0)}}{\partial q_1} \right)^2 + V(q_1, t) + \frac{\partial S_1^{(0)}}{\partial t} = 0,$$

(21)

and

$$\frac{1}{2} \sum_{k=0}^{n} \frac{\partial S_1^{(k)}}{\partial q_1} \frac{\partial S_1^{(n-k)}}{\partial q_1} - \frac{i}{2} \frac{\partial^2 S_1^{(n-1)}}{\partial q_1^2} + \frac{\partial S_1^{(n)}}{\partial t} = 0, \quad n \geq 1.$$  

(22)

Given the solution $S_1^{(0)}$ of the classical Hamilton-Jacobi equation (21), we solve Eq. (22) to find $S_1^{(1)}$. $S_1^{(2)}$ can be determined subsequently from the knowledge of $S_1^{(0)}$ and $S_1^{(1)}$, and so forth. We note that Eq. (22) is linear in $S_1^{(n)}$ and first-order differential in $q_1$ for $S_1^{(n)}$. Thus, from a practical viewpoint, Eqs. (21) and (22) could be more advantageous to deal with than Eq. (19) as long as the classical Hamilton’s principal function that is the solution of Eq. (21) is readily available.

The present formalism provides an encouraging point that the well-ordered operator counterpart of the quantum Hamilton’s principal function gives also the solutions of the Heisenberg equations through Eq. (2). If we consider the case $\dot{U}(t) = \dot{T}(t)$, we can obtain in the Heisenberg picture the relations $(\hat{q}_H, \hat{p}_H) = (\dot{T}^\dagger \hat{q}_S \dot{T}, \dot{T}^\dagger \hat{p}_S \dot{T})$ and $(\hat{Q}_H, \hat{P}_H) = (\dot{T}^\dagger \hat{Q}_S \dot{T}, \dot{T}^\dagger \hat{P}_S \dot{T}) = (\hat{q}_S, \hat{p}_S)$, where we attached the subscript $_S$ and $_H$ to operators to explicitly denote, respectively, the Schrödinger and the Heisenberg pictures. Thus, when expressed in the Heisenberg picture Eq. (2) turns into

$$\dot{\hat{p}}_H = \frac{\partial S_1(\hat{q}_H, \hat{q}_S, t)}{\partial \hat{q}_H}, \quad \dot{\hat{p}}_S = -\frac{\partial S_1(\hat{q}_H, \hat{q}_S, t)}{\partial \hat{q}_S},$$

(23)

and from these transformation relations we can obtain $\hat{q}_H$ and $\hat{p}_H$ as functions of time and the initial operators $\hat{q}_S$ and $\hat{p}_S$. Obviously, $\hat{q}_H(\hat{q}_S, \hat{p}_S, t)$ and $\hat{p}_H(\hat{q}_S, \hat{p}_S, t)$ obtained in this way evolve according to the Heisenberg equations.

### IV. QUANTUM PHASE-SPACE DISTRIBUTION FUNCTIONS AND CANONICAL TRANSFORMATIONS

Since our theory of the quantum canonical transformations is formulated with the canonical position $\hat{q}$ and momentum $\hat{p}$ variables on an equal footing, it would be relevant to consider the phase-space picture of quantum mechanics, exploiting the distribution functions in relation to the present theory.

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3For a stationary state of a system whose Hamiltonian does not depend explicitly on time, one may put $S(q,t) = W(q) - Et$ and obtain a differential equation for $W(q)$. To find a solution to the resulting equation, one may then use the expansion of $W$ in powers of $\hbar$. This approach has been extensively considered in connection with the well-known WKB approximation. In the present paper, the formalism is developed for general nonstationary states (of systems that can possibly have time-dependent Hamiltonians).
A. Distribution functions

For a given density operator \( \hat{\rho} \), a general way of defining quantum distribution functions proposed by Cohen [14] is that
\[
F^f(q_1, p_1, t) = \frac{1}{2\pi\hbar} \int \int dx dy dq_2 (q_2 + y|\hat{\rho}|q_2 - y)f(x, 2y/\hbar) e^{ix(q_2 - q_1)} e^{-ixp_1/\hbar}.
\]
(24)
Various choices of \( f(x, 2y/\hbar) \) lead to a wide class of quantum distribution functions [15]. To mention only a few, the choice \( f = 1 \) produces the well-known Wigner distribution function [16], while the choice \( f(x, 2y/\hbar) = e^{-hx^2/4am_e y^2/\hbar} \) yields the Husimi distribution function that recently has found its application in nonlinear dynamical problems [17]. The transformed distribution function is defined in \((Q_1, P_1)\) phase space likewise by
\[
G^f(Q_1, P_1, t) = \frac{1}{2\pi\hbar} \int \int dx dy dq_2 (q_2 + y|\hat{\rho}|q_2 - y)f(X, 2Y/\hbar) e^{iX(Q_1 - Q_1)} e^{-i2YP_1/\hbar}.
\]
(25)

Our main objective here is to find a relation between the old and the transformed distribution functions. After a straightforward algebra, which is displayed in Appendix B, it turns out that the transformation relation between the two distribution functions can be expressed as
\[
G^f(Q_1, P_1, t) = \int dq_2 dp_2 \kappa(Q_1, Q_1, q_2, p_2, t) F^f(q_2, p_2, t),
\]
(26)
where the kernel \( \kappa \) is given by
\[
\kappa(Q_1, P_1, q_2, p_2, t) = \frac{1}{2\pi\hbar} \int \int dx dy dq_2 \int \int dx dy dq_2 \frac{f(X, 2Y/\hbar)}{f(x, 2y/\hbar)} \times e^{i[F_1(q_2 + a - y, q_2 - Y, t) - F_1'(q_2 + a + y, Q_2 + Y, t)]/\hbar} e^{i[X(Q_2 - Q_1) - \alpha x]/\hbar} e^{i[p_2 - YP_1]/\hbar}.
\]
(27)
This expression for the kernel can be further simplified if integrations in Eq. (27) can be performed with a specific choice of the function \( f \). For instance, the simple choice \( f = 1 \) provides the following kernel for the Wigner distribution function,
\[
\kappa(Q_1, P_1, q_2, p_2, t) = \frac{2}{\pi\hbar} \int dY dy e^{i[F_1(q_2 - y, Q_1 - Y, t) - F_1'(q_2 + y, Q_1 + Y, t)]/\hbar} e^{i[p_2 - YP_1]/\hbar}.
\]
(28)
This equation was first derived by Garcia-Calderón and Moshinsky [18] without employing the idea of the quantum generating function. Curtright et al. [19] also obtained an equivalent expression in their recent discussion of the time-independent Wigner distribution functions.

We wish to point out that the quantum canonical transformation described here is basically different from that considered earlier by Kim and Wigner [12]. While the present approach deals with the transformation between operators \((\hat{q}, \hat{p})\) and \((\hat{Q}, \hat{P})\), their approach is about the transformation between c-numbers \((q, p)\) and \((Q, P)\). For the transformation \( Q = Q(q, p, t) \) and \( P = P(q, p, t) \), their approach yields for the kernel the expression
\[
\kappa(Q_1, P_1, q_2, p_2, t) = \delta(Q_1 - Q(q_2, p_2, t)) \delta(P_1 - P(q_2, p_2, t)),
\]
(29)
where \( Q(q, p, t) \) and \( P(q, p, t) \) satisfy the classical Poisson brackets relation, \([Q, P]_{RB} = [q, p]_{RB} = 1\). The kernels of Eq. (28) and Eq. (29) coincide with each other for the special case of a linear canonical transformation, as was shown by Garcia-Calderón and Moshinsky [18]. Specifically, for the case of the Wigner distribution function, they showed that the linear transformation for operators, \( \hat{Q} = a\hat{q} + b\hat{p} \) and \( \hat{P} = c\hat{q} + d\hat{p} \), and that for c-number variables, \( Q = aq + bp \) and \( P = cq + dp \), yield the same kernel \( \kappa(Q_1, P_1, q_2, p_2) = \delta(Q_1 - (aq_2 + bp_2)) \delta(P_1 - (cq_2 + dp_2)) \). In general cases, however, Eq. (27) and Eq. (29) give rise to different kernels. As an example, let us consider the unitary transformation \( \hat{U} = e^{i\hat{q}\hat{q}/\hbar} \) considered in Sec. II. The first-type quantum generating function has the form \( e^{iF_1(q, Q)/\hbar} = e^{i\hat{q}_1/\hbar} \delta(q_1 - Q_2) \). This nonlinear canonical transformation yields for the Wigner distribution function the kernel
\[
\kappa(Q_1, P_1, q_2, p_2) = \frac{\delta(Q_1 - q_2)}{\pi\hbar} \int dy e^{i[q_1 - y - (q_2 + y)]/\hbar} e^{i[p_2 - P_1]/\hbar}.
\]
(30)
It is apparent that the integral of the above equation cannot generally be reduced to the \( \delta \)-function of Eq. (29) except for some trivial cases, e.g., \( g = \text{const}, g = q \), and \( g = q^2 \). Distribution functions other than the Wigner distribution function do not usually allow the simple expression for the kernel in the form of Eq. (29), even if one considers a linear canonical transformation.
B. Dynamics

In this subsection we describe how the quantum Hamilton-Jacobi theory can lead to dynamical solutions in the phase-space picture of quantum mechanics. For this task, we first consider the time evolution of the transformed distribution function in \((Q_1, P_1)\) phase space. Differentiating Eq. (25) with respect to time, we can get

\[
\frac{\partial G^f}{\partial t} = \frac{1}{2\pi^2\hbar} \int \int dX dY dQ_2 \left[ \left( \frac{\partial}{\partial t} (Q_2 + Y) \right) \hat{\rho}(Q_2 - Y)_t + \iota (Q_2 + Y) \frac{\partial \hat{\rho}}{\partial t} (Q_2 - Y)_t \right. \\
\left. + \iota (Q_2 + Y) \hat{\rho} \left( \frac{\partial}{\partial t} (Q_2 - Y)_t \right) \right] f(X, 2Y/\hbar) e^{iX(Q_2 - Q_1)} e^{-i2YP_1/\hbar}.
\]  

(31)

We now substitute into Eq. (31) the time evolution equations

\[
\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}],
\]

(32)

\[
\frac{\partial}{\partial t} \langle Q_2 + Y \rangle = \iota \langle Q_2 + Y \rangle \hat{U} \frac{\partial \hat{U}^\dagger}{\partial t},
\]

(33)

\[
\frac{\partial}{\partial t} \langle Q_2 - Y \rangle = \frac{\partial \hat{U}}{\partial t} \langle Q_2 - Y \rangle = -\hat{U} \frac{\partial \hat{U}^\dagger}{\partial t} \langle Q_2 - Y \rangle_t,
\]

(34)

where \(\hat{H} = H(\hat{q}, \hat{p}, t)\) is the Hamiltonian governing the dynamics of the system, and obtain

\[
\frac{\partial G^f}{\partial t} = \frac{1}{2\pi^2\hbar} \int \int dX dY dQ_2 \langle Q_2 + Y \rangle \left( -i \frac{\partial}{\partial t} [\hat{K}, \hat{\rho}] \right) \langle Q_2 - Y \rangle_t f(X, 2Y/\hbar) e^{iX(Q_2 - Q_1)} e^{-i2YP_1/\hbar},
\]

(35)

where \(\hat{K} = K(\hat{Q}, \hat{P}, t)\) is just the transformed Hamiltonian already defined in Eq. (11). Eq. (35) should be compared with the following equation that governs the time evolution of the distribution function in \((q_1, p_1)\) phase space,

\[
\frac{\partial F^f}{\partial t} = \frac{1}{2\pi^2\hbar} \int \int dx dy d\hat{q}_2 \langle q_2 + y \rangle \left( -i \frac{\partial}{\partial \hat{t}} [\hat{\hat{H}}, \hat{\rho}] \right) \langle q_2 - y \rangle f(x, 2y/\hbar) e^{iX(q_2 - q_1)} e^{-i2yp_1/\hbar}.
\]

(36)

We can easily see that, through the quantum canonical transformation, the role played by \(\hat{H}\) is turned over to \(\hat{K}\).

Just as the wave function has a trivial solution in the representation where the transformed Hamiltonian \(\hat{H}(\hat{q}, \hat{p}, t)\) vanishes, so does the distribution function in the corresponding phase space, as can be seen from Eq. (35). With the trivial solution \(G^f = \text{const.}\), we go back to the original space via the inverse of the transformation equation (26) to obtain \(F^f(q_1, p_1, t)\). For example, for the case of the Wigner distribution function the transformation can be accomplished by

\[
F^W(q_1, p_1, t) = \int \int dQ_2 dP_2 \hat{k}(q_1, p_1, Q_2, P_2, t) G^W(Q_2, P_2),
\]

(37)

where \(\hat{k}\) is given in terms of the quantum principal function by

\[
\hat{k} = \frac{2}{\pi \hbar} \int dydY e^{i[S_1(q_1+y,Q_2+Y,t)-S_1^*(q_1-y,Q_2-Y,t)]} e^{iX(Q_2-Q_1)} e^{-i2yp_1/\hbar}.
\]

(38)

Thus, once the quantum Hamilton-Jacobi equation is solved and the quantum principal function \(S_1\) is obtained, the dynamics of the distribution function, as well as that of the wave function, can be determined.

V. BOUNDARY CONDITIONS AND APPLICATIONS

Up to this point the whole theory has been developed for the case \(\hat{U}(t) = \hat{T}(t)\hat{A}\) with \(\hat{A}\) taken to be arbitrary unless otherwise mentioned. To see how the quantum Hamilton-Jacobi theory is used to achieve the dynamical solutions of quantum problems, it would be sufficient, though, to consider the case of \(\hat{A} = I\), the unit operator. This case was considered by Dirac in connection with his action principle (see Sec. 32 of Ref. [3]). He showed that \(S_1\) defined by Eq. (15) equals the classical action function in the limit \(\hbar \to 0\). It should be mentioned that this particular case allows the quantum generating functions to attain the property that \(e^{iS_1/\hbar}\) is the propagator in position space and \(e^{iS_1/\hbar}\) the
propagator in momentum space. We will henceforth work on the case \( \hat{U}(t) = \hat{T}(t) \). The general case \( \hat{U}(t) = \hat{T}(t)\hat{A} \) will be briefly treated in Appendix C.

Before applying the theory it is necessary to provide some remarks concerning the quantum Hamilton-Jacobi equation (17) and its solution. First, if the Hamiltonian depends only on either \( \hat{q} \) or \( \hat{p} \), we do not need to solve Eq. (17). Instead, since the unitary operator has the simple form \( \hat{U} = e^{-i\bar{H}(\hat{q})/\hbar} \) or \( e^{-i\bar{H}(\hat{p})/\hbar} \), we can obtain \( S_1 \) directly from Eq. (15) by calculating the matrix elements of \( \hat{U} \). For example, for a free particle, \( \hat{U} = e^{-ij\hat{p}^2/2\hbar} \), it is convenient to calculate \( e^{iS_2/\hbar} = \langle q_1 | e^{-i\hat{p}^2t/2\hbar} | q_2 \rangle \), and we get \( S_2(q_1, P_2, t) = -\frac{P_2^2}{2} + q_1P_2 + \frac{i\hbar}{2} \ln 2\pi\hbar \). Second, in order to solve Eq. (17), we need to impose proper boundary conditions on \( S_1 \). Since here we are dealing with unitary transformations, we immediately get from the definition of \( S_1 \) the condition

\[
\int dQd\psi e^{i[S_1(q_1, Q_3, t) - S_1'(q_2, Q_3, t)]/\hbar} = \delta(q_1 - q_2), \tag{39}
\]

which follows from the calculation of the matrix elements of \( \hat{U}(t)\hat{U}^\dagger(t) = \hat{I} \). This unitary condition ensures that the well-ordered operator counterpart of \( S_1 \) yields Hermitian operators for \( \hat{Q} \) and \( \hat{P} \) from Eq. (2). Mathematically, Eq. (17) can have several solutions, and there is an arbitrariness in the choice of the new position variable, because any function of the constant of integration of Eq. (17) can be a candidate for the new position variable. Not all the possible solutions correspond to the unitary transformations, and from the possible solutions we choose only those which satisfy Eq. (39) and thus give Hermitian position and momentum operators that are observables. These solutions correspond to the unitary transformations of the type \( \hat{U}(t) = \hat{T}(t)\hat{A} \). Further, from these solutions we single out the one that corresponds to the case \( \hat{A} = \hat{I} \) by imposing the condition \( e^{iS_1(q_1, Q_2, t=0)/\hbar} = \delta(q_1 - Q_2) \) as an initial condition. The appropriate form for \( S_2 \) corresponding to this condition is that \( e^{iS_2(q_1, P_2, t=0)/\hbar} = \frac{1}{\sqrt{2\pi\hbar}} e^{i\hat{q}_1\hat{P}_2/\hbar} \). In the limit \( \hbar \to 0 \), \( S_2 \) in this equation reduces to the correct classical generating function for the identity transformation, \( S_2 = q_1P_2 \). In solving the Hamilton-Jacobi equation perturbatively using Eqs. (21) and (22), in order to consistently satisfy the initial condition, we start with the classical Hamilton’s principal function \( S_1^{(0)} \) that gives at initial time the relations \( q_1 = Q_2 \) and \( p_1 = P_2 \) from the classical c-number counterpart of Eq. (2). An arbitrary additive constant \( c \) to the solution of Eq. (17) that always appears in the form \( S_1 + c \) when we deal with a partial differential equation such as Eq. (19) which contains only partial derivatives of \( S_1 \) can also be fixed by the initial condition. Depending whether boundary conditions can readily be expressed in a simple form, one type of the quantum generating function may be favored over another. The existence and uniqueness of the independent solution of Eq. (17) satisfying the above conditions can be guaranteed from the consideration of the equation \( e^{iS_1(q_1, Q_2, t)/\hbar} = \langle q_1 | \hat{T}(t) | q_2 \rangle \), in which \( S_1 \) is just given by the matrix elements of \( \hat{T}(t) \). It is clear that these matrix elements exist and are uniquely defined.

As illustrations of the application of the theory, we consider the following two simple systems.

Example 1. A particle under a constant force.

As a first example, let us consider a particle moving under a constant force of magnitude \( a \), for which the Hamiltonian is \( \hat{H} = \hat{p}^2/2 - a\hat{q} \). We start with the following classical principal function that is the solution of Eq. (21),

\[
S_1^{(0)} = \frac{(q_1 - Q_2)^2}{2t} + at(q_1 + Q_2) - \frac{a^2t^3}{24}. \tag{40}
\]

Substituting \( S_1^{(0)} \) into Eq. (22) and solving the resulting equation, we find that the first order term in \( \hbar \) has the general solution

\[
S_1^{(1)} = \frac{i}{2} \ln t + f \left( \frac{q_1 - Q_2}{t} - \frac{a^3}{2t^3} \right), \tag{41}
\]

where \( f \) is an arbitrary differentiable function. To satisfy the proper boundary condition \( e^{iS_1(q_1, Q_2, t=0)/\hbar} = \delta(q_1 - Q_2) \), \( f \) and all higher order terms of \( S_1 \) are chosen to be zero, and the overall additive constant to be \( c = \hbar \frac{i}{2} \ln 2\pi\hbar \). By well-ordering terms, we get the generating operator

\[
\hat{S}_1(\hat{q}, \hat{Q}, t) = \frac{\hat{q}^2 - 2\hat{q}\hat{Q} + \hat{Q}^2}{2t} + at(\hat{q} + \hat{Q}) - \frac{a^2t^3}{24} + \hbar \frac{i}{2} \ln 2\pi\hbar. \tag{42}
\]

We can easily check that the operator form of the quantum Hamilton-Jacobi equation (13) is satisfied by the above generating operator.

From Eq. (14) we obtain the wave function

\[
\psi^q(q_1, t) = \int \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{1}{2\hbar}\left[(q_1 - Q_3)^2 + at(q_1 + Q_2) - \frac{a^2t^3}{24}\right]} \psi^Q(Q_2) dQ_2. \tag{43}
\]
Because $\psi^Q(Q_2)$ is constant in time, we can express it in terms of the initial wave function. For the present case in which we use the first-type quantum generating function $S_1$ and $\hat{A} = \hat{I}$, we have simply $\psi^q(q_2 = Q_2, t = 0) = \psi^Q(Q_2)$. We note that Eq. (43) is in exact agreement with the result of Feynman’s path-integral approach \[20\].

For the time evolution of the distribution function, we find from Eq. (38) the following kernel for the Wigner distribution function,

$$\tilde{\kappa}(q_1, p_1, Q_2, P_2, t) = \frac{1}{\pi^2 \hbar t} \int \int dY dYe^{-\frac{i}{\hbar} (q_2 - q_1 + pt - \frac{a^2}{2})} \sum e^{i p_2 \frac{q_1}{t} - \frac{a^2}{2t^2}}$$

$$= \delta(Q_2 - q_1 + pt - at^2/2)\delta\left(P_2 - \frac{q_1 - Q_2 - at^2/2}{t}\right). \quad (44)$$

Substituting Eq. (44) into Eq. (37), we obtain

$$F^W(q_1, p_1, t) = F^W(q_1 - pt + at^2/2, p_1 - at, 0), \quad (45)$$

where use has been made of the relation $F^W(q_1, p_1, t = 0) = G^W(q_1, p_1)$.

As has been mentioned, the present Hamilton-Jacobi theory also provides the solutions of the Heisenberg equations via the transformation relations between the two sets of canonical operators. From Eqs. (2) and (42) we can obtain

$$\dot{q}_S = \dot{Q}_S(t) + \hat{P}_S(t)t + \frac{a}{2} t^2, \quad (46)$$

$$\dot{p}_S = \hat{P}_S(t) + at. \quad (47)$$

In the Heisenberg picture, the above equations become

$$\dot{q}_H(t) = \dot{q}_S + \dot{p}_S t + \frac{a}{2} t^2, \quad (48)$$

$$\dot{p}_H(t) = \dot{p}_S + at, \quad (49)$$

which are the solutions of the Heisenberg equations.

By setting $a = 0$, we can obtain the free particle solution.

**Example 2. The harmonic oscillator**

For the harmonic oscillator whose Hamiltonian is given by $\hat{H} = \hat{p}^2/2 + \hat{q}^2/2$, the classical Hamilton-Jacobi equation (21) can be solved to give the classical principal function

$$S_1^{(0)} = \frac{1}{2} (q_1^2 + Q_2^2) \cot t - q_1 Q_2 \csc t. \quad (50)$$

With the boundary condition $e^{iS_1(q_1, Q_2, t = 0)/\hbar} = \delta(q_1 - Q_2)$, Eq. (22) can be solved to give

$$S_1^{(1)} = \frac{i}{2} \ln \sin t, \quad (51)$$

and $S_1^{(2)} = \cdots = 0$. The additive constant has the form $c = \hbar \frac{1}{2} \ln i2\pi \hbar$. The well-ordered generating operator is then written as

$$S_1(\hat{q}, \hat{Q}, t) = \frac{1}{2} (\hat{q}^2 + \hat{Q}^2) \cot t - \hat{q}\hat{Q} \csc t + \hbar \frac{i}{2} \ln i2\pi \hbar \sin t. \quad (52)$$

The wave function takes the form

$$\psi^q(q_1, t) = \int \frac{1}{\sqrt{i2\pi \hbar \sin t}} e^{\frac{i}{\hbar} \sin t (q_1^2 + Q_2^2) \cos t - 2q_1Q_2} \psi^q(Q_2, 0) dQ_2, \quad (53)$$

and the kernel and the distribution function are given respectively by

$$\tilde{\kappa}(q_1, p_1, Q_2, P_2, t) = \delta(Q_2 - q_1 \cos t + p_1 \sin t)\delta(P_2 + Q_2 \cos t - q_1 \sin t), \quad (54)$$

and

$$F^W(q_1, p_1, t) = F^W(q_1 \cos t - p_1 \sin t, q_1 \sin t + p_1 \cos t, 0). \quad (55)$$
This equation shows that the Wigner distribution function for the harmonic oscillator rotates clockwise in phase space. The quantum Hamilton-Jacobi equation for other types of generating operators can be solved by a similar technique. For instance, we can obtain the following solution for the second-type generating operator,

\[ S_2(\hat{q}, \hat{P}, t) = -\frac{1}{2}(\hat{q}^2 + \hat{P}^2) \tan t + \hat{q}\hat{P} \sec t + \frac{i\hbar}{2} \ln 2\pi \hbar \cos t. \] (56)

The solutions of the Heisenberg equations can be obtained from Eqs. (2) and (52) (or Eqs. (3) and (56)). In the Heisenberg picture we have

\[ \hat{q}_H(t) = \hat{q}_S \cos t + \hat{p}_S \sin t, \]  
(57)

\[ \hat{p}_H(t) = -\hat{q}_S \sin t + \hat{p}_S \cos t. \] (58)

It should be mentioned that, even though we restricted our discussion in this section only to the case \( \hat{A} = \hat{I} \) by imposing the special initial condition, it is very probable that another choice of \( \hat{A} \) satisfying the quantum Hamilton-Jacobi equation happens to be more readily obtainable. In that case, the initial condition that is derived from \( e^{iS_1(q_1, q_2, 0)/\hbar} = \langle q_1 | \hat{A} | q_2 \rangle \) is of course different from that described above. As an example, for the harmonic oscillator, we presented a different solution for \( S_1 \) in Appendix C where the unitary operator \( \hat{A} \) corresponds to the transformation that interchanges the position and momentum operators.

VI. CONCLUDING REMARKS

We wish to give some final remarks concerning the quantum Hamilton-Jacobi theory. In this approach, the quantum Hamilton-Jacobi equation takes the place of the time-dependent Schrödinger equation for solving dynamical problems, and the quantum Hamilton’s principal function \( S_1 \) that is the solution of the latter equation gives the solution of the former through Eq. (14). As mentioned in Sec. V, \( e^{iS_1(q_1, q_2, 0)/\hbar} \) becomes the propagator in position space for the case \( \hat{A} = \hat{I} \). To find the propagator, Feynman’s path-integral approach divides the time difference between a given initial state and a final state into infinitesimal time intervals, and then lets the quantum generating function for the infinitesimal transformation equal the classical action function plus a proper additive constant that vanishes in the limit \( \hbar \to 0 \), and finally takes the sum of the infinitesimal transformations. On the other hand, the present approach seeks the quantum generating function that directly transforms the initial state to the final state. The present formalism gives also the solutions of the Heisenberg equations through the transformation relations which in the Heisenberg picture can be expressed as Eq. (23). In conclusion, it is clear that the present approach, which has its origin in Dirac’s canonical transformation theory, helps better comprehend the interrelations among the existing different formulations of quantum mechanics.

Finally, one more remark may be worth making as to the extent to which the quantum Hamilton-Jacobi theory can stretch the range of its validity. Even though our work here deals with the unitary transformation to ensure that the new operators become Hermitian, and hence observables, the main idea presented in this paper could be extended so as to include the non-unitary transformation that deals with non-Hermitian operators. The theory would then have the form of the quantum Hamilton-Jacobi equation, but it would be associated with different types of transformations, such as \( \hat{U}(t) = \hat{T}(t) \hat{B} \) where \( \hat{U}(t) \) and \( \hat{B} \) are not unitary. However, it may then be necessary to pay particular attention and care to the completeness of the eigenstates of the new operators \( \hat{Q} \) and \( \hat{P} \), for the property is crucial to several relations derived and has been used implicitly throughout the paper.

APPENDIX A: PROOF OF THE EQUIVALENCE OF EQUATIONS (11) AND (12)

Eq. (12) can be derived from Eq. (11) by considering the matrix element of the second term on the right hand side of Eq. (11) as follows,

\[ \langle q_1 | i\hbar \frac{\partial}{\partial t} \hat{U}^\dagger | q_2 \rangle = -\langle q_1 | i\hbar \frac{\partial}{\partial t} \hat{U}^\dagger | q_2 \rangle, \] (A1)

\[ = -\int dq_3 \langle q_1 | i\hbar \frac{\partial}{\partial t} | q_3 \rangle \langle q_3 | \hat{U}^\dagger | q_2 \rangle, \] (A2)

\[ = \int dQ_3 \left( -i\hbar \frac{\partial}{\partial t} \langle q_1 | \hat{U} | q_3 \rangle \right) \langle Q_3 | q_2 \rangle, \] (A3)
where the identity $\hat{U}\hat{U}^\dagger = \hat{I}$ is used to obtain Eq. (A1). Using the definition of the quantum generating function (1), we can obtain

$$
\langle q_1 | i\hbar \frac{\partial \hat{U}^\dagger}{\partial t} | q_2 \rangle = \int dQ_5 \frac{\partial F_1(q_1, Q_3)}{\partial t} \langle q_1 | Q_5 \rangle_t \langle Q_5 | q_2 \rangle,
$$

(A4)

$$
= \int dQ_5 \langle q_1 | \frac{\partial \hat{F}_1(\hat{q}, \hat{Q}, t)}{\partial t} | Q_5 \rangle_t \langle Q_5 | q_2 \rangle,
$$

(A5)

$$
= \langle q_1 | \frac{\partial \hat{F}_1(\hat{q}, \hat{Q}, t)}{\partial t} | q_2 \rangle.
$$

(A6)

Since $i\hbar \frac{\partial \hat{U}^\dagger}{\partial t}$ and $\frac{\partial \hat{F}_1(\hat{q}, \hat{Q}, t)}{\partial t}$ have the same matrix element, we conclude that the two operators are identical.

**APPENDIX B: DERIVATION OF THE KERNEL $\kappa$**

In order to find the relation between $F^f$ and $G^f$, we first make use of the completeness of the eigenvectors of $\hat{q}$ in Eq. (25) and get

$$
G^f(Q_1, P_1, t) = \frac{1}{2\pi^2} \int \int \int \int \int dX dY dQ_2 dq_3 dq_4 \langle Q_2 + Y | q_3 | \hat{p} | q_4 \rangle \langle q_4 | Q_2 - Y \rangle_t
\times f(X, 2Y/h) e^{iX(Q_2 - Q_1)} e^{-iY P_1/h}.
$$

(B1)

Changing variables with $q_5 = (q_3 + q_1)/2$ and $y = (q_5 - q_6)/2$, and using the relation $\int dy' dq_6 \delta(y - y') \delta(q_5 - q_6) g(y', q_6) = g(y, q_5)$ where the $\delta$-functions are written in the forms

$$
\delta(y - y') = \frac{1}{\hbar} \int dp_3 e^{-2i p_3(y - y')/\hbar},
$$

(B2)

and

$$
\delta(q_5 - q_6) = \frac{1}{2\pi} \int dx e^{ix(q_6 - q_5)},
$$

(B3)

we obtain

$$
G^f(Q_1, P_1, t) = \frac{1}{2\pi^4} \int \int \int \int \int dX dY dQ_2 dq_3 dy dq_6 dx f(X, 2Y/h) \langle Q_2 + Y | q_5 + y' \rangle
\times \langle q_6 + y' | \hat{p} | q_6 \rangle \langle q_5 - y' | Q_2 - Y \rangle_t e^{iX(Q_2 - Q_1)} e^{-iY P_1/h} e^{-2i p_3(y - y')/h} e^{i x(q_6 - q_5)}.
$$

(B4)

Next, we multiply this equation by

$$
\int \int dx'' dy'' \frac{f(x, 2y/h)}{f(x'', 2y''/h)} \delta(x'' - x) \delta(y'' - y) = 1,
$$

(B5)

where

$$
\delta(x'' - x) \delta(y'' - y) = \frac{1}{2\pi^2} \int \int dx dx' e^{-i(x'' - x)} e^{-2i(x'' - x)/h}.
$$

(B6)

In the resulting equation, we replace the integrations over $q_5$ and $p_3$, respectively, with those over $q_2 = q_5 - \alpha$ and $p_2 = p_3 - \beta$, and then integrate over $\beta$ and $y'$. We then obtain

$$
G^f(Q_1, P_1, t) = \int \int dq_2 dp_2 \left[ \frac{1}{2\pi^3} \int \int \int \int dX dY dQ_2 dx'' dy'' d\alpha \langle Q_2 + Y | q_2 + \alpha + y'' \rangle
\times \langle q_2 + \alpha - y'' | Q_2 - Y \rangle \frac{f(X, 2Y/h)}{f(x'', 2y''/h)} e^{iX(Q_2 - Q_1)} e^{-2i Y P_1/h} e^{-i\alpha x''} e^{2i p_2 y''/h} \right]
\times \left[ \frac{1}{2\pi^2} \int \int dx dy dq_6 \langle q_6 + y | \hat{p} | q_6 - y \rangle f(x, 2y/h) e^{ix(q_6 - q_2)} e^{-2i p_2/h} \right],
$$

(B7)

which leads immediately to Eq. (26).
APPENDIX C: SOLUTIONS OF THE QUANTUM HAMILTON-JACOBI EQUATION

In Sec. V we considered the case $\hat{A} = \hat{I}$ only for convenience, because, as can be noticed from the two examples of Sec. V, this case not only gives a simple relation between the initial wave function $\psi^0(q_1,0)$ (distribution function $F^f(q_1,p_1,0)$) in $q$-representation and the constant wave function $\psi^0(Q_2)$ (distribution function $G^f(Q_2,P_2)$) in $Q$-representation, but also makes it easy to express the new operators $(\hat{Q}_H, \hat{P}_H)$ in the Heisenberg picture in terms of the old operators $(\hat{q}_S, \hat{p}_S)$ in the Schrödinger picture. In doing so, we required the solution to satisfy the specific initial condition described in the first part of Sec. V. This specialization is of course not of necessity, and if this initial condition is discarded with the unitary condition of the transformation still retained, we have a group of general solutions each member of which corresponds to a specific choice of $\hat{A}$. As an illustration, we present below another possible solution of the quantum Hamilton-Jacobi equation (19) for the harmonic oscillator that belongs to unitary transformations of the type $\hat{U}(t) = \hat{T}(t)\hat{A}$,

$$\hat{S}_1(\hat{q}, \hat{Q}, t) = -\frac{1}{2}(\hat{q}^2 + \hat{Q}^2) \tan t + \hat{q}\hat{Q}\sec t + \frac{i}{2} \ln 2\pi \hbar \cos t. \quad (C1)$$

Equation (C1) satisfies at initial time $e^{i\hat{S}_1(q_1,Q_2,0)/\hbar} = \frac{1}{\sqrt{2\pi \hbar}} e^{iq_1Q_2/\hbar}$, which equals $(q_1|\hat{A}|q_2)$, i.e., the matrix element of the unitary operator $\hat{A}$. In this case, the operator $\hat{A}$ corresponds to the exchange transformation which generates the transformation relations

$$\hat{p} = \frac{\partial \hat{S}_1(\hat{q}, \hat{Q}, 0)}{\partial \hat{q}} = \hat{Q}, \quad (C2)$$
$$\hat{P} = -\frac{\partial \hat{S}_1(\hat{q}, \hat{Q}, 0)}{\partial \hat{Q}} = -\hat{q}. \quad (C3)$$

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