Linear Canonical Transformations and the Hamilton-Jacobi Theory in Quantum Mechanics

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Abstract

We investigate two methods of constructing a solution of the Schrödinger equation from the canonical transformation in classical mechanics. One method shows that we can formulate the solution of the Schrödinger equation from linear canonical transformations, the other focuses on the generating function which satisfies the Hamilton-Jacobi equation in classical mechanics. We also show that these two methods lead to the same solution of the Schrödinger equation.
1 Introduction

The idea of canonical transformations provides us with a powerful technique for solving mechanical problems. Not only does this enable us to solve classical problems but it also gives us a clue to the quantization of classical systems. In particular, the Hamilton-Jacobi theory provides the key for connecting classical and quantum mechanics.

However, there are few problems in which a solution to the Schrödinger equation can be found by a canonical transformation or the Hamilton-Jacobi theory in classical mechanics. One of the reasons may be the restriction of the non-commutativity of physical variables in quantum systems. The analogy of the canonical transformation in classical mechanics with the unitary transformation in quantum mechanics was pointed out by Dirac [1] just after the birth of the quantum mechanics in 1926. Originally, he considered the transformation function \( \langle q | P ; t \rangle \) between the old position \( q \) and new momentum \( P \) with the corresponding generating function \( W_2(q, P, t) \)

\[
\langle q | P ; t \rangle = \exp \left[ i \frac{\hbar}{\bar{\hbar}} W_2(q, P, t) \right].
\]  

(1)

In his next papers [2, 3], he changed the variable from \( P \) to the new position \( Q \) and constructed the transformation function

\[
\langle q | Q ; t \rangle = \exp \left[ i \frac{\hbar}{\bar{\hbar}} W_1(q, Q, t) \right].
\]  

(2)

This form of the transformation function inspired Feynman to invent the celebrated path integrals [4].

Recently, some authors [5, 6, 7] have reconsidered the validity of these transformation functions (2) for solving the quantum mechanical problems. Especially, Lee and l’Yi [5] derived a solution of the time-independent Schrödinger equation in the transformed \( Q \)-space, which was then transformed to the original \( q \)-space by the transformation function (2). The relationship with the Hamilton-Jacobi theory has been investigated by Kim and Lee [6].
In this paper, we show two methods for constructing solutions of the Schrödinger equation. One method is that by which we construct the transformation function $\langle q|Q; t \rangle$ from linear canonical transformations in classical mechanics. The other method is closely related to the Hamilton-Jacobi theory. Using the generating function $W_1(q, Q; t)$ which satisfies the Hamilton-Jacobi equation, we construct the solution of the Schrödinger equation. It is shown that these two method leads to identical solutions.

This paper is organized in the following way. In section 2, we construct the quantum transformation function from linear canonical transformations in classical mechanics. In section 3, the solution of the Schrödinger equation is obtained with the aid of the Hamilton-Jacobi theory in classical mechanics. In section 4, we will show some applications to ideal systems. Section 5 is devoted to a discussion.

2 Linear canonical transformations and their transformation function

We consider the following linear canonical transformations;

$$\begin{cases} Q(t) = a(t)q + b(t)p \\ P(t) = c(t)q + d(t)p, \end{cases}$$

where $(q, p)$ and $(Q, P)$ describe the old and new canonical variables. We assume that the coefficients $a(t), b(t), c(t)$ and $d(t)$ are all real functions of time $t$. In order for these linear transformations to be canonical transformations, the Poisson bracket $[A, B]_c$ should be satisfied. Thus, the coefficients $a(t), b(t), c(t)$ and $d(t)$ are constrained;

$$[Q(t), P(t)]_c = \frac{\partial Q(t)}{\partial q} \frac{\partial P(t)}{\partial p} - \frac{\partial P(t)}{\partial q} \frac{\partial Q(t)}{\partial p} = a(t)d(t) - b(t)c(t) = 1.$$ (4)

Now, we construct the transformation function from the canonical transformations in classical mechanics. The canonical variables in eq.(3) are raised to quantum
numbers: we attach ˆ to the variables to distinguish the q-numbers from c-numbers,
\[
\begin{align*}
\hat{Q}(t) & = a(t)\hat{q} + b(t)\hat{p} \\
\hat{P}(t) & = c(t)\hat{q} + d(t)\hat{p}.
\end{align*}
\] (5)

With the condition (4) and the commutation relation for the old variables
\[
[\hat{q}, \hat{p}] = \hat{q}\hat{p} - \hat{p}\hat{q} = i\hbar,
\] (6)
we have the commutation relation for the new variables
\[
\left[\hat{Q}(t), \hat{P}(t)\right] = i\hbar.
\] (7)

We proceed by constructing a transformation function [8]. Firstly, we define the eigenstate \(|Q; t\rangle\) of the operator \(\hat{Q}(t)\) with eigenvalue \(Q\) to form the \(Q\)-representation:
\[
\hat{Q}(t)|Q; t\rangle = Q|Q; t\rangle.
\] (8)

Secondly, the \(q\)-representation for the eigenstate \(|Q; t\rangle\) can be obtained from the differential equation
\[
\langle q|\hat{Q}(t)|Q; t\rangle = \left\{a(t)q - i\hbar b(t)\frac{\partial}{\partial q}\right\} \langle q|Q; t\rangle = Q\langle q|Q; t\rangle. \quad (9)
\]
Integrating (9) with the normalization condition
\[
\langle Q; t|Q'; t\rangle = \delta(Q - Q'), \quad (10)
\]
we have
\[
\langle q|Q; t\rangle = \Phi(Q) \times \sqrt{\frac{1}{2\pi(-i)\hbar b(t)}} \exp \left[\frac{i}{\hbar} \frac{2qQ - a(t)q^2}{2b(t)}\right], \quad (11)
\]
where \(\Phi(Q)\) is an arbitrary phase factor which depends on \(Q\). Here, the meaning of \((-i)\) in the square root is clarified later. Note that hereafter we consider the \(b(t) \neq 0\) case so as not to lose generality in our discussion.

Thirdly, we consider the matrix element of the operator \(\hat{P}(t)\) with an arbitrary state \(|\psi\rangle\),
\[
\langle Q; t|\hat{P}(t)|\psi\rangle = \int dq \langle Q; t|q\rangle \langle q|\hat{P}(t)|\psi\rangle \quad (12)
\]  
\[
= \int dq \langle Q; t|q\rangle \left\{c(t)q - ihd(t)\frac{\partial}{\partial q}\right\} \langle q|\psi\rangle. \quad (13)
\]
Integrating by parts and using the $q$-derivative of eq.(11), we have

$$\langle Q; t | \hat{P}(t) | \psi \rangle = \left\{ \frac{d(t)}{b(t)} Q - \frac{i}{\hbar} \frac{\partial}{\partial Q} + \frac{i}{\hbar} \frac{\partial \Phi^*}{\partial Q} \right\} \langle Q; t | \psi \rangle. \quad (14)$$

If we set

$$\Phi^*(Q) = \exp \left[ \frac{i}{\hbar} \frac{d(t)}{2b(t)} Q^2 \right], \quad (15)$$

$\langle Q; t | \hat{P} | \psi \rangle$ is given by

$$\langle Q; t | \hat{P}(t) | \psi \rangle = -i \frac{\hbar}{\partial Q} \langle Q; t | \psi \rangle, \quad (16)$$

so that the $q$-representation of the eigenstate $|Q; t\rangle$ turns out to be

$$\langle q|Q; t\rangle = \sqrt{-1} \frac{1}{2\pi i \hbar b(t)} \exp \left[ \frac{i}{\hbar} \frac{2qQ - a(t)q^2 - d(t)Q^2}{2b(t)} \right]. \quad (17)$$

This is the first result in this paper. We have the linear canonical transformation (3) which is neither a point transformation, nor a transformation from position to momentum space. Next, all variables are raised to $q$-number variables and we take the old and new positions as bases and form the transformation function $q \leftrightarrow Q$.

It is noted that the exponential factor, except for $(i/\hbar)$,

$$W_1(q, Q, t) = \frac{qQ}{b(t)} - \frac{a(t)}{2b(t)} q^2 - \frac{d(t)}{2b(t)} Q^2 \quad (18)$$

is a type-1 generating function which causes a canonical transformation (3) according to the ordinary prescription:

$$p = \frac{\partial}{\partial q} W_1(q, Q, t), \quad P = -\frac{\partial}{\partial Q} W_1(q, Q, t). \quad (19)$$

The other types of generating functions are given by Legendre transformations,

$$W_2(q, P, t) = \frac{qP}{d(t)} - \frac{c(t)}{2d(t)} q^2 + \frac{b(t)}{2d(t)} P^2 \quad (20)$$

$$W_3(p, Q, t) = -\frac{pQ}{a(t)} + \frac{b(t)}{2a(t)} p^2 - \frac{c(t)}{2a(t)} Q^2 \quad (21)$$

$$W_4(p, P, t) = -\frac{pP}{c(t)} + \frac{d(t)}{2c(t)} p^2 + \frac{a(t)}{2c(t)} P^2. \quad (22)$$
while the transformation functions are given by Fourier transformations \[6\],

\[
\langle q|P; t \rangle = \sqrt{\frac{1}{2\pi\hbar(d(t)}} \exp \left[ \frac{i}{\hbar} W_2(q, P, t) \right]
\]

(23)

\[
\langle p|Q; t \rangle = \sqrt{\frac{1}{2\pi\hbar(a(t)}} \exp \left[ \frac{i}{\hbar} W_3(p, Q, t) \right]
\]

(24)

\[
\langle p|P; t \rangle = \sqrt{\frac{1}{2\pi\hbar c(t)}} \exp \left[ \frac{i}{\hbar} W_4(p, P, t) \right].
\]

(25)

### 3 Schrödinger equation and Hamilton-Jacobi theory

In this section, we find a solution to the Schrödinger equation

\[
i\hbar \frac{\partial}{\partial t} \psi(q, t) = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} + V(q) \right] \psi(q, t),
\]

(26)

with the aid of the Hamilton-Jacobi theory in classical mechanics.

Let us write the wave function as

\[
\psi(q, t) = \exp \left[ \frac{i}{\hbar} S(q, t) \right],
\]

(27)

and putting this into the above Schrödinger equation (26), we obtain

\[
\frac{1}{2m} \left( \frac{\partial S}{\partial q} \right)^2 + V(q) + \frac{\partial S}{\partial t} - \frac{i\hbar}{2m} \frac{\partial^2 S}{\partial q^2} = 0.
\]

(28)

This form of the equation has been well studied in the classical limit using the WKB formalism where the focus is on the stationary-state solution. Here, we consider this equation from a different point of view. We define the new function

\[
F \equiv \frac{1}{2m} \frac{\partial^2 S}{\partial q^2}.
\]

(29)

If the function \( S \) is given by a polynomial with respect to \( q \) up to the second order, \( F \) is independent of \( q \) and depends only on \( t \). We consider this case hereafter. Under this condition, the function \( S \) is divided into two parts; one depending only on time \( t \), and the other \( W(q, t) \) depending on \( q \) and \( t \),

\[
S(q, t) = W(q, t) + i\hbar \int_t^t dt' F(t').
\]

(30)
Putting this back into eq.(28), we obtain

$$\frac{1}{2m} \left( \frac{\partial W}{\partial q} \right)^2 + V(q) + \frac{\partial W}{\partial t} = 0. \quad (31)$$

This is the Hamilton-Jacobi equation that appears in classical mechanics. This indicates the possibility of obtaining a solution to the Schrödinger equation from the Hamilton-Jacobi theory in classical mechanics. The procedure for this is as follows.

(i) Once we have the function $W$ which satisfies the Hamilton-Jacobi equation (31),

(ii) we calculate the function $F$ from eq.(29). The second term in (30) is a function of $t$, so (29) becomes

$$F = \frac{1}{2m} \frac{\partial^2 S}{\partial q^2} = \frac{1}{2m} \frac{\partial^2 W}{\partial q^2}. \quad (32)$$

(iii) Next, putting $F$ back into (30) and integrating the second term, we derive the function $S$.

(iv) Accordingly, putting this $S$ back into (27), we obtain the solution to the Schrödinger equation (26).

Now, we apply this method to the generating function $W_1(q, Q, t)$ which appears in (18). It is easy to check that

$$a(t) = -m\dot{b}(t) \quad (33)$$

is required in order for $W_1(q, Q, t)$ to satisfy the Hamilton-Jacobi equation (31), where $\dot{b}(t)$ describes the time derivative of $b(t)$. We have two other conditions but these have no bearing on the following discussion. Calculating the function $F$ from (32) with (33)

$$F(t) = \frac{1}{2m} \frac{-a(t)}{b(t)} = \frac{1}{2m} \frac{mb(t)}{b(t)} = \frac{d}{dt} \ln \sqrt{b(t)}, \quad (34)$$
we have the exponential factor \( S(q, t) \)

\[
S(q, t) = W_1(q, Q, t) + \frac{i\hbar}{\hbar} \ln \sqrt{b(t)}.
\]  

(35)

Thus, the solution of the Schrödinger equation is

\[
\psi = \exp \left[ \frac{i}{\hbar} S(q, t) \right] = \sqrt{\frac{1}{b(t)}} \exp \left[ \frac{i}{\hbar} W_1(q, Q, t) \right].
\]  

(36)

This is identical to eq.(17) without the trivial constant in the square root which is obtained from the normalization of the wave function.

This is the second result in this paper. We assume the solution of the Schrödinger equation to be like (27). Part of the function \( S \) is the generating function \( W_1 \) which satisfies the Hamilton-Jacobi equation. Once we have the generating function which satisfies the Hamilton-Jacobi equation, then the solution of the Schrödinger equation is calculated according to the procedure stated above.

4 Applications to simple systems

In this section, we will apply the method to two ideal systems.

4.1 Free particle

The Hamiltonian is

\[
H = \frac{p^2}{2m},
\]  

(37)

where \( m \) and \( p \) are the mass and momentum of the particle.

We consider the canonical transformation

\[
\begin{pmatrix}
a(t) \\
b(t) \\
c(t) \\
d(t)
\end{pmatrix} = \begin{pmatrix}
1 & \frac{i}{m} \\
0 & 1
\end{pmatrix},
\]  

(38)

whose physical meaning is the Galilean transformation. The constraints (4) and (33) are satisfied by these coefficients. The generating function (18) that results in the above transformation is

\[
W_1(q, Q, t) = -\frac{m}{t} qQ + \frac{m}{2t} q^2 + \frac{m}{2t} Q^2 = \frac{m}{2t} (q - Q)^2.
\]  

(39)
Since this is the Galilean transformation, the transformed Hamiltonian \( K = H + \frac{\partial W_1}{\partial t} \) must be zero. So, \( W_1 \) also satisfies the Hamilton-Jacobi equation.

From the above canonical transformation, we obtain the transformation function or the solution to the Schrödinger equation

\[
\langle q | Q; t \rangle = \exp \left[ \frac{i}{\hbar} S \right] = \sqrt{\frac{m}{2\pi i \hbar t}} \exp \left[ \frac{i m}{\hbar 2t} (q - Q)^2 \right].
\]

It is interesting that this function is identical to the Feynman propagator in the free Hamiltonian.

### 4.2 Harmonic Oscillator

The Hamiltonian is

\[
H = \frac{p^2}{2m} + \frac{m \omega^2}{2} q^2,
\]

where \( m, p \) and \( \omega \) are the mass, momentum and frequency of the particle.

We consider the canonical transformation

\[
\begin{pmatrix}
    a(t) \\
    b(t) \\
    c(t) \\
    d(t)
\end{pmatrix} = \begin{pmatrix}
    \cos \omega t & \frac{1}{m \omega} \sin \omega t \\
    -m \omega \sin \omega t & \cos \omega t
\end{pmatrix},
\]

whose physical meaning is a rotation in phase space. The constraints (4) and (33) are satisfied by these coefficients. The generating function (18) that causes the above transformation is

\[
W_1(q, Q, t) = -\frac{m \omega}{\sin \omega t} qQ + \frac{m \omega}{2 \tan \omega t} (q^2 + Q^2).
\]

Since this is a rotation in phase space, the transformed Hamiltonian \( K = H + \frac{\partial W_1}{\partial t} \) must be zero. So, \( W_1 \) also satisfies the Hamilton-Jacobi equation.

From the above canonical transformation, we obtain the transformation function or the solution to the Schrödinger equation

\[
\langle q | Q; t \rangle = \exp \left[ \frac{i}{\hbar} S \right] = \sqrt{\frac{m \omega}{2\pi i \hbar \sin \omega t}} \exp \left[ \frac{i}{\hbar} \left\{ -\frac{m \omega}{\sin \omega t} qQ + \frac{m \omega}{2 \tan \omega t} (q^2 + Q^2) \right\} \right].
\]
It is interesting that this function is identical to the Feynman propagator of the harmonic oscillator.

5 Discussion

We have investigated two methods which construct solutions to the Schrödinger equation from classical canonical transformations. For linear canonical transformations in classical mechanics, we have constructed the quantum counterpart and this is related to the Hamilton-Jacobi theory.

However, our method is restricted only to linear canonical transformations. There is a variety of canonical transformations in classical mechanics. For example, the generating function

$$W_1(q, Q, t) = \frac{m\omega q^2}{2\tan Q}$$

(45)

is a good choice for obtaining a solution to the classical harmonic oscillator, while a naive application of Dirac’s (2) does not work in quantum mechanics [5].

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