Canonical Transformations for Time-Dependent Harmonic Oscillators

Tae Jun Park

Department of Chemistry, Dongguk University, Seoul 100-715, Korea

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A canonical transformation changes variables such as coordinates and momenta to new variables preserving either the Poisson bracket or the commutation relations depending on whether the problem is classical or quantal respectively. Classically canonical transformations are well established as a powerful tool for solving differential equations. Quantum canonical transformations have been defined and used relatively recently because of the non-commutativeness of the quantum variables. Three elementary canonical transformations and their composite transformations have quantum implementations. Quantum canonical transformations have been mostly used in time-independent Schrödinger equations and a harmonic oscillator with time-dependent angular frequency is probably the only time-dependent problem solved by these transformations. In this work, we apply quantum canonical transformations to a harmonic oscillator in which both angular frequency and equilibrium position are time-dependent.

Key Words : Canonical, Transformation, Time-dependent, Harmonic, Oscillator

Introduction

In order to integrate the equations of motion in classical mechanics, we solve the second-order differential equations directly or trivialize the Hamiltonian by eliminating conjugate variables using canonical transformations. There is one situation where the equation of motion is trivial. That is when all the coordinates are cyclic[1] and the conjugate momenta are all constant and as a consequence the Hamiltonian becomes a function of constants. In this case the solutions of the Hamilton's equations are simple. Since the generalized coordinates would not normally be cyclic, we need to transform one set of variables to some other set so that new variables contain more than one cyclic coordinate. Classically a canonical transformation is a change of variables which preserves Poisson bracket $\{p, q\} = -1$ in which q is a coordinate and p is its conjugate momentum.

Due to the non-commutability of operators, canonical transformations have not been fully realized in quantum mechanics. Unitary transformations have been more often used instead because quantum canonical transformations are mistakenly understood to be unitary. In quantum mechanics, a canonical transformation is naturally defined[2] as a change of the non-commuting variables which preserves the commutation relation $[p, q] = -i$. Although unitary transformations possess the same property they do not represent the full class of canonical transformations. A canonical transformation is implemented by a function $C(q, p)$ such that $(p, q) \rightarrow (p', q')$ where $p' = CpC^{-1}$, $q' = CqC^{-1}$ and C is not necessarily unitary since the definition does not require the Hilbert space or inner product. As a consequence, quantum canonical transformations may not be unitary and they are norm-preserving isometric transformations.[3] In order to define a quantum canonical transformation, followings must be considered; 1) the ordering of new variables q' and p' are given; 2) the inverse and fractional powers of differential operators are defined. Three elementary transformations are widely used and they are the interchange transformation, the similarity transformation, and the point transformation.[3,4] A general quantum canonical transformation can be decomposed into a sequence of these elementary transformations. Solving a Schrödinger equation is facilitated by transforming the Hamiltonian to a simpler one with the elementary canonical transformations. Tools for solving differential equations including raising and lowering operators,[5] intertwining operators,[6,7] and Lie algebraic methods[8] may also be regarded as canonical transformations.

The quantum canonical transformations provide a unified approach to the integrability of many time-independent systems and exact solutions of the Schrödinger equation are obtained for systems including the harmonic oscillator,[4] the Morse potential, and the Pöschl-Teller potential, etc.[9] For time-dependent problems, however, a harmonic oscillator with time-dependent angular frequency is probably the only system solved by these transformations.[3]

In this work, we apply quantum canonical transformations to a harmonic oscillator in which both angular frequency and equilibrium position are time-dependent.

Quantum Canonical Transformations

A quantum canonical transformation is defined to change variables preserving the commutator bracket

$$[q, p] = i = [q'(q, p), p'(q, p)] \tag{1}$$

New variables are generated by an arbitrary complex function $C(q, p)$ as below;

$$q'(q, p) = CqC^{-1}, \qquad p'(q, p) = CpC^{-1} \tag{2}$$

There are three elementary canonical transformations which have quantum implementations as finite transformations.

They are interchange transformations, similarity transformations, and point transformations. A general canonical transformation can be obtained as products of these elementary transformations. Each of the elementary canonical transformations will be briefly reviewed in the following and the readers who are interested in more details are referred to ref. 3.

The interchange of coordinates and momenta

$$p \rightarrow IpI^{-1} = -q, \quad q \rightarrow IqI^{-1} = p \tag{3}$$

is done by the Fourier transform operator

$$I = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dq' e^{iqq'} \tag{4}$$

The wavefunction is transformed

$$\psi^{(1)}(q) = I\psi^{(0)}(q) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dq' e^{iqq'} \psi^{(0)}(q') \tag{5}$$

where $\psi^{(0)}$ is the original wavefunction. The inverse interchange is

$$p \rightarrow q, \quad q \rightarrow -p \tag{6}$$

implemented by the inverse Fourier transform

$$I^{-1} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dq' e^{-iqq'} \tag{7}$$

The similarity transformation is carried out by $e^{-f(q)}$ where $f(q)$ is an arbitrary complex function of the coordinate(s). Applying the generator to q and p, the coordinate is unchanged and the momentum is transformed

$$q \rightarrow e^{-f(q)} q e^{f(q)} = q, \quad p \rightarrow e^{-f(q)} p e^{f(q)} = p - i\frac{\partial f}{\partial q} \tag{8}$$

which can be obtained from Baker-Hausdorff formula.[4] The wavefunction is transformed

$$\psi^{(1)}(q) = e^{-f(q)}\psi^{(0)}(q) \tag{9}$$

The composite similarity transformation is done by the generator

$$e^{-f(p)} = Ie^{-f(q)}I^{-1} \tag{10}$$

which is obtained by applying the interchange transformation to $e^{-f(q)}$ to exchange coordinates for momenta. This transformation changes q while leaving p unchanged

$$q \rightarrow e^{-f(p)} q e^{f(p)} = q + i\frac{\partial f}{\partial p}, \quad p \rightarrow p \tag{11}$$

The wavefunction changes

$$\psi^{(1)}(q) = e^{-f(p)}\psi^{(0)}(q) = Ie^{-f(q)}I^{-1}\psi^{(0)}(q) \tag{12}$$

The point transformation is not explicitly expressed as the exponential form, but representatively as $P_{f(q)}$ and it is implemented

$$q \rightarrow P_{f(q)} q P_{f^{-1}(q)} = f(q), \quad p \rightarrow P_{f(q)} p P_{f^{-1}(q)} = \frac{1}{\left(\frac{\partial f}{\partial q}\right)} p \tag{13}$$

where $f^{-1}(q)$ represents the inverse function of $f(q)$. Actual forms of transformed variables are easily realized when $f(q)$ is explicitly given. The wavefunction changes by the point transformation as

$$\psi^{(1)}(q) = P_{f(q)}\psi^{(0)}(q) = \psi^{(0)}(f(q)) \tag{14}$$

The composite point transformation is done by the generator $P_{f(p)} = IP_{f(q)}I^{-1}$ which is obtained by applying the interchange transformation to $P_{f(q)}$. Variables change

$$q \rightarrow \left(\frac{\partial f}{\partial p}\right)^{-1} q, \quad p \rightarrow f(p) \tag{15}$$

which are obtained from Eq. (13) by interchanging variables in both sides of equality. The wavefunction is transformed

$$\psi^{(1)}(q) = P_{f(p)}\psi^{(0)}(q) = IP_{f(q)}I^{-1}\psi^{(0)}(q) \tag{16}$$

Application: Time-Dependent Harmonic Oscillator

The quantum canonical transformations have been used to solve the Schrödinger equation for many time-independent systems.[9] However they have not been often used in other time-dependent problems than a harmonic oscillator with time-dependent angular frequency.[3] The time-dependent harmonic oscillators have been widely studied by a variety of methods including the invariant operator,[10] the propagator,[11] and the time-space transformation.[12,13] It is useful to have analytical solutions for the time-dependent harmonic oscillator since it may be used as an instructive model[14] to represent the solute vibrations in solutions. We apply quantum canonical transformations to a harmonic oscillator in which both angular frequency and equilibrium position are time-dependent.

Let us start with the Hamiltonian operator $H^{(0)}$ for the time-dependent harmonic oscillator

$$H^{(0)} = p_t + p^2 + w^2(t)(q-u(t))^2 \tag{17}$$

where $p_t = -i(\partial/\partial t)$ and $p = -i(\partial/\partial q)$ are momentum operators in time and in the coordinate respectively. The angular frequency $w(t)$ and the equilibrium position $u(t)$ are functions of time. Mass of the system is scaled and $\hbar$ is assumed to be 1. The Schrödinger equation to be solved is $H^{(0)}\psi^{(0)}(q, t) = 0$.

The quadratic term in q in Eq. (17) is cancelled by making a two-variable similarity transformation

$$p_t \rightarrow p_t - \frac{i}{2}\left(\frac{\partial f}{\partial t}\right)q^2, \quad p \rightarrow p - ifq \tag{18}$$

and the Hamiltonian operator becomes

$$\begin{aligned} H^{(a)} = {} & p_t + p^2 - 2ifqp + \left(2w^2 - i\frac{\partial f}{\partial t} - 2f^2\right)\frac{q^2}{2} \\ & -2w^2uq + w^2u^2 - f \end{aligned} \tag{19}$$

The condition that the quadratic potential be cancelled is

$$i\frac{\partial f}{\partial t} + 2f^2 = 2w^2 \tag{20}$$

This first-order nonlinear equation can be linearized by the substitution $f = \frac{i}{2\phi}\left(\frac{\partial\phi}{\partial t}\right)$ as

$$\frac{\partial^2\phi}{\partial t^2} = -4w^2\phi \tag{21}$$

If a specific form of $w(t)$ is given, Eq. (21) can be solved to determine f and thus the generator $\exp\left(-f(t)\frac{q^2}{2}\right)$.

The second two-variable similarity transformation is carried out to remove the quadratic term in the momentum

$$p_t \to p_t - \frac{i}{2}\left(\frac{\partial g}{\partial t}\right)p^2, \qquad q \to q + igp \tag{22}$$

This changes the Hamiltonian operator to be

$$H^{(b)} = p_t + \left(2 - i\frac{\partial g}{\partial t} + 4fg\right)\frac{p^2}{2} - 2ifqp - 2iw^2ugp$$
$$- 2w^2uq + w^2u^2 - f \tag{23}$$

To eliminate the quadratic term of momentum, we have

$$i\frac{\partial g}{\partial t} = 4fg + 2 \tag{24}$$

With f determined from above, Eq. (24) is integrated to give

$$g = -2ie^{-4i\int fdt}\int e^{4i\int fdt}dt \tag{25}$$

The third two-variable similarity transformation is performed to remove the linear term in q,

$$p_t \to p_t - i\left(\frac{\partial h}{\partial t}\right)q, \qquad p \to p - ih \tag{26}$$

and the Hamiltonian operator will be

$$H^{(c)} = p_t - \left(i\frac{\partial h}{\partial t} + 2fh + 2w^2u\right)q - 2ifqp$$
$$-2iw^2ugp - 2w^2ugh + w^2u^2 - f \tag{27}$$

From the condition that the linear term of coordinate be cancelled, h is determined

$$h = 2ie^{2i\int fdt}\int w^2ue^{-2i\int fdt}dt \tag{28}$$

The next two-variable similarity transformation is done to eliminate the linear term in p,

$$p_t \to p_t - i\left(\frac{\partial r}{\partial t}\right)p, \qquad q \to q + ir \tag{29}$$

and the Hamiltonian operator changes to

$$H^{(d)} = p_t - \left(i\frac{\partial r}{\partial t} + 2iw^2ug - 2fr\right)p - 2ifqp$$
$$-2w^2ugh + w^2u^2 - f \tag{30}$$

The linear term in p would be cancelled if r is to be

$$r = 2e^{2i\int fdt}\int w^2uge^{-2i\int fdt}dt \tag{31}$$

with g given in Eq. (25).

Next, the following point transformation eliminates the coordinate from $H^{(d)}$

$$p \to e^{-q}p, \qquad q \to e^q \tag{32}$$

and the Hamiltonian operator will be

$$H^{(e)} = p_t - 2ifp - 2w^2ugh + w^2u^2 - f \tag{33}$$

Finally, the two-variable similarity transformation

$$p_t \to p_t + 2ifp + 2w^2ugh - w^2u^2 + f, \quad q \to q - 2i\int fdt \tag{34}$$

is carried out to trivialize the Hamiltonian operator

$$H^{(1)} = p_t \tag{35}$$

Since the Schrödinger equation would be trivialized as

$$H^{(1)}\psi^{(1)} = p_t\psi^{(1)} = 0 \tag{36}$$

and $\psi^{(1)}$ is any t-independent function, $\psi^{(0)}(q, t)$ is formally obtained

$$\psi^{(0)}(q, t) = e^{f(t)q^2/2}e^{g(t)p^2/2}e^{h(t)q}e^{r(t)p}$$
$$\times P_{\ln q}e^{-2p\int fdt + i\int(2w^2ugh - w^2u^2 + f)dt}\psi^{(1)}(q) \tag{37}$$

Due to the ambiguity in $\psi^{(1)}(q)$, the explicit form of $\psi^{(0)}(q, t)$ can not be determined by Eq. (37). This ambiguity can be eliminated if $\psi^{(0)}(q, t)$ is sought starting from $\psi^{(e)}(q, t)$ which is the wavefunction of $H^{(e)}$ in Eq. (33)

$$\psi_c^{(e)}(q, t) = e^{cq}e^{i\int[(2w^2ugh - w^2u^2 + (2c+1)f)]dt} \tag{38}$$

where c is a constant. This constant turns out to be a non-negative integer n according to the normalizability requirement. $\psi_n^{(0)}(q, t)$ is then obtained

$$\psi_n^{(0)}(q, t) = e^{f(t)q^2/2}e^{g(t)p^2/2}e^{h(t)q}e^{r(t)p}P_{\ln q}\psi_n^{(e)}(q)$$
$$= e^{i\int[(2w^2ugh - w^2u^2 + (2n+1)f)]dt}$$
$$\times e^{f(t)q^2/2}e^{g(t)p^2/2}e^{h(t)q}(q - ir(t))^n \tag{39}$$

Application of $e^{g(t)p^2/2}$ on $e^{h(t)q}(q - ir(t))^n$ produces the shifted Hermite polynomial[15] and the final expression of unnormalized $\psi_n^{(0)}(q, t)$ would be

$$\psi_n^{(0)}(q, t) = g^{\frac{3n}{2}}e^{-\frac{1}{2}gh^2 + i\int[2w^2ugh - w^2u^2 + (2n+1)f]dt}$$
$$\times e^{\frac{1}{2}fq^2 + hq}H_n\left(\sqrt{\frac{g}{2}}\left(\frac{q - ir}{g} - h\right)\right) \tag{40}$$

with $f(t)$, $g(t)$, $h(t)$, and $r(t)$ are determined from Eqs. (21), (25), (28), and (31) respectively.

Conclusion

In this work, we have solved the Schrödinger equation by a series of elementary canonical transformations for the time-dependent harmonic oscillator in which both angular frequency and equilibrium position change in time. Successive applications of canonical transformations are carried out until the Hamiltonian operator is trivialized. Solutions of the trivialized Hamiltonian operator are sequentially transformed back to obtain solutions of the original Schrödinger equation.

The canonical transformations will be a good approach to many other time-dependent problems than the harmonic oscillators and they are expected to extend to problems like time-dependent Morse oscillators and time-dependent Eckart barriers.

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