Constructing Green functions of the Schrödinger equation by elementary transformations

Gin-yih Tsaur[a)]
Department of Mathematics, Tunghai University, Taichung 407, Taiwan

Jyhpyng Wang
Institute of Atomic and Molecular Sciences, Academia Sinica, P. O. Box 23-166, Taipei 106, Taiwan

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The initial value problem in quantum mechanics is most conveniently solved by the Green function method. Instead of the conventional methods of eigenfunction expansion and path integration, we present a new method for constructing the Green functions systematically. By using suitable elementary transformations, one of the conjugate variables in the Hamiltonian can be eliminated and the Green function for the simplified Hamiltonian can be easily derived. We then obtain the Green function for the original Hamiltonian by the reverse sequence of the elementary transformations. The method is illustrated for the linear potential, the harmonic oscillator, the centrifugal potential, and the centripetal barrier oscillator.
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I. INTRODUCTION

The Green function $K(x,x';t)$ of the Schrödinger equation is the solution of $i(\partial/\partial t)K=HK$ with the initial value $K(x,x';0)=\delta(x-x')$, where $H=H(p,x)$ is the Hamiltonian and $p=-i(\partial/\partial x)$. The Green function can be a powerful tool for solving the initial value problem because the solution of $i(\partial/\partial t)\psi=H\psi$ with any initial value $\psi(x,0)$ can be obtained directly from the Green function by the convolution

$$\psi(x,t) = \int_{-\infty}^{+\infty} \psi(x',0)K(x,x';t)dx'. \tag{1}$$

A well-known method for constructing the Green function of the Schrödinger equation is given by the eigenfunction expansion[1]

$$K(x,x';t) = \int \psi_E^*(x')\psi_E(x)\exp(-iEt)dE, \tag{2}$$

where $\psi_E(x)$ is the normalized eigenfunction of H with the eigenvalue E. Equation (2) is only a formal solution. Even if we have solved the eigenvalue problem $H\psi=E\psi$ to obtain $\psi_E(x)$, it might not be obvious how to convert the expansion to a closed form.

Another formal solution can be expressed as the Feynman path integral[2]

$$K(x,x';t) = \int \exp\left[i\int_0^t L(\dot{x},x,t)dt\right]\mathcal{D}x(t), \tag{3}$$

where the outer integration is over all paths from $(x',0)$ to (x,t) and $L(\dot{x},x,t)$ is the Lagrangian of the system. It is also difficult to reduce Eq. (3) to a closed form, except for the elementary case in which L is quadratic in $\dot{x}$ and x. Some recent developments in Green function theory for localization problems of quasi-periodic lattice Schrödinger operators can be found in Ref. 3.

In this paper, we present a new method for constructing the Green function. It is similar to the canonical-transformation method of classical mechanics. In classical mechanics, the use of a canonical transformation to simplify the Hamiltonian is a standard procedure for solving the equations of motion. If the Hamiltonian $H(p,x)$ can be canonically transformed into a one-variable form $\tilde{H}(P)$, then the equation of motion is greatly simplified. Namely, $\dot{P}=-\partial\tilde{H}/\partial X=0$ implies that P is a constant of the motion and $\dot{X}=\partial\tilde{H}/\partial P=$constant implies that X evolves linearly in time. For example, the Hamiltonian $H(p,x)=\frac{1}{2}p^2+x$ can be transformed into the one-variable form $\tilde{H}(P)=P$ by canonical transformations as follows. By the interchange transformation $(p,x)=(x_1,-p_1)$, one transforms $H=\frac{1}{2}p^2+x$ to $H_1=\frac{1}{2}x_1^2-p_1$, then by the similarity transformation $(p_1,x_1)=(p_2+x_2^2/2,x_2)$ to $H_2=-p_2$, finally by the point transformation $(p_2,x_2)=(-P,-X)$ to $\tilde{H}=P$. As we shall see in Sec. II, these elementary canonical transformations have analogs in quantum mechanics and can all be written in the form

$$p = CPC^{-1}, \tag{4a}$$

$$x = CXC^{-1}, \tag{4b}$$

where C represents an integral transformation, multiplication by a function, or an algebraic substitution.

In quantum mechanics, the reduction of the Hamiltonian by elementary transformations is slightly more involved because p and x do not commute. For $p=-i(\partial/\partial x)$, one has the commutation relation $[p,x]\equiv px-xp=-i$. By using Eq. (4), it might be possible to transform the Hamiltonian from $H(p,x)$ to a simpler form $\tilde{H}(P,X)$,

$$\tilde{H}(P,X) = H(CPC^{-1},CXC^{-1}) = CH(P,X)C^{-1}. \tag{5}$$

By using a sequence of elementary transformations, it might even be possible to reduce the Hamiltonian to a one-variable form $\tilde{H}(P)$.

For the eigenvalue problem of the Schrödinger equation, the identity of $\tilde{H}=CHC^{-1}$ in Eq. (5) implies

$$\tilde{H}\Psi = E\Psi \Leftrightarrow H(C^{-1}\Psi) = E(C^{-1}\Psi). \tag{6}$$

That is, the eigenfunction ψ of the original Hamiltonian H can be obtained from the eigenfunction Ψ of the simplified

Hamiltonian $\tilde{H}$ by the inverse wavefunction transformation

$$\psi = C^{-1}\Psi. \tag{7}$$

Because $[p,x]=C[P,X]C^{-1}$, the commutation relation $[p,x]=-i$ implies $[P,X]=-i$ or $P=-i(\partial/\partial X)$. The eigenfunction of P is e^{ikX} with constant k. Therefore, the eigenfunction of the one-variable Hamiltonian $\tilde{H}(P)$ is also $\Psi(X)=e^{ikX}$. From Eq. (7), the eigenfunction of the original $H(p,x)$ is $\psi(x)=C^{-1}e^{ikX}$. As we shall see, the effect of C^{-1} can be readily evaluated. This method has been used to derive the energy eigenfunctions for all known solvable quantum models.[4–6]

The method will be extended in this paper to solve the initial value problem of the Schrödinger equation. The identity of $\tilde{H}=CHC^{-1}$ in Eq. (5) implies

$$i\frac{\partial}{\partial t}\Psi = \tilde{H}\Psi \Leftrightarrow i\frac{\partial}{\partial t}(C^{-1}\Psi) = H(C^{-1}\Psi). \tag{8}$$

That is, the solution of the original Schrödinger equation $i(\partial/\partial t)\psi=H\,\psi$ can be obtained from the solution of the simplified Schrödinger equation $i(\partial/\partial t)\Psi=\tilde{H}\,\Psi$ by the inverse wavefunction transformation $\psi=C^{-1}\Psi$. If the simplified Hamiltonian depends on only one variable, the equation for the Green function becomes

$$i\frac{\partial}{\partial t}\tilde{K}(X,x';t) = \tilde{H}(P)\tilde{K}(X,x';t). \tag{9}$$

As we shall see, Eq. (9) with the initial value $\tilde{K}(X,x';0)=C\delta(x-x')$ can be easily solved. Then by the inverse wavefunction transformation $K(x,x';t)=C^{-1}\tilde{K}(X,x';t)$, we obtain the Green function of the original Schrodinger equation.

In Sec. II, we discuss the definitions and the corresponding wavefunction transformations of the elementary transformations. In Sec. III, we show how to find the sequence of elementary transformations that eliminates one of the conjugate variables in the Hamiltonian. The corresponding wavefunction transformations can then be used to construct the Green functions. To illustrate the method Green functions are constructed for the linear potential, the harmonic oscillator, the centrifugal potential, and the centripetal barrier oscillator.

II. ELEMENTARY TRANSFORMATIONS

In this section, the interchange, similarity, and point transformations are introduced and their corresponding wavefunction transformations are discussed.[5,6] The transformations are

$$\text{interchange:}(p,x) = (X,-P), \tag{10}$$

$$\text{similarity:}(p,x) = (P+f'(X),X), \tag{11}$$

$$\text{point:}(p,x) = \left(\frac{1}{g'(X)}P, g(X)\right), \tag{12}$$

where $f'=df/dX$ and $g'=dg/dX$. For simplicity, we will often use **I** to replace the "interchange" or "the interchange transformation," **S** to replace "similarity" or "the similarity transformation," and **P** to replace "point" or "the point transformation." The transformations can all be written in the form

$$(p,x) = (CPC^{-1}, CXC^{-1}). \tag{13}$$

The corresponding wavefunction transformations $\Psi=C\psi$ and inverse wavefunction transformations $\psi=C^{-1}\Psi$ are summarized in the following.

For the interchange transformation, we compare the right-hand sides of Eqs. (10) and (13) and obtain

$$X = C_{\mathrm{I}}PC_{\mathrm{I}}^{-1}, \tag{14a}$$

$$-P = C_{\mathrm{I}}XC_{\mathrm{I}}^{-1}. \tag{14b}$$

If we multiply Eq. (14) by C_{I} from the right, it becomes $XC_{\mathrm{I}}=C_{\mathrm{I}}P$ and $-PC_{\mathrm{I}}=C_{\mathrm{I}}X$. The C_{I} transformation can be implemented by the Fourier transformation,

$$C_{\mathrm{I}}\psi = \int_{-\infty}^{+\infty} e^{-iX\xi}\psi(\xi,t)d\xi, \tag{15}$$

because

$$X(C_{\mathrm{I}}\psi) = \int_{-\infty}^{+\infty}\left(i\frac{\partial}{\partial\xi}e^{-iX\xi}\right)\psi(\xi,t)d\xi = \int_{-\infty}^{+\infty} e^{-iX\xi}\left[-i\frac{\partial}{\partial\xi}\psi(\xi,t)\right]d\xi = C_{\mathrm{I}}(P\psi), \tag{16a}$$

$$-P(C_{\mathrm{I}}\psi) = i\frac{\partial}{\partial X}\int_{-\infty}^{+\infty} e^{-iX\xi}\psi(\xi,t)d\xi = \int_{-\infty}^{+\infty} e^{-iX\xi}[\xi\psi(\xi,t)]d\xi = C_{\mathrm{I}}(X\psi). \tag{16b}$$

For the similarity transformation, we compare the right-hand sides of Eqs. (11) and (13) and obtain

$$P+f'(X) = C_{\mathrm{S}}PC_{\mathrm{S}}^{-1}, \tag{17a}$$

$$X = C_{\mathrm{S}}XC_{\mathrm{S}}^{-1}. \tag{17b}$$

If we multiply Eq. (17) by C_{S} from the right, it becomes $[P+f'(X)]C_{\mathrm{S}}=C_{\mathrm{S}}P$ and $XC_{\mathrm{S}}=C_{\mathrm{S}}X$. The C_{S} transformation can be implemented by multiplying ψ with $e^{-if(X)}$,

$$C_{\mathrm{S}}\psi = e^{-if(X)}\psi(X,t), \tag{18}$$

because

$$[P+f'(X)](C_{\mathrm{S}}\psi) = \left[-i\frac{\partial}{\partial X}+f'(X)\right]\left[e^{-if(X)}\psi(X,t)\right], = e^{-if(X)}\left[-i\frac{\partial}{\partial X}\psi(X,t)\right] = C_{\mathrm{S}}(P\psi), \tag{19a}$$

$$X(C_{\mathrm{S}}\psi) = X[e^{-if(X)}\psi(X,t)] = e^{-if(X)}[X\psi(X,t)] = C_{\mathrm{S}}(X\psi). \tag{19b}$$

For the point transformation we compare the right-hand sides of Eqs. (12) and (13) and find

$$\frac{1}{g'(X)}P = C_{\mathrm{P}}PC_{\mathrm{P}}^{-1}, \tag{20a}$$

$$g(X)=C_{\rm P}XC_{\rm P}^{-1}. \tag{20b}$$

If we multiply Eq. (20) by $C_{\rm P}$ from the right, it becomes $[1/g'(X)]PC_{\rm P}=C_{\rm P}P$ and $g(X)C_{\rm P}=C_{\rm P}X$. The $C_{\rm P}$ transformation can be implemented by changing variables,

$$C_{\rm P}\psi=\psi(g(X),t), \tag{21}$$

because

$$\frac{1}{g'(X)}P(C_{\rm P}\psi)=\frac{1}{g'(X)}\left(-i\frac{\partial}{\partial X}\right)\psi(g(X),t),$$
$$=\left[-i\frac{\partial}{\partial x}\psi(x,t)\right]_{x=g(X)}=C_{\rm P}(P\psi), \tag{22a}$$

$$g(X)(C_{\rm P}\psi)=g(X)\psi(g(X),t)=C_{\rm P}(X\psi). \tag{22b}$$

As an example, we show how the x-linear Hamiltonian $H=a+bx$ with $a=F(p)$ and $b=G(p)$ can be reduced to $\widetilde{H}=P$ by the three elementary transformations. This reduction will be used repeatedly in the rest of this paper. The x-linear Hamiltonian $H=F(p)+G(p)x$ can be transformed by $\mathbf{I}$ to the p-linear form $H=F(x)-G(x)p$, then transformed to $H=-G(x)p$ by the $\mathbf{S}$ transformation with $f'(x)=F(x)/G(x)$, and finally reduced to $\widetilde{H}=P$ by the inverse point $\mathbf{P}^{-1}$ transformation with $1/g'(x)=-G(x)$. We define the ordered combination of the particular $\mathbf{I}$, $\mathbf{S}$, and $\mathbf{P}^{-1}$ transformations described above to be the x-linear transformation

$$\mathbf{L}_x: F(p)+G(p)x=P, \tag{23}$$

where $\mathbf{L}_x$ represents the word x-linear or the x-linear transformation. It transforms the x-linear form to P. Its corresponding wavefunction transformation is

$$C_{{\rm L}_x}\psi=C_{\rm P}^{-1}C_{\rm S}C_{\rm I}\psi=\left[e^{-if(\xi)}\int_{-\infty}^{+\infty}e^{-i\xi\eta}\psi(\eta,t)d\eta\right]_{\xi=g^{-1}(X)}, \tag{24}$$

where

$$f'(x)=F(x)/G(x), \tag{25a}$$

$$g'(x)=-1/G(x). \tag{25b}$$

In summary, the $\mathbf{I}$, $\mathbf{S}$, $\mathbf{P}$, and $\mathbf{L}_x$ transformations and their corresponding wavefunction transformations are

$$\mathbf{I}:(p,x)=(X,-P),\quad \Psi=C_{\rm I}\psi=\int_{-\infty}^{\infty}e^{-iX\xi}\psi(\xi,t)d\xi, \tag{26a}$$

$$\mathbf{S}:(p,x)=(P+f'(X),X),\quad \Psi=C_{\rm S}\psi=e^{-if(X)}\psi(X,t), \tag{26b}$$

$$\mathbf{P}:(p,x)=\left(\frac{1}{g'(X)}P,g(X)\right),\quad \Psi=C_{\rm P}\psi=\psi(g(X),t), \tag{26c}$$

$$\mathbf{L}_x: F(p)+G(p)x=P,\quad \Psi=C_{{\rm L}_x}\psi$$
$$=\left[e^{-if(\xi)}\int_{-\infty}^{+\infty}e^{-i\xi\eta}\psi(\eta,t)d\eta\right]_{\xi=g^{-1}(X)}, \tag{26d}$$

where ψ is the eigenfunction before the transformation and Ψ is the eigenfunction after the transformation. The inverse wavefunction transformations are

$$\psi=C_{\rm I}^{-1}\Psi=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{ix\xi}\Psi(\xi,t)d\xi, \tag{27a}$$

$$\psi=C_{\rm S}^{-1}\Psi=e^{if(x)}\Psi(x,t), \tag{27b}$$

$$\psi=C_{\rm P}^{-1}\Psi=\Psi(g^{-1}(x),t), \tag{27c}$$

$$\psi=C_{{\rm L}_x}^{-1}\Psi=\frac{1}{2\pi}\int_{-\infty}^{+\infty}e^{ix\xi}e^{if(\xi)}\Psi(g(\xi),t)d\xi. \tag{27d}$$

III. CONSTRUCTING THE GREEN FUNCTIONS

We now show how to construct the Green functions of the Schrödinger equation by using the elementary transformations. The first step is bringing $H(p,x)=p^2/2+V(x)$ to a one-variable form. A general scheme is to use a point transformation $\mathbf{P}: x\rightarrow g(x)$ to simplify the potential $V(x)$, followed by a similarity transformation $\mathbf{S}: p\rightarrow p+f'(x)$ to bring in additional terms from $p^2/2$ to eliminate the simplified $V(x)$. If we make the right choice of $g(x)$ and $f(x)$, the transformed Hamiltonian will become much simpler. For example, it may become an x-linear form, a p-linear form, or a $\widetilde{p}$-linear form.[6] A p-linear form $F(x)+G(x)p$ can be transformed to an x-linear form by $\mathbf{I}$. A $\widetilde{p}$-linear form is $F(q)+G(q)p$, where $q=x+h(p)$. It can also be transformed to an x-linear form by $\mathbf{I}$ and an $\mathbf{S}$ transformation. Then, the x-linear form can be reduced to P by $\mathbf{L}_x$ as shown in Sec. II.

If the Hamiltonian depends only on one variable, that is, $H=H(P)$, the solution of $i\partial K/\partial t=H(P)K$ in terms of its initial condition $K(X,x';0)$ can be written as

$$K(X,x';t)=e^{-iH(P)t}K(X,x';0). \tag{28}$$

By Eq. (14a), one has $P=C_{\rm I}^{-1}XC_{\rm I}$ and hence $e^{-iH(P)t}=C_{\rm I}^{-1}e^{-iH(X)t}C_{\rm I}$. Consequently, Eq. (28) is equivalent to

$$K(X,x';t)=C_{\rm I}^{-1}e^{-iH(X)t}C_{\rm I}K(X,x';0), \tag{29a}$$

$$=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{iX\xi}e^{-iH(\xi)t}\left[\int_{-\infty}^{\infty}e^{-i\xi\eta}K(\eta,x';0)d\eta\right]d\xi, \tag{29b}$$

$$=\int_{-\infty}^{\infty}\left[\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{-iH(\xi)t+i\xi(X-\eta)}d\xi\right]K(\eta,x';0)d\eta. \tag{29c}$$

Equation (29) shows that the Green function $\widetilde{K}(X,x';t)$ of the Schrödinger equation for a one-variable Hamiltonian can be obtained from its initial value $\widetilde{K}(X,x';0)$ by an integral transformation. For example, for the free particle $H(p)=p^2/2$, the Green function $K(x,x';t)$ with the initial condition $K(x,x';0)=\delta(x-x')$ is

$$K(x,x';t)=\int_{-\infty}^{\infty}\left[\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{-i(\xi^2/2)t+i\xi(x-\eta)}d\xi\right]\delta(\eta-x')d\eta, \tag{30a}$$

$$=\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i(\xi^2/2)t+i\xi(x-x')}d\xi, \tag{30b}$$

$$=\sqrt{\frac{1}{2\pi it}}\exp\left[-\frac{(x-x')^2}{2it}\right], \tag{30c}$$

where for the last step, we used

$$\int_{-\infty}^{+\infty}\exp(-a\xi^2+b\xi)d\xi=\sqrt{\frac{\pi}{a}}\exp\left(\frac{b^2}{4a}\right). \tag{31}$$

In the following examples, the Hamiltonian depends on both conjugate variables. We illustrate how to transform the Hamiltonian to a one-variable form to derive the Green function $\widetilde{K}(X,x';t)$ and then transform it back to obtain $K(x,x';t)$. For the transformation of the initial value $\widetilde{K}(X,x';0)=C\delta(x-x')$, we use the wavefunction transformations in Eq. (26), and for the transformation of the Green function $K(x,x';t)=C^{-1}\widetilde{K}(X,x';t)$, we use the inverse wavefunction transformations in Eq. (27).

Linear potential, $H=p^2/2-Ux$, where U is an arbitrary positive constant. This Hamiltonian is an x-linear form and can be reduced to $\widetilde{H}=P$ by the x-linear transformation

$$\mathbf{L}_x\text{:}\frac{p^2}{2}-Ux=P, \tag{32}$$

which is the $\mathbf{L}_x$ in Eq. (26d) with $F(p)=p^2/2$ and $G(p)=-U$. The corresponding wavefunction transformation is the C_{L_x} in Eq. (26d), where by Eq. (25) $f(x)=-x^3/(6U)$ and $g(x)=x/U$, and hence $g^{-1}(X)=UX$. The initial value $K(x,x';0)=\delta(x-x')$ is transformed to the new variable as

$$\widetilde{K}(X,x';0)=C_{\mathrm{L}_x}\delta(x-x'), \tag{33a}$$

$$=\left[e^{i\xi^3/(6U)}\int_{-\infty}^{+\infty}e^{-i\xi\eta}\delta(\eta-x')d\eta\right]_{\xi=UX}, \tag{33b}$$

$$=\exp\left(\frac{iU^2X^3}{6}-iUXx'\right). \tag{33c}$$

Because the Hamiltonian $\widetilde{H}=P$ now depends only on one variable, the Green function can be obtained from its initial value by Eq. (29c),

$$\widetilde{K}(X,x';t)=\int_{-\infty}^{\infty}\left[\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{i\xi(X-t-\eta)}\right]\widetilde{K}(\eta,x';0)d\eta, \tag{34a}$$

$$=\int_{-\infty}^{\infty}\delta(X-t-\eta)\widetilde{K}(\eta,x';0)d\eta, \tag{34b}$$

$$=\widetilde{K}(X-t,x';0). \tag{34c}$$

Therefore, the Green function in the new variable is

$$\widetilde{K}(X,x';t)=\exp\left[\frac{iU^2(X-t)^3}{6}-iU(X-t)x'\right]. \tag{35}$$

By using the inverse wavefunction transformation corresponding to Eq. (32), we can transform $\widetilde{K}(X,x';t)$ back to $K(x,x';t)$, that is,

$$K(x,x';t)=C_{\mathrm{L}_x}^{-1}\widetilde{K}(X,x';t), \tag{36a}$$

$$=\frac{1}{2\pi}\int_{-\infty}^{+\infty}e^{ix\xi}e^{-i\xi^3/(6U)}\widetilde{K}\left(\frac{\xi}{U},x';t\right)d\xi, \tag{36b}$$

$$=\frac{1}{2\pi}\exp\left(-\frac{iU^2t^3}{6}+iUtx'\right)\times \int_{-\infty}^{+\infty}\exp\left[-\frac{it}{2}\xi^2+i\xi\left(x-x'+\frac{Ut^2}{2}\right)\right]d\xi. \tag{36c}$$

By Eq. (31), $K(x,x';t)$ is

$$K(x,x';t)=\sqrt{\frac{1}{2\pi it}}\exp\left[-\frac{iU^2t^3}{6}+iUtx'-\frac{1}{2it}\times\left(x-x'+\frac{Ut^2}{2}\right)^2\right]. \tag{37}$$

As $U\to 0$, the solution reduces to the Green function for the free particle.

Harmonic oscillator, $H=p^2/2+Ux^2$. The Hamiltonian can be reduced to $\widetilde{H}=P-\alpha/2$ by the transformations

$$\mathbf{S}\text{:}(p,x)=(p_1+i\alpha x_1,x_1), \tag{38a}$$

$$\mathbf{L}_x\text{:}p_1^2/2+i\alpha p_1x_1=P, \tag{38b}$$

where $\alpha=\pm\sqrt{2U}$. The $\mathbf{S}$ transformation is used to bring in additional terms from $p^2/2$ to eliminate the potential. After that $p^2/2=p_1^2/2+i\alpha p_1x_1-\alpha/2-\alpha^2x_1^2/2$. The last term eliminates the potential $V=Ux_1^2$ when $\alpha=\pm\sqrt{2U}$, and the Hamiltonian becomes the x-linear form $H_1=p_1^2/2+i\alpha p_1x_1-\alpha/2$. It is reduced to $\widetilde{H}=P-\alpha/2$ by the x-linear transformation in Eq. (38b), which is the $\mathbf{L}_x$ in Eq. (26d) with $F(p)=p^2/2$ and $G(p)=i\alpha p$. Therefore, for the wavefunction transformation C_{L_x}, we have by Eq. (25) $f(x)=-ix^2/(4\alpha)$ and $g(x)=i\ln x/\alpha$, and, hence, $g^{-1}(X)=e^{-i\alpha X}$. We transform the initial value $K(x,x';0)=\delta(x-x')$ to the new variable by the wavefunction transformations corresponding to Eq. (38a),

$$\widetilde{K}(X,x';0)=C_{\mathrm{L}_x}C_{\mathrm{S}}\delta(x-x'), \tag{39a}$$

$$=\left[e^{-\xi^2/(4\alpha)}\int_{-\infty}^{+\infty}e^{-i\xi\eta}e^{\alpha\eta^2/2}\delta(\eta-x')d\eta\right]_{\xi=e^{-i\alpha X}}, \tag{39b}$$

$$=\exp\left(-\frac{1}{4\alpha}e^{-2i\alpha X}-ix'e^{-i\alpha X}+\frac{\alpha x'^2}{2}\right). \quad (39c)$$

In the new variable the Hamiltonian is $\widetilde{H}=P-\alpha/2$, and the Green function can be obtained from its initial value by Eq. (29c). It is

$$\widetilde{K}(X,x';t)=e^{i\alpha t/2}\widetilde{K}(X-t,x';0), \quad (40a)$$

$$=e^{i\alpha t/2}\exp\left[-\frac{1}{4\alpha}e^{-2i\alpha(X-t)}-ix'e^{-i\alpha(X-t)}+\frac{\alpha x'^2}{2}\right]. \quad (40b)$$

By using the inverse wavefunction transformations in the reverse order, we can transform $\widetilde{K}(X,x';t)$ back to $K(x,x';t)$, that is,

$$K(x,x';t)=C_{\mathrm{S}}^{-1}C_{\mathrm{L}_x}^{-1}\widetilde{K}(X,x';t), \quad (41a)$$

$$=\frac{e^{-\alpha x^2/2}}{2\pi}\int_{-\infty}^{+\infty}e^{ix\xi}e^{\xi^2/(4\alpha)}\widetilde{K}(i\ln\xi/\alpha,x';t)d\xi. \quad (41b)$$

Because

$$\widetilde{K}(i\ln\xi/\alpha,x';t)=e^{i\alpha t/2}\exp\left(-\frac{\xi^2}{4\alpha}e^{2i\alpha t}-ix'\xi e^{i\alpha t}+\frac{\alpha x'^2}{2}\right), \quad (42)$$

we have

$$K(x,x';t)=\exp\left[\frac{\alpha}{2}(x'^2-x^2)\right]\frac{e^{i\alpha t/2}}{2\pi}\times\int_{-\infty}^{+\infty}\exp\left[-\frac{\xi^2}{4\alpha}(e^{2i\alpha t}-1)+i\xi(x-x'e^{i\alpha t})\right]d\xi. \quad (43)$$

By Eq. (31), $K(x,x';t)$ is

$$K(x,x';t)=\exp\left[\frac{\alpha}{2}(x'^2-x^2)\right]\frac{e^{i\alpha t/2}}{2\pi}\sqrt{\frac{4\alpha\pi}{e^{2i\alpha t}-1}}\times\exp\left[-\frac{\alpha(x-x'e^{i\alpha t})^2}{e^{2i\alpha t}-1}\right], \quad (44a)$$

$$=\sqrt{\frac{\alpha}{\pi(e^{i\alpha t}-e^{-i\alpha t})}}\exp\left[\frac{\alpha}{2}(x'^2-x^2)-\frac{\alpha(x-x'e^{i\alpha t})^2}{e^{2i\alpha t}-1}\right], \quad (44b)$$

$$=\sqrt{\frac{\alpha}{2\pi i\sin\alpha t}}\exp\left[-\frac{\alpha}{2i\sin\alpha t}\left(x^2\cos\alpha t-2xx'+x'^2\cos\alpha t\right)\right]. \quad (44c)$$

Note that the solution in Eq. (44c) is the same for $\alpha=\sqrt{2U}$ and $\alpha=-\sqrt{2U}$.

Centrifugal potential, $H=p^2/2+U/x^2$ with $x>0$. The Hamiltonian can be reduced to $\widetilde{H}=P$ by the sequence of transformations

$$\mathbf{P}:(p,x)=(2\sqrt{x_1}p_1,\sqrt{x_1}), \quad (45a)$$

$$\mathbf{S}:(p_1,x_1)=(p_2+i\beta/x_2,x_2), \quad (45b)$$

$$\mathbf{L}_x:2p_2^2x_2+i(4\beta+3)p_2=P, \quad (45c)$$

where $\beta=(-1\pm\sqrt{1+8U})/4$. The $\mathbf{P}$ transformation is used to simplify the potential, after which $V=U/x_1$ and $p^2/2=2(\sqrt{x_1}p_1)^2$. By the $\mathbf{S}$ transformation, $p^2/2$ is further transformed to $2(\sqrt{x_2}p_2)^2+4i\beta p_2-(2\beta^2+\beta)/x_2$. The last term eliminates the simplified potential when $\beta=(-1\pm\sqrt{1+8U})/4$, and the Hamiltonian becomes the x-linear form $H_2=2(\sqrt{x_2}p_2)^2+4i\beta p_2=2p_2^2x_2+i(4\beta+3)p_2$. The Hamiltonian H_2 is reduced to $\widetilde{H}=P$ by the x-linear transformation in Eq. (45c),which is the $\mathbf{L}_x$ in Eq. (26d) with $F(p)=i(4\beta+3)p$ and $G(p)=2p^2$. Therefore, for the wavefunction transformation C_{L_x}, we have by Eq. (25) $f(x)=i(2\beta+3/2)\ln x$ and $g(x)=1/(2x)$, and hence $g^{-1}(X)=1/(2X)$. The initial value $K(x,x';0)=\delta(x-x')$ is transformed to the new variable by the wavefunction transformations corresponding to Eq. (45) as

$$\widetilde{K}(X,x';0)=C_{\mathrm{L}_x}C_{\mathrm{S}}C_{\mathrm{P}}\delta(x-x'), \quad (46a)$$

$$=\left[\xi^{2\beta+3/2}\int_0^{+\infty}e^{-i\xi\eta}\eta^{\beta}\delta(\sqrt{\eta}-x')d\eta\right]_{\xi=1/(2X)}. \quad (46b)$$

We set $\eta=\zeta^2$ and obtain

$$\widetilde{K}(X,x';0)=\left[\xi^{2\beta+3/2}\int_0^{+\infty}e^{-i\xi\zeta^2}\zeta^{2\beta}\delta(\zeta-x')2\zeta d\zeta\right]_{\xi=1/(2X)}, \quad (47a)$$

$$=2x'^{2\beta+1}\left(\frac{1}{2X}\right)^{2\beta+3/2}\exp\left(\frac{-ix'^2}{2X}\right). \quad (47b)$$

In the new variable the Hamiltonian is $\widetilde{H}=P$, and hence is similar to the linear potential,

$$\widetilde{K}(X,x';t)=\widetilde{K}(X-t,x';0), \quad (48a)$$

$$=2x'^{2\beta+1}\left[\frac{1}{2(X-t)}\right]^{2\beta+3/2}\exp\left[\frac{-ix'^2}{2(X-t)}\right]. \tag{48b}$$

By using the inverse wavefunction transformations in the reverse order, we can transform $\tilde{K}(X,x';t)$ back to $K(x,x';t)$, that is,

$$K(x,x';t)=C_{\mathrm{P}}^{-1}C_{\mathrm{S}}^{-1}C_{\mathrm{L}_x}^{-1}\tilde{K}(X,x';t), \tag{49a}$$

$$=\left[\frac{\eta^{-\beta}}{2\pi}\int_{-\infty}^{+\infty}e^{i\eta\xi}\xi^{-(2\beta+3/2)}\tilde{K}\left(\frac{1}{2\xi},x';t\right)d\xi\right]_{\eta=x^2}, \tag{49b}$$

$$=\frac{x'^{2\beta+1}x^{-2\beta}}{\pi}\int_{-\infty}^{+\infty}e^{ix^2\xi}\left(\frac{1}{1-2\xi t}\right)^{2\beta+3/2}\times\exp\left(\frac{-i\xi x'^2}{1-2\xi t}\right)d\xi. \tag{49c}$$

If we set $u=1-2\xi t$, namely $\xi=(1-u)/(2t)$ and $\int_{-\infty}^{+\infty}d\xi=1/(2t)\int_{-\infty}^{+\infty}du$, Eq. (49c) becomes

$$K(x,x';t)=\frac{x'^{2\beta+1}x^{-2\beta}}{2\pi t}\exp\left(\frac{ix^2}{2t}+\frac{ix'^2}{2t}\right)\int_{-\infty}^{+\infty}u^{-2\beta-3/2}\times\exp\left(-\frac{ix^2u}{2t}-\frac{ix'^2}{2tu}\right)du \tag{50a}$$

$$=i^{2\beta-1/2}\frac{\sqrt{xx'}}{t}\exp\left(\frac{ix^2}{2t}+\frac{ix'^2}{2t}\right)J_{-2\beta-1/2}\left(\frac{xx'}{t}\right), \tag{50b}$$

where $J_\nu(r)\equiv 1/(-2\pi i)(r/2)^\nu\int s^{\nu-1}\exp(-r^2s/4+1/s)ds$ is the Bessel function. If $-2\beta-1/2<0$, the term $J_{-2\beta-1/2}$ diverges as $x\to 0$. Hence, the root $\beta=(-1+\sqrt{1+8U})/4$ should be excluded.

Centripetal barrier oscillator, $H=p^2/2+U(x-1/x)^2$ with $x>0$. This example is given as an exercise in the appendix.

IV. SUMMARY

We have shown that by using elementary transformations it is possible to simplify the Hamiltonian so that its Green function can be derived easily. The Green functions of the linear potential, the harmonic oscillator, and the centrifugal potential can be found in Refs. 1 and 7, where they are solved by the eigenfunction expansion method described in Eq. (2). The Green function of the harmonic oscillator can also be found in Ref. 2, where it is solved by Feynman's path integral method described in Eq. (3). Because the elementary transformations preserve the commutation relation $[p,x]=-i$, they are canonical transformations in quantum mechanics. The interchange transformation corresponds to the interchange of coordinate and momentum, the similarity transformation corresponds to a gauge transformation, and the point transformation corresponds to a change of variables. They are the simplest canonical transformations in both classical and quantum mechanics.

The method used in this paper is analogous to the canonical methods of analysis of classical mechanics.[8] We hope that further development of this method may help establish links to the wealth of powerful techniques in classical mechanics, such as superconvergent perturbation theory[9,10] and the Kolmogorov–Arnold–Moser theorem[10,11] for the analysis of quantum dynamics.

APPENDIX: SOLUTION OF THE CENTRIPETAL BARRIER OSCILLATOR

The Hamiltonian of the centripetal barrier oscillator is $H=p^2/2+U(x-1/x)^2$ with $x>0$. To reduce H to a one-variable form, the first step is to use the point transformation $x=g(x_1)$ to simplify the potential. The original potential contains quadratic terms, such as x^2 and $1/x^2$. If we wish to change them to x and $1/x$, respectively, what should be the choice of $g(x_1)$? What is the corresponding change of $p^2/2$? Hint: Use Eq. (12).

Solution: By choosing $g(x_1)=\sqrt{x_1}$, the potential is changed to $V=U(x_1+1/x_1-2)$ and $p^2/2$ is changed to $2(\sqrt{x_1}p_1)^2=2p_1^2x_1+3ip_1$.

To eliminate the potential $V=U(x_1+1/x_1-2)$ a similarity transformation should be used. Note that now the $p^2/2$ term has been changed to $2p_1^2x_1+3ip_1$, which means a similarity transformation $p_1=p_2+i\alpha+i\beta/x_2$ would give extra terms in x and $1/x$. By a suitable choice of α and β, these extra terms cancel the potential. To achieve this goal, what values should be chosen for α and β?

Solution: If we substitute (p_1,x_1) by $(p_2+i\alpha+i\beta/x_2,x_2)$, we find that the choice $\alpha=\pm\sqrt{U/2}$ and $\beta=(-1\pm\sqrt{1+8U})/4$ eliminates the potential. The Hamiltonian becomes the x-linear form $H_2=2p_2(p_2+2i\alpha)x_2+2a(p_2+2i\alpha)+2bp_2$, where $a=i(\alpha+\beta+3/4)$ and $b=i(-\alpha+\beta+3/4)$.

Now the Hamiltonian becomes an x-linear form, which can be reduced to $\tilde{H}=P$ by an x-linear transformation $F(p_2)+G(p_2)x_2=P$. What are the forms of $F(p_2)$ and $G(p_2)$?

Solution: They are $F(p_2)=2a(p_2+2i\alpha)+2bp_2$ and $G(p_2)=2p_2(p_2+2i\alpha)$. Therefore, for the wavefunction transformation C_{L_x}, we have by Eq. (25) $f(x)=a\ln x+b\ln(x+2i\alpha)$ and $g(x)=i/(4\alpha)\ln[x/(x+2i\alpha)]$, hence $g^{-1}(X)=2i\alpha/(e^{4i\alpha X}-1)$.

The initial value of the Green function for the original Hamiltonian is $K(x,x';0)=\delta(x-x')$, and that for the simplified $\tilde{H}$ is $\tilde{K}(X,x';0)=C_{\mathrm{L}_x}C_{\mathrm{S}}C_{\mathrm{P}}\,\delta(x-x')$. Evaluate $\tilde{K}(X,x';0)$ using Eq. (26).

Solution: According to Eq. (26), we have

$$\tilde{K}(X,x';0)=C_{\mathrm{L}_x}C_{\mathrm{S}}C_{\mathrm{P}}\delta(x-x'), \tag{A1a}$$

$$=\left[\xi^{-ia}(\xi+2i\alpha)^{-ib}\int_0^{+\infty}e^{-i\xi\eta}e^{\alpha\eta}\eta^\beta\delta(\sqrt{\eta}-x')d\eta\right]_{\xi=2i\alpha/(e^{4i\alpha X}-1)}. \tag{A1b}$$

If we set $\eta=\zeta^2$, we find

$$\tilde{K}(X,x';0)=\left[\xi^{-ia}(\xi+2i\alpha)^{-ib}\int_0^{+\infty}e^{-i\xi\zeta^2}e^{\alpha\zeta^2}\zeta^{2\beta}\delta(\zeta-x')2\zeta d\zeta\right]_{\xi=2i\alpha/(e^{4i\alpha X}-1)}, \tag{A2a}$$

$$=2e^{\alpha x'^2}x'^{2\beta+1}\Big[\xi^{-ia}(\xi + 2i\alpha)^{-ib}e^{-i\xi x'^2}\Big]_{\xi=2i\alpha/(e^{4i\alpha X}-1)}, \quad \text{(A2b)}$$

$$=2e^{\alpha x'^2}x'^{2\beta+1}e^{4b\alpha X}\left(\frac{2i\alpha}{e^{4i\alpha X}-1}\right)^{-i(a+b)} \times\exp\left(\frac{2\alpha x'^2}{e^{4i\alpha X}-1}\right). \quad \text{(A2c)}$$

According to Eq. (34c), the Green function $\widetilde{K}(X,x';t)$ for $\widetilde{H}$ is $\widetilde{K}(X-t,x';0)$. We can now transform $\widetilde{K}(X,x';t)$ back to the original variables by $K(x,x';t)=C_{\mathrm{P}}^{-1}C_{\mathrm{S}}^{-1}C_{\mathrm{L}_x}^{-1}\widetilde{K}(X,x';t)$. Evaluate $K(x,x';t)$ using Eq. (27).

Solution: According to Eq. (34c), we have

$$\widetilde{K}(X,x';t)=\widetilde{K}(X-t,x';0), \quad \text{(A3a)}$$

$$=2e^{\alpha x'^2}x'^{2\beta+1}e^{4b\alpha(X-t)} \times\left[\frac{2i\alpha}{e^{4i\alpha(X-t)}-1}\right]^{-i(a+b)}\exp\left[\frac{2\alpha x'^2}{e^{4i\alpha(X-t)}-1}\right]. \quad \text{(A3b)}$$

According to Eq. (27), we have

$$K(x,x';t)=C_{\mathrm{P}}^{-1}C_{\mathrm{S}}^{-1}C_{\mathrm{L}_x}^{-1}\widetilde{K}(X,x';t), \quad \text{(A4a)}$$

$$=e^{-\alpha x^2}x^{-2\beta}\frac{1}{2\pi}\int_{-\infty}^{+\infty}e^{ix^2\xi}\xi^{ia}(\xi + 2i\alpha)^{ib}\widetilde{K}\left(\frac{i}{4\alpha}\ln\frac{\xi}{\xi+2i\alpha},x';t\right)d\xi, \quad \text{(A4b)}$$

$$=e^{-\alpha x^2}x^{-2\beta}\frac{1}{\pi}e^{\alpha x'^2}x'^{2\beta+1}e^{-4b\alpha t}(2i\alpha)^{-i(a+b)} \times\int_{-\infty}^{+\infty}e^{ix^2\xi}\left[\frac{1}{(\xi+2i\alpha)e^{-4i\alpha t}-\xi}\right]^{-i(a+b)} \times\exp\left[\frac{2\alpha x'^2\xi}{(\xi+2i\alpha)e^{-4i\alpha t}-\xi}\right]d\xi. \quad \text{(A4c)}$$

Set $u=(\xi+2i\alpha)e^{-4i\alpha t}-\xi$, namely $\xi=(u-2i\alpha e^{-4i\alpha t})/f(t)$, where $f(t)=e^{-4i\alpha t}-1$. Then Eq. (A4c) becomes

$$K(x,x';t)=\frac{(2i\alpha)^{-i(a+b)}}{\pi f(t)}x^{-2\beta}x'^{2\beta+1} \times\exp\left[\alpha(x'^2-x^2-4bt)+\frac{2\alpha x'^2+2\alpha x^2e^{-4i\alpha t}}{f(t)}\right]\times\int u^{i(a+b)} \times\exp\left[\frac{ix^2u}{f(t)}-\frac{4i\alpha^2x'^2e^{-4i\alpha t}}{f(t)u}\right]du, \quad \text{(A5)}$$

where $b=i(-\alpha+\beta+3/4)$ and $i(a+b)=-2\beta-3/2$. Note that $f(t)=-2ie^{-2i\alpha t}\sin(2\alpha t)$ and, therefore,

$$K(x,x';t)=i^{2\beta+3/2}\frac{2\alpha\sqrt{xx'}}{\sin(2\alpha t)}\exp[4i\alpha^2t+i\alpha\cot(2\alpha t)(x'^2+x^2)]J_{-2\beta-1/2}\left[\frac{2\alpha xx'}{\sin(2\alpha t)}\right]. \quad \text{(A6)}$$

The solution in Eq. (A6) is the same for $\alpha=\pm\sqrt{U/2}$ and the root $\beta=(-1+\sqrt{1+8U})/4$ should be excluded because the corresponding $J_{-2\beta-1/2}$ diverges as $x\to 0$.

[a]Electronic mail: gytsaur@thu.edu.tw

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