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Unitary transformation approach to the exact solutions of time-dependent quantum systems with $SU(1,1)$ dynamical group

Shengli Zhang and Fuli Li

CCAST (World Laboratory) PO Box 8730, Beijing 100080, People's Republic of China
Division of Theoretical Physics, Department of Physics, Xian Jiaotong University, Xi'an 710049, People's Republic of China†

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Abstract. A unitary transformation is introduced to determine the exact solution of the time-dependent quantum system. As examples, two quantum systems with Hamiltonian including the quadratic term of generators of $SU(1,1)$ are solved analytically.

Since quantum mechanics was established, finding out the exact solutions of quantum systems has been significant. Many approaches and skills for finding the stationary state of quantum systems have been developed [1]. In contrast to this case, the studies of solving time-dependent quantum systems are principally on the basis of perturbation approximation and numerical computation [2]. However, there are many time-dependent quantum systems, such as the time-dependent harmonic oscillator [3], the quantum motion of a particle in a Paul trap [4], the interaction between atom and radiation [5], and the time-dependent shell models [6], which have to be dealt with exactly or non-perturbativelly. Therefore, it is very necessary and significant to develop non-perturbation and analytical approaches for time-dependent quantum systems.

Some investigations for this purpose have been done. For a time-dependent system in which the Hamiltonian is a linear function of operators of a Lie algebra, Wei and Norman [7] showed that solving the corresponding time-dependent Schrödinger equation can be transformed to solving a set of coupled second-order differential equations by introducing the local evolution operators. In studying the time-dependent harmonic oscillator, Lewis and Riesenfeld [8] developed the invariant operator method and showed that the general solution of the time-dependent Schrödinger equation for the oscillator can be expressed as a linear superposition of eigenstates of the invariant operator. Hagedorn *et al* [9] studied the connection between the classical and quantum motion of a system in which the Hamiltonian is self-adjoint quadratic polynomial in coordinate q and momentum p, and showed that the spectrum of the Floquet operator is either a pure point or purely transient absolutely continuous.

It is well known that group theory plays a powerful role in quantum mechanics [10]. When the stationary Schrödinger equation of a time-independent system is related to the

† Mailing address.

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Casimir operator of a Lie algebra by performing a proper transformation, the quantum states of the system can be connected to the unitary representation of the corresponding group. Not only can the bound states be determined, but also the scattering problem may be studied by a group theory approach. Alhassid *et al* [11] researched the one-dimensional Schrödinger equation with a Morse or Poschl–Teller potential by imbedding the original one-dimensional problem into a two-dimensional space and connecting it with the $SU(1,1)$ group. Generally, when the Hamiltonian of a time-independent system can be written as a function of operators of a Lie algebra, the method of group theory may also be powerful in calculating various physical quantities of the system. The studies of time-dependent quantum systems in which the Hamiltonians are linear functions of operators of $su(1,1)$ or $su(2)$ algebra have been performed by means of the algebraic dynamics approach [12]. The success of these studies stimulates us to apply this approach to a time-dependent quantum system in which the Hamiltonian is a nonlinear function of operators of a Lie algebra. Since the nonlinear case is very challenging, as the first step of attack, in this paper we will study two examples in which the Hamiltonians include the quadratic term of the operators of $su(1,1)$.

For a time-dependent quantum system, the state vector evolves in time according to the Schrödinger equation

$$\mathrm{i}\partial_t \Psi(\boldsymbol{r},t) = \hat{H}(\hat{\boldsymbol{r}},\hat{\boldsymbol{p}},t)\Psi(\boldsymbol{r},t) \tag{1}$$

where we take $\hbar = 1$. In order to solve the equation, let us introduce a transformation

$$\Psi(\boldsymbol{r},t) = U(\hat{\boldsymbol{r}},\hat{\boldsymbol{p}},t)\Psi'(\boldsymbol{r},t) \tag{2}$$

with $U(\hat{\boldsymbol{r}},\hat{\boldsymbol{p}},0) = 1$. Substituting (2) into (1), we obtain

$$\mathrm{i}\partial_t \Psi'(\boldsymbol{r},t) = \hat{H}'(\hat{\boldsymbol{r}},\hat{\boldsymbol{p}},t)\Psi'(\boldsymbol{r},t) \tag{3}$$

in which

$$\hat{H}'(\hat{\boldsymbol{r}},\hat{\boldsymbol{p}},t) = U^{-1}\hat{H}U - \mathrm{i}U^{-1}\partial_t U. \tag{4}$$

The above expression is often called a unitary transformation. With the proper choice of transformation U, we may make the transformed Hamiltonian $\hat{H}'$ possessing the following form,

$$\hat{H}'(\hat{\boldsymbol{r}},\hat{\boldsymbol{p}},t) = f(t)\hat{H}_0(\hat{\boldsymbol{r}},\hat{\boldsymbol{p}}) \tag{5}$$

where $\hat{H}_0$ is time-independent and $f(t)$ is a function of time. If the solutions of the eigenequation of $\hat{H}_0$,

$$\hat{H}_0\phi_n = E_n\phi_n \tag{6}$$

are found, the general solution of (3) can be written as

$$\Psi'(\boldsymbol{r},t) = \sum_n C_n \exp\left[-\mathrm{i}E_n\int_0^t \mathrm{d}\sigma f(\sigma)\right]\phi_n(\boldsymbol{r}) \tag{7}$$

where C_n are time-independent superposition coefficients to be determined by the initial condition for $\Psi(\boldsymbol{r},t)$. Then, we obtain the general solution of equation (1):

$$\Psi(\boldsymbol{r},t) = \sum_n C_n \exp\left[-\mathrm{i}E_n\int_0^t \mathrm{d}\sigma f(\sigma)\right]U(\hat{\boldsymbol{r}},\hat{\boldsymbol{p}},t)\phi_n(\boldsymbol{r}). \tag{8}$$

Suppose that the system is in the kth eigenstate of $\hat{H}_0$ initially, at time t the system evolves to the state

$$\Psi(\boldsymbol{r},t) = \exp\left[-\mathrm{i}E_k\int_0^t \mathrm{d}\sigma f(\sigma)\right]U(\hat{\boldsymbol{r}},\hat{\boldsymbol{p}},t)\phi_k(\boldsymbol{r}). \tag{9}$$

The expectation value of $\hat{H}$ in (9) is

$$E(t) = \frac{\langle \Psi(\boldsymbol{r}, t)|\hat{H}|\Psi(\boldsymbol{r}, t)\rangle}{\langle \Psi(\boldsymbol{r}, t)|\Psi(\boldsymbol{r}, t)\rangle} = f(t)E_k + \mathrm{i}\frac{\langle \phi_k|U^+\partial_t U|\phi_h\rangle}{\langle \phi_k|U^+U|\phi_k\rangle}. \tag{10}$$

Therefore, the dynamic phase acquired in the evolution from $t = 0$ to T is

$$\theta_\mathrm{d} = \int_0^T E(t)\,\mathrm{d}t = E_k\int_0^T f(t)\,\mathrm{d}t + \mathrm{i}\int_0^T \mathrm{d}t\,\frac{\langle \phi_k|U^+\partial_t U|\phi_k\rangle}{\langle \phi_k|U^+U|\phi_k\rangle}. \tag{11}$$

If $U(\hat{\boldsymbol{r}}, \hat{\boldsymbol{p}}, T + t) = U(\hat{\boldsymbol{r}}, \hat{\boldsymbol{p}}, t)$, from (9), the total phase acquired over a period T is given by

$$\theta_\mathrm{t} = -\int_0^t E_k f(\sigma)\,\mathrm{d}\sigma. \tag{12}$$

Thus, the non-adiabatic Berry phase [13] is

$$\theta_\mathrm{B} = \theta_\mathrm{t} + \theta_\mathrm{d} = \mathrm{i}\int_0^T \mathrm{d}t\,\frac{\langle \phi_k|U^+\partial_t U|\phi_k\rangle}{\langle \phi_k|U^+U|\phi_k\rangle}. \tag{13}$$

We see that the Berry phase is determined totally by the unitary transformation.

In the following section, we will apply the above general formalism to two time-dependent systems in which the Hamiltonians include the quadratic term of the generators of $su(1, 1)$.

Firstly, let us consider the time-dependent quantum system with the Hamiltonian

$$\hat{H} = A_1(t)\hat{I}_0\hat{I}_- + \mathrm{i}B_1\hat{I}_0 + C_1(t) \tag{14}$$

in which $A_1(t)$, $B_1(t)$ are real functions of t and $C_1(t)$ is a complex function of t, and $\hat{I}_0$, $\hat{I}_\pm$ constitute a $su(1, 1)$ algebra. For this system, we consider the transformation

$$U_1 = \exp\{u_1\hat{I}_0\hat{I}_- + v_1\} \tag{15}$$

where $u_1(t)$ and $v_1(t)$ are two functions of t to be determined. Using (4) and (14), one has

$$\hat{H}' = (\mathrm{i}\dot{u}_1 - \mathrm{i}B_1u_i + A_1)\hat{I}_0\hat{I}_- + \mathrm{i}B\hat{I}_0 + \mathrm{i}\dot{v}_1 + C_1 \tag{16}$$

in which $\dot{u}_1(t)$ and $\dot{v}_1(t)$ stand for the differentiation of $u_1(t)$ and $v_1(t)$ with respect to time. If $u_1(t)$ and $v_1(t)$ satisfy the equations

$$\mathrm{i}\dot{u}_1(t) - \mathrm{i}B_1(t)u_1(t) + A_1(t) = 0 \tag{17}$$

$$\mathrm{i}\dot{v}_1(t) + C_1(t) = \mathrm{i}\tfrac{1}{2}B_1(t) \tag{18}$$

the Hamiltonian (19) becomes

$$\hat{H}_1' = f_1(t)\hat{H}_{01} \tag{19}$$

with

$$f_1(t) = B_1(t) \qquad \hat{H}_{01} = \mathrm{i}\hat{I}_0 - \mathrm{i}\tfrac{1}{2}. \tag{20}$$

Now we can write the solution of the time-dependent Schrödinger equation with the Hamiltonian (14) as follows,

$$\Psi_1(x, t) = \exp\left\{-\mathrm{i}E_{01}\int_0^t f_1(\sigma)\,\mathrm{d}\sigma\right\}\phi_1(x) \tag{21}$$

where

$$\hat{H}_{01}\phi_1(x) = E_{01}\phi_1(x). \tag{22}$$

For concreteness, let us choose the following realization of $su(1,1)$

$$\hat{I}_- = -\frac{\mathrm{d}}{\mathrm{d}x} \qquad \hat{I}_0 = x\frac{\mathrm{d}}{\mathrm{d}x} + 1 \qquad \hat{I}_+ = x^2\frac{\mathrm{d}}{\mathrm{d}x} + 2x. \tag{23}$$

With this realization, equation (22) becomes

$$\mathrm{i}\left(x\frac{\mathrm{d}\phi_1}{\mathrm{d}x} + \tfrac{1}{2}\phi_1\right) = E_{01}\phi_1. \tag{24}$$

We see that the Hamiltonian $\hat{H}_{01}$ in the above equation is Hermitian. Furthermore, under the realization (23) the Hamiltonian (14) is also Hermitian if the functions in (14) satisfy

$$\mathrm{Im}\{C_1(t)\} = -\frac{B_1(t)}{2} \tag{25}$$

and $A_1(t)$ is real. It should be pointed out that the model (14) is not only significant in the methodology, but also is meaningful in physics. In fact, the Hamiltonian (14) stands for a quantum system with position-dependent effective mass, $m = (2A_1x)^{-1}$, under realization (23). The position-dependent mass problem is known associating with the theory of semiconductor heterostructures and inhomogeneous crystals [14] in the last decade. Recently, it has attracted much attention and some approaches have been considered [15]. The solution of equation (24) is

$$\phi_{1E} = \frac{1}{\sqrt{2\pi}}x^{-\mathrm{i}E_{01}-\frac{1}{2}}. \tag{26}$$

Substituting (28) and (23) into (21), we obtain the wavefunction of the system with the Hamiltonian (14)

$$\begin{aligned}\Psi_{1E}(x,t) = {} & \frac{1}{\sqrt{2\pi}}\exp\left\{U_1(t)\left(x\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\mathrm{d}}{\mathrm{d}x}\right) + v_1(t)\right\} \\ & \times \exp\left\{-\mathrm{i}E_{01}\int_0^t B_1(\sigma)\,\mathrm{d}\sigma\right\}x^{-\mathrm{i}E_{01}-\frac{1}{2}}.\end{aligned} \tag{27}$$

From (17) and (18), we can derive $u_1(t)$ and $v_1(t)$ as follows:

$$u_1(t) = \exp\left[\int_0^t B_1(\sigma)\,\mathrm{d}\sigma\right]\left\{\mathrm{i}\int_0^t A_1(\sigma)\exp\left[-\int_0^\sigma B_1(\rho)\,\mathrm{d}\rho\right]\mathrm{d}\sigma + u_1(0)\right\} \tag{28}$$

$$v_1(t) = \int_0^t \{\mathrm{i}C_1(\sigma) - \tfrac{1}{2}B_1(\sigma)\}\,\mathrm{d}\sigma + v_1(0). \tag{29}$$

The wavefunction (27) can now be written

$$\begin{aligned}\Psi_{1E}(x,t) = {} & \frac{1}{\sqrt{2\pi}}\exp\left\{-\mathrm{i}E_{01}\int_0^t B_1(\sigma)\,\mathrm{d}\sigma + \int_0^t [\mathrm{i}C_1(\sigma) - \tfrac{1}{2}B_1(\sigma)]\,\mathrm{d}\sigma\right\} \\ & \times \exp\left\{-u_1(t)\left(x\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\mathrm{d}}{\mathrm{d}x}\right)\right\}x^{-\mathrm{i}E_{01}-\frac{1}{2}} \\ = {} & \frac{1}{\sqrt{2\pi}}\exp\left\{-\mathrm{i}E_{01}\int_0^t B_1(\sigma)\,\mathrm{d}\sigma + \int_0^t [\mathrm{i}C_1(\sigma) - \tfrac{1}{2}B_1(\sigma)]\,\mathrm{d}\sigma\right\} \\ & \times \sum_{n=0}^{+\infty}\prod_{l=0}^{n}(\mathrm{i}E + \tfrac{1}{2} + l)^2[-u_1(t)]^n\frac{x^{-\mathrm{i}E_{01}-n-\frac{1}{2}}}{n!}.\end{aligned} \tag{30}$$

According to [11], the diabatic energy level reads

$$E_1(t) = \frac{\langle \Psi_{1E}(t)|\hat{H}_1|\Psi_{1E}(t)\rangle}{\langle \Psi_{1E}|\Psi_{1E}\rangle}$$
$$= B_1(t)E_{01} + \mathrm{i}\frac{\langle \psi_{1E}(t)|U^+\partial_t U|\psi_{1E}(t)\rangle}{\langle \psi_{1E}|U^+U|\psi_{1E}\rangle}$$
$$= B_1(t)E_{01} + \mathrm{i}\dot{u}_1\frac{\langle \phi_{1E}|U_1^+U_1\hat{I}_0\hat{I}_-|\phi_{1E}\rangle}{\langle \phi_{1E}|U^+U|\phi_{1E}\rangle} + \mathrm{i}\dot{v}_1(t). \tag{31}$$

With the initial condition $U_1(\hat{r}, \hat{p}, 0) = 1$, which implies that

$$u_1(0) = 0 \qquad v_1(0) = 0 \tag{32}$$

from (28) and (23) we can show that the transformation (15) is indeed unitary. Therefore,

$$E_1(t) = B_1(t)E_{01} + \mathrm{i}\dot{v}_1(t) + \mathrm{i}\dot{u}_1(t)\frac{\langle \phi_{1E}|\hat{I}_0\hat{I}_-|\phi_{1E}\rangle}{\langle \phi_{1E}|\phi_{1E}\rangle}. \tag{33}$$

Using (18), (20) and (22) and the commutation relation of the operators of $su(1, 1)$, we find

$$E_1(t) = B_1(t)E_{01} - C_1(t) - \tfrac{1}{2}\mathrm{i}B_1(t). \tag{34}$$

When the functions $B_1(t)$ and $C_1(t)$ satisfy equation (25), i.e. the Hamiltonian (14) is Hermitian, the diabatic energy becomes

$$E_1(t) = B_1(t)E_{01} + \mathrm{Re}[C_1(t)]. \tag{35}$$

Using (13), it can be shown that the Berry Phase [13] of the present time-dependent quantum system is zero although the parameter functions evolve periodically.

Now let us consider another time-dependent quantum system with the Hamiltonian

$$\hat{H}_2(t) = A_2(t)\hat{I}_-^2 + \mathrm{i}B_2(t)\hat{I}_0 + C_2(t) \tag{36}$$

where $A_2(t)$ and $B_2(t)$ are two real functions of t and $C_2(t)$ is a complex function. For this system, we choose the transformation to be

$$U_2 = \exp\{u_2(t)\hat{I}_0 + v_2(t)\}. \tag{37}$$

According to (4), the transformed Hamiltonian of (36) is given as

$$\hat{H}_2' = A_2(t)\exp[2u_2(t)]\hat{I}_-^2 + \mathrm{i}(B_2 - \dot{u}_2(t))\hat{I}_0 + (C_2 - \mathrm{i}\dot{v}_2). \tag{38}$$

If $u_2(t)$ and $v_2(t)$ satisfy the equations

$$\dot{u}_2(t) - B_2(t) = 0 \tag{39}$$
$$\mathrm{i}\dot{v}_2(t) + 2\mu A_2(t)\exp[2u_2(t)] = C_2(t) \tag{40}$$

the Hamiltonian (38) becomes

$$\hat{H}_2'(t) = f_2(t)\hat{H}_{02} \tag{41}$$

where we define

$$f_2(t) = -2A_2(t)\exp[2u_2(t)] \qquad H_{02} = -\tfrac{1}{2}\hat{I}_-^2 + \mu. \tag{42}$$

In (40), μ is a constant. The solutions of (39) and (40) are as follows,

$$u_2(t) = \int_0^t B_2(\sigma)\,\mathrm{d}\sigma \tag{43}$$

$$v_2(t) = -\mathrm{i}\int_0^t \mathrm{d}\sigma\left\{C_2(\sigma) - 2\mu A_2(\sigma)\exp\left[2\int_0^\sigma B_2(\rho)\,\mathrm{d}\rho\right]\right\} \tag{44}$$

in which we have used the initial conditions $u_2(0) = 0$ and $v_2(0) = 0$ in deriving (43) and (44). These conditions are consistent with $U(\hat{\boldsymbol{r}}, \hat{\boldsymbol{p}}, 0) = 1$.

From (3), we find the wavefunction of the time-dependent system with Hamiltonian (36) as

$$\Psi_2(x,t) = \exp[u_2(t)I_0 + v_2(t)] \exp\left[-\mathrm{i}E_{02} \int_0^t f_2(\sigma)\,\mathrm{d}\sigma \right] \phi_2(x) \tag{45}$$

where $\phi_2(x)$ is a solution of the equation

$$\hat{H}_{02}\phi_2(x) = E_{02}\phi_2(x). \tag{46}$$

Under the realization (23), the Hamiltonian in (46) can be written as ($b = 0$)

$$\hat{H}_{02} = \tfrac{1}{2}\hat{p}^2 + \mu.$$

Then the solutions of (46) are

$$E_{02} = E_{01k} = \tfrac{1}{2}k^2 + \mu \tag{47}$$

$$\phi_2(x) = \phi_{2k}(x) = \frac{1}{\sqrt{2\pi}} \exp(\mathrm{i}kx). \tag{48}$$

Finally, we obtain the wavefunction (45) as follows:

$$\begin{aligned}\Psi_{2k}(x,t) = \frac{1}{\sqrt{2\pi}} \exp&\left\{ \mathrm{i}2(\tfrac{1}{2}k^2 + \mu) \int_0^t A_2(\sigma) \exp\left[2\int_0^\sigma B_2(\rho)\,\mathrm{d}\rho \right] \mathrm{d}\sigma \right\} \\ &\times \exp\left\{ -\mathrm{i}\int_0^t \mathrm{d}\sigma \left[C_2(\sigma) - 2\mu A_2(\sigma) \exp\left[\int_0^\sigma B_2(\rho)\,\mathrm{d}\rho \right] \right] \right\} \\ &\times \exp\left\{ \left[\int_0^t B_2(\sigma)\,\mathrm{d}\sigma \right] x\frac{\mathrm{d}}{\mathrm{d}x} \right\} \exp(\mathrm{i}kx).\end{aligned} \tag{49}$$

From (10), (37), and (49), the diabatic energy level is given by

$$E_{2k}(t) = f_2(t)E_{02k} + \mathrm{Re}[C_2(t)] - 2\mu A_2(t) \exp\left\{ 2\int_0^t B_2(\sigma)\,\mathrm{d}\sigma \right\}. \tag{50}$$

Using (13), we can show that the non-adiabatic Berry phase [13] of the present system is also zero even though the parameters in (36) are periodic functions of time.

On the other hand, we would like to point out that our discussion for the system (36) is different from [9] in some respects. The authors of [3] showed that the quantum mechanical evolution generated by the Hamiltonian, which is a quadratic polynomial in coordinate q and momentum p with time-dependent coefficients, is determined by a unitary implementation of the phase flow of the corresponding classical Hamiltonian and studied the spectrum of the Floquet operator. In our paper, we suggest an approach to find out a unitary transformation for the system.

In conclusion, we have studied the time-dependent systems in which the Hamiltonian contains the quadratic terms of the generators of $su(1,1)$ by means of the algebraic dynamics approach. With the proper choice of transformation, we have analytically found out the exact solutions of these systems. The non-adiabatic Berry phase of these systems have also been calculated. The results have shown that the Berry phases are zero although the parameters in the Hamiltonians are periodic functions of time. The present study shows that the algebraic dynamics approach to time-dependent quantum systems is not only effective for the cases in which the Hamiltonian is a linear function of the generators of an algebra, but also for the cases that the Hamiltonian is a nonlinear function of the operators.

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