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Solution of the Schrödinger equation for time-dependent 1D harmonic oscillators using the orthogonal functions invariant

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Abstract

An extension of the classical orthogonal functions invariant to the quantum domain is presented. This invariant is expressed in terms of the Hamiltonian. Unitary transformations which involve the auxiliary function of this quantum invariant are used to solve the time-dependent Schrödinger equation for a harmonic oscillator with time-dependent parameter. The solution thus obtained is in agreement with the results derived using other methods which invoke the Lewis invariant in their procedures.

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1. Introduction

The existence of invariants in mechanical systems with an explicitly time-dependent Hamiltonian has evoked considerable interest [1]. These constants of motion are of central importance in the study of dynamical systems. A wide variety of methods has been developed in order to obtain the invariants of systems with one degree of freedom [2]. In particular, the time-dependent harmonic oscillator (TDHO) has received much attention due to its applications in many areas of physics [3]. Among the procedures developed for obtaining invariants, a straightforward derivation for the classical TDHO has been presented which leads directly to the orthogonal functions invariant or, if preferred, to the Lewis invariant [4]. The study of exact invariants has led to the nonlinear superposition principle as well as obtaining general solutions, provided that a particular solution is known.

The extension of the theory of invariants to the quantum realm has evolved in, at least, two directions. On the one hand, the one-dimensional time-independent Schrödinger equation is formally equivalent to the TDHO equation. The translation between equations requires the

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exchange of temporal and spatial variables as well as a constant shift of the potential $V(x)$ with the appropriate scaling for the initially time-dependent parameter $\Omega^2(t) \rightarrow \frac{2m}{\hbar^2}(\mathcal{E} - V(x))$. The results obtained in the classical invariant theory are thus applicable for spatially arbitrary time-independent potentials in stationary one-dimensional quantum theory. On the other hand, quantum mechanical expressions of the classical invariant operators have been used in order to obtain exact solutions to the time-dependent Schrödinger equation. To this end, the classical Hamiltonian is translated into a quantum Hamiltonian by considering the canonical coordinate and momentum as time-independent operators obeying the commutation relationship $[\hat{q}, \hat{p}] = \mathrm{i}\hbar$. The quantum treatment then becomes a (1+1)-dimensional problem where the wavefunction depends on a spatial as well as the temporal variable. A potential with an arbitrary time dependence is identified with the coordinate operator of the Hamiltonian. Exact invariants have been derived to tackle a limited class of admissible potentials [5]. The most relevant cases are the quadratic spatial dependence which leads to the quantum mechanical time-dependent harmonic oscillator (QM-TDHO) and the linear potential [6].

The QM-TDHO has been solved under various circumstances such as damping and a time-dependent mass. This problem has been worked out in terms of time-dependent Green functions using a path integral method [7]. Other techniques have also been used such as the time–space rescaling or transformation method and the time-dependent invariant method [8]. The constant of motion that has been invoked in the latter procedure is the well-known Lewis invariant [9]. Unitary transformations then provide a useful tool for simplifying the invariant and for constructing more general states, such as coherent or squeezed states of the QM-TDHO. The analytical solutions thus obtained are functions of a c-number quantity whose differential equation needs to be solved.

The present paper, in contrast to previous derivations which invoke the Lewis invariant, considers the orthogonal functions quantum invariant as the starting point of the derivation. This invariant is a quantum version of the classical orthogonal functions invariant that arises from the linearly independent solutions of the TDHO. A closely related operator with complex coefficients is also referred to in the literature as a linear integral of motion operator [10]. Unitary transformations are then applied to the invariant in order to obtain an explicitly time-independent quantity. The transformations map the orthogonal functions quantum invariant directly onto the momentum operator. Once these transformations are established, the wavefunction is transformed in order to obtain a simplified Schrödinger equation which is readily integrable. The procedure is then compared with the transformations which arise from the Ermakov–Lewis invariant.

2. Orthogonal functions quantum invariant

Consider the time-dependent Hamiltonian of the QM-TDHO:

$$\hat{H}(t) = \tfrac{1}{2}(\hat{p}^2 + \Omega^2(t)\hat{q}^2). \tag{1}$$

The orthogonal functions invariant of this Hamiltonian's classical counterpart is given by

$$G = q_1\dot{q}_2 - q_2\dot{q}_1 \tag{2}$$

where q_1 and q_2 are linearly independent solutions of the TDHO equation [4]. In order to translate this invariant to the quantum domain, let the function q_2 and its time derivative become the quantum coordinate and momentum operators. The remaining function is then treated as a real c-number, which obeys the classical TDHO equation:

$$\ddot{u}(t) + \Omega^2(t)u(t) = 0. \tag{3}$$

The orthogonal functions quantum invariant is then

$$\hat{G} = u(t)\hat{p} - \dot{u}(t)\hat{q} \tag{4}$$

where the dot denotes differentiation with respect to time. The invariance of this linear integral of motion may be corroborated by direct evaluation of its time derivative. The partial time derivative reads

$$\frac{\partial \hat{G}}{\partial t} = \dot{u}\hat{p} - \ddot{u}\hat{q}. \tag{5}$$

This quantity does not vanish since the invariant is explicitly time dependent. However, its total time derivative is indeed zero:

$$\frac{\mathrm{d}\hat{G}}{\mathrm{d}t} = \frac{\partial \hat{G}}{\partial t} - \frac{\mathrm{i}}{\hbar}[\hat{G}, \hat{H}(t)] = (\ddot{u} + \Omega^2 u)\hat{q} = 0. \tag{6}$$

This constant of motion is closely related to the Lewis invariant and is appealing for its physical significance in the adiabatic limit [11].

3. Unitary transformations

The goal of the transformations in this context is to map the invariant onto an explicitly time-independent quantity. The transformed 'invariant' is then no longer time independent although its partial time derivative does vanish. Such a transformation leads to the solution of the Schrödinger equation as we shall demonstrate in the following sections. Unitary transformations of the form

$$\hat{D}(f) = \exp\left(-\frac{\mathrm{i}}{2\hbar} f(t)\hat{q}^2\right) \tag{7}$$

represent a position-dependent displacement of the momentum operator $\hat{D}(f)\hat{p}\hat{D}^\dagger(f) = \hat{p} + f(t)\hat{q}$, whereas the position operator is unaffected by this transformation. In order to eliminate the $\dot{u}(t)$ dependence in the invariant expression (4), consider the transformation

$$\hat{D}_u = \exp\left(-\mathrm{i}\frac{\dot{u}(t)}{2\hbar u(t)}\hat{q}^2\right) \tag{8}$$

so that when applied to the invariant it yields

$$\hat{G}_{\text{disp}} = \hat{D}_u \hat{G} \hat{D}_u^\dagger = u\hat{p} \tag{9}$$

provided that the function u in the transformation obeys the TDHO equation (3). In the present case, this shift not only eliminates the $\dot{u}(t)$ dependence but it also happens to eliminate the position operator $\hat{q}$ in the transformed invariant.

A further unitary transformation realized by the squeeze operator [12]

$$\hat{S}(g) = \exp\left(\mathrm{i}\frac{g(t)}{2\hbar}(\hat{q}\hat{p} + \hat{p}\hat{q})\right) \tag{10}$$

generates a scaling of the position and momentum operators $\hat{S}(g)\hat{q}\hat{S}^\dagger(g) = \hat{q}\,\mathrm{e}^{g(t)}$ and $\hat{S}(g)\hat{p}\hat{S}^\dagger(g) = \hat{p}\,\mathrm{e}^{-g(t)}$. Squeezing or stretching is produced depending on the sign of $g(t)$. For the displaced invariant (9), the unitary transformation

$$\hat{S}_u = \exp\left(\mathrm{i}\frac{\ln u(t)}{2\hbar}(\hat{q}\hat{p} + \hat{p}\hat{q})\right) \tag{11}$$

generates an explicitly time-independent expression $\hat{G}' = \hat{S}_u \hat{G}_{\text{disp}} \hat{S}_u^\dagger = \hat{p}$. The complete transformation may then be written as

$$\hat{T}_u = \hat{S}_u \hat{D}_u = \exp\left(\mathrm{i}\frac{\ln u(t)}{2\hbar}(\hat{q}\hat{p} + \hat{p}\hat{q})\right)\exp\left(-\mathrm{i}\frac{\dot{u}(t)}{2\hbar u(t)}\hat{q}^2\right). \tag{12}$$

This operator may also be written as a single exponential

$$\hat{T}_u = \exp\left(\mathrm{i}\frac{\ln u(t)}{2\hbar}\left(\hat{q}\hat{p} + \hat{p}\hat{q} + \frac{2u(t)\dot{u}(t)}{1-u(t)^2}\hat{q}^2\right)\right) \tag{13}$$

since the commutator of the operators in the exponentials is proportional to one of the operators $[\hat{q}\hat{p} + \hat{p}\hat{q}, \hat{q}^2] \propto \hat{q}^2$ [13]. The orthogonal functions quantum invariant (4) is then transformed into the momentum operator:

$$\hat{G}' = \hat{T}_u \hat{G} \hat{T}_u^\dagger = \hat{p}. \tag{14}$$

Unitary transformations in quantum mechanics correspond to canonical transformations in classical mechanics [14]. In this case, the transformed invariant becomes the new momentum just as the canonical transformation of the adiabatic invariant turns it into the action variable [15]. However, in the present case the invariant is exact since it has been established without the need for adiabatic approximation.

3.1. Invariant in terms of the Hamiltonian

Let us define an invariant which involves the square of the coordinate and momentum operators:

$$\hat{I}_u = \tfrac{1}{2}\hat{G}^2 = \tfrac{1}{2}(u\hat{p} - \dot{u}\hat{q})^2. \tag{15}$$

Quadratic integrals of motion of this type have been used before in order to introduce even and odd coherent states (see for example [16] and references therein). The Hamiltonian, with the aid of the classical TDHO equation (3), may be written as $u^2\hat{H}(t) = \frac{1}{2}(u^2\hat{p}^2 - u\ddot{u}\hat{q}^2)$. On the other hand, the partial time derivative of the transpose transformation is

$$\frac{\partial \hat{T}_u^\dagger}{\partial t} = \frac{\mathrm{i}}{2\hbar}\frac{1}{u^2}[(u\ddot{u} + \dot{u}^2)\hat{q}^2 - u\dot{u}(\hat{p}\hat{q} + \hat{q}\hat{p})]\hat{T}_u^\dagger \tag{16}$$

so that the invariant and the Hamiltonian are related by

$$\hat{I}_u = u^2\left(H(t) - \mathrm{i}\hbar\frac{\partial \hat{T}_u^\dagger}{\partial t}\hat{T}_u\right). \tag{17}$$

The representation of the Hamiltonian in terms of its invariants is relevant in several applications [17] since it provides an eigenvalue which may be related to the energy of the system. If we apply the transformation from the left and its inverse from the right, the transformed invariant yields

$$\hat{I}'_u = \hat{T}_u\hat{I}_u\hat{T}_u^\dagger = u^2\left(\hat{T}_u H(t)\hat{T}_u^\dagger - \mathrm{i}\hbar\hat{T}_u\frac{\partial \hat{T}_u^\dagger}{\partial t}\right). \tag{18}$$

In summary, the invariant operators $\hat{G}$, $\hat{I}_u$ are time independent although their partial time derivatives are different from zero. On the other hand, the transformed operators $\hat{G}'$, $\hat{I}'_u$ are implicitly time dependent but their partial time derivative is zero.

4. Solution to the Schrödinger equation

Consider the Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = \hat{H}(t)|\psi(t)\rangle \tag{19}$$

for the QM-TDHO Hamiltonian given in equation (1). In order to solve this equation, allow for the unitary transformation $\hat{T}_u$ which maps the orthogonal functions quantum invariant onto an explicitly time-independent operator:

$$|\phi_u(t)\rangle = \hat{T}_u|\psi(t)\rangle \tag{20}$$

where u is the solution to the TDHO equation (3). Substitution in the Schrödinger equation (19) leads to

$$\mathrm{i}\hbar\left(\hat{T}_u^\dagger\frac{\partial|\phi_u(t)\rangle}{\partial t} + \frac{\partial\hat{T}_u^\dagger}{\partial t}|\phi_u(t)\rangle\right) = \hat{H}(t)\hat{T}_u^\dagger|\phi_u(t)\rangle. \tag{21}$$

Multiplying by $\hat{T}_u$ from the left and rearranging, we obtain

$$\mathrm{i}\hbar\frac{\partial|\phi_u(t)\rangle}{\partial t} = \left[\hat{T}_u\hat{H}(t)\hat{T}_u^\dagger - \mathrm{i}\hbar\hat{T}_u\frac{\partial\hat{T}_u^\dagger}{\partial t}\right]|\phi_u(t)\rangle \tag{22}$$

where

$$\hat{\mathcal{H}}(t) = \hat{T}_u\hat{H}(t)\hat{T}_u^\dagger = \frac{1}{2}\left(\left(\frac{\hat{p}}{u} + \dot{u}\hat{q}\right)^2 + \Omega^2(t)u^2\hat{q}^2\right) \tag{23}$$

stands for the transformed Hamiltonian. Although in appearance a less tractable Hamiltonian, its simplification with the term involving the time derivative of the transformation

$$\frac{\partial\hat{T}_u^\dagger}{\partial t} = \frac{\mathrm{i}}{2\hbar}\hat{T}_u^\dagger\left[(u\ddot{u} - \dot{u}^2)\hat{q}^2 - \frac{\dot{u}}{u}(\hat{p}\hat{q} + \hat{q}\hat{p})\right] \tag{24}$$

leads to an integrable form of equation (22):

$$\mathrm{i}\hbar\frac{\partial|\phi_u(t)\rangle}{\partial t} = \frac{1}{2}\left[\frac{\hat{p}^2}{u^2} + (\Omega^2u + \ddot{u})u\hat{q}^2\right]|\phi_u(t)\rangle = \frac{1}{2}\frac{\hat{p}^2}{u^2}|\phi_u(t)\rangle. \tag{25}$$

The solution of this equation is

$$|\phi_u(t)\rangle = \exp\left(-\frac{\mathrm{i}}{2\hbar}\hat{p}^2\int_0^t\frac{\mathrm{d}t'}{u^2(t')}\right)|\phi_u(0)\rangle \tag{26}$$

where $|\phi_u(0)\rangle$ is the wavefunction at $t = 0$. Finally, going back to the initial wavefunction, the solution to the original Schrödinger equation (19) is

$$|\psi(t)\rangle = \hat{T}_u^\dagger\exp\left(-\frac{\mathrm{i}}{2\hbar}\hat{p}^2\int_0^t\frac{\mathrm{d}t'}{u^2(t')}\right)\hat{T}_{u_0}|\psi(0)\rangle \tag{27}$$

where $\hat{T}_{u_0}$ is the transformation at time $t = 0$. This solution may be applied to any initial condition $|\psi(0)\rangle$. It may be easily checked that the above solution is indeed correct by evaluating its partial time derivative:

$$\frac{\partial|\psi(t)\rangle}{\partial t} = \frac{\mathrm{i}}{2\hbar}\left[\frac{u\ddot{u} + (\dot{u})^2}{u^2}\hat{q}^2 - \frac{\dot{u}}{u}(\hat{q}\hat{p} + \hat{p}\hat{q}) - \left(\hat{p} - \frac{\dot{u}}{u}\hat{q}\right)^2\right]|\psi(t)\rangle = -\frac{\mathrm{i}}{\hbar}H(t)|\psi(t)\rangle \tag{28}$$

which recovers the original Schrödinger equation (19). This derivation has considered the simplest case of a Hamiltonian with only quadratic terms in the operators. However, the extension to a complete second-order polynomial in the coordinate operator is also possible [2]. Such an extension permits forced oscillations as well as a time-dependent energy shift. The formalism presented here is also applicable to this general case as shown in the appendix.

4.1. Solution in terms of the invariant

The above procedure used to solve the Schrödinger equation does not necessarily involve the use of the invariant. Nonetheless, in order to choose the appropriate transformation, the guiding principle was to transform the invariant into an explicitly time-independent quantity. We are now in a position where this assertion may be justified. Returning to the transformed Schrödinger equation (22), substitution of the relationship between the invariant and the Hamiltonian (18) yields

$$\mathrm{i}\hbar\frac{\partial|\phi(t)\rangle}{\partial t} = \left(\frac{\hat{T}_u\hat{I}_u\hat{T}_u^\dagger}{u^2}\right)|\phi(t)\rangle = \frac{\hat{I}'_u}{u^2}|\phi(t)\rangle. \tag{29}$$

If the transformed invariant is explicitly time independent, the above equation is formally integrable. The solution of the initial wavefunction in terms of the transformed and the original invariant is then

$$|\psi(t)\rangle = \hat{T}_u^\dagger \exp\left(-\frac{\mathrm{i}}{\hbar}\hat{T}_u\hat{I}_u\hat{T}_u^\dagger\int_0^t\frac{\mathrm{d}t'}{u^2(t')}\right)\hat{T}_{u_0}|\psi(0)\rangle \tag{30}$$

$$= \exp\left(-\frac{\mathrm{i}}{\hbar}\hat{I}_u\int_0^t\frac{\mathrm{d}t'}{u^2(t')}\right)\hat{T}_u^\dagger\hat{T}_{u_0}|\psi(0)\rangle. \tag{31}$$

5. Ermakov–Lewis invariant

The transformation method has been extensively used in order to obtain exact solutions of the Schrödinger equation [18]. This method involves an appropriate rescaling of the space and time variables in the Schrödinger equation as well as a unitary transformation of the wavefunction [8]. An equivalent procedure has been to invoke the Ermakov–Lewis invariant and perform a suitable transformation in order to obtain the eigenvalue equation [19]. Let us recreate this method in order to compare it with the results derived in the previous sections. Consider the transformation

$$\hat{T}_\rho = \mathrm{e}^{\mathrm{i}\frac{\ln\rho}{2\hbar}(\hat{q}\hat{p}+\hat{p}\hat{q})}\,\mathrm{e}^{-\mathrm{i}\frac{\dot{\rho}}{2\hbar\rho}\hat{q}^2} \tag{32}$$

where ρ satisfies the auxiliary equation

$$\ddot{\rho} - \rho^{-3} = -\Omega^2\rho. \tag{33}$$

This transformation is formally equivalent to that implemented in the preceding sections except for the auxiliary function ρ which now obeys the Ermakov equation. Recall that the Ermakov–Lewis invariant is given by

$$\hat{I}_\rho = \frac{1}{2}\left(\left(\frac{\hat{q}}{\rho}\right)^2 + (\rho\hat{p} - \dot{\rho}\hat{q})^2\right). \tag{34}$$

The transformed invariant then reads

$$\hat{I}'_\rho = \hat{T}_\rho\hat{I}_\rho\hat{T}_\rho^\dagger = \tfrac{1}{2}[\hat{q}^2 + \hat{p}^2]. \tag{35}$$

This invariant is again explicitly time independent as in the previous case although it retains the spatial operator. It corresponds to that derived by Hartley and Ray [19] where the spatial rescaling made in their communication has been included here in the squeezing transformation. The transformed wavefunction $|\phi_\rho(t)\rangle = \hat{T}_\rho|\psi(t)\rangle$, then translates the Schrödinger equation (19) into

$$\mathrm{i}\hbar\frac{\partial|\phi_\rho(t)\rangle}{\partial t} = \frac{1}{2\rho^2}(\hat{q}^2 + \hat{p}^2)|\phi_\rho(t)\rangle = \frac{\hat{I}'_\rho}{\rho^2}|\phi_\rho(t)\rangle. \tag{36}$$

The solution is then

$$|\psi(t)\rangle = \exp\left(-\frac{\mathrm{i}}{\hbar}\hat{I}_\rho \int_0^t \frac{\mathrm{d}t'}{\rho^2}\right)\hat{T}_\rho^\dagger \hat{T}_{\rho 0}|\psi(0)\rangle. \tag{37}$$

The relationship between the Lewis invariant and the Hamiltonian is obtained in an analogous fashion to the derivation of equation (17):

$$\hat{I}_\rho = \rho^2\left(H(t) - \mathrm{i}\hbar\frac{\partial \hat{T}_\rho^\dagger}{\partial t}\hat{T}_\rho\right). \tag{38}$$

These last three equations are formally equivalent to those obtained with the orthogonal functions invariant (29), (31) and (17) provided that the invariant together with the transformation and its associated auxiliary function are substituted. The Lewis–Risenfeld orthonormal states have been used to obtain expansions of coherent states [20] as well as squeezed states [21] of the QM-TDHO.

6. Conclusions

A quantum version of the orthogonal functions classical invariant has been economically derived in order to establish unitary transformations that map this operator onto an explicitly time-independent operator. The quantum invariant and its transformed operator have been expressed in terms of the Hamiltonian. The orthogonal functions invariant (4) is equally suitable as the Ermakov–Lewis invariant in order to solve the one-dimensional QM-TDHO although the former does not require an auxiliary Ermakov equation.

Appendix. Generalized Hamiltonian

Consider the Schrödinger equation for a Hamiltonian which in addition to the quadratic terms has a linear term in the position operator with an arbitrary time-dependent function and an operator-free time-dependent term:

$$\mathrm{i}\hbar\frac{\partial|\epsilon(t)\rangle}{\partial t} = \left(\frac{\hat{p}^2}{2} + \frac{\Omega^2(t)\hat{q}^2}{2} + g_1(t)\hat{q} + g_0(t)\right)|\epsilon(t)\rangle. \tag{A.1}$$

Allow for the unitary transformation

$$|\epsilon(t)\rangle = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\tilde{u}(t)\hat{p} - \dot{\tilde{u}}(t)\hat{q})}|\xi(t)\rangle \tag{A.2}$$

where $\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\tilde{u}(t)\hat{p} - \dot{\tilde{u}}(t)\hat{q})}$ is the Glauber displacement operator (see, for instance, [22]). The Schrödinger equation is then mapped to

$$\mathrm{i}\hbar\frac{\partial|\xi(t)\rangle}{\partial t} = \left(\frac{\hat{p}^2}{2} + \frac{\Omega^2(t)\hat{q}^2}{2} + \theta(t)\right)|\xi(t)\rangle \tag{A.3}$$

where $\tilde{u}$ obeys an inhomogeneous time-dependent harmonic differential equation

$$\ddot{\tilde{u}} + \Omega^2\tilde{u} = g_1 \tag{A.4}$$

and

$$\theta = g_0 + \tfrac{3}{2}(\Omega^2\tilde{u}^2 - \dot{\tilde{u}}^2) + -2\tilde{u}g_1. \tag{A.5}$$

The term θ represents an overall phase or time-dependent shift of the energy. It may be easily eliminated by performing a phase transformation

$$|\psi(t)\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int\theta\,\mathrm{d}t}|\xi(t)\rangle \tag{A.6}$$

in order to obtain the Schrödinger equation (19) which was the starting point of our previous derivations:

$$i\hbar\frac{\partial|\psi(t)\rangle}{\partial t}=\left(\frac{\hat{p}^2}{2}+\frac{\Omega^2(t)\hat{q}^2}{2}\right)|\psi(t)\rangle. \tag{A.7}$$

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