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Remarks on solving the one-dimensional time-dependent Schrödinger equation on the interval $[0,\infty]$: the case of a quantum bouncer

S T Dembiński and L Wolniewicz
Institute of Physics, Nicholas Copernicus University, ul. Grudziadzka 5, 87-100 Torun, Poland

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Abstract. It is shown that the 1D Hamiltonian, which is a sum of operators which generate a finite nilpotent Lie algebra and depends explicitly on time existing closed form solutions of the time-dependent Schrödinger equation, cannot fulfil in general boundary and normalization conditions on a positive semi-axis. An explanation of the controversy surrounding the solutions of the quantum bouncer model, which appeared recently in the literature, is given.

1. Introduction

Quantum theory of systems which are subjected to constraints has attracted far less interest in the literature than the classical theory of such systems, the latter being in fact an inherent part of any textbook on classical mechanics. There are of course quite well understood reasons for such a state of affairs. Recently, however, when it became fashionable to look for 'finger prints' of classical chaos in quantum physics, quantization of the simplest possible classical nonlinear models attracted much interest. Among these models there are, in particular, models of infinitely deep wells, gravitational bouncers, stadia of different shapes and so on. Particles in these models are allowed to occupy only some restricted volumes of space and this fact alone introduces nonlinearity to the equations of motion. In order to have chaotic behaviour in such systems, boundaries of these volumes may also be time dependent. This holonomic (time-dependent) type of constraint is a necessary condition for the chaos to appear in one-dimensional models. To restrict motions of a quantum particle to some domain Ω in the configurational space one assumes that the potential is infinite at the boundaries and outside of Ω. This fact in turn implies vanishing of the state vector (in the position representation) on the boundary and outside Ω. In this way the infinite potential, which is responsible for the constraints, is in practice in all further considerations represented exclusively by the boundary conditions imposed on the state function. It will be demonstrated and explained in this paper why, when trying to solve problems with time-dependent boundary conditions, this fact may lead to confusion. An example from the very recent literature will be quoted in this context.

We consider here the one-dimensional gravitational bouncer, i.e. a point mass m in the potential $U(x) : U(x) = mgx$ for $x > l(t)$ and $U(x) = \infty$ for $x \leqslant l(t)$. The function $l(t)$ is a real-valued function of time t.

The Schrödinger equation reads ($m = 1, \hbar = 1$)

$$\mathrm{i}\partial_t \Psi = (-\tfrac{1}{2}\partial_x^2 + gx)\Psi \tag{1}$$

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and physically acceptable solutions must obey the condition

$$\forall t : \left\{ \Psi(x,t) = 0 \quad \text{for } x = l(t) \quad \text{and} \int_{l(t)}^{\infty} |\Psi(x,t)|^2 \, \mathrm{d}x = 1 \right\}. \tag{2}$$

The Schrödinger equation (1) with the boundary conditions given in (2) has been studied in a number of papers, (see the bibliography in [1]). It is well known that the simple change of variable, $x \to y : y = x - l(t)$, transforms (1) to the following form:

$$\mathrm{i}\partial_t \Psi = [-\tfrac{1}{2}\partial_y^2 + \mathrm{i}\dot{l}(t)\partial_y + gy + gl(t)]\Psi \equiv \boldsymbol{H}(t)\Psi \tag{3}$$

and the boundary condition now reads

$$\forall t : \left\{ \Psi(y,t) = 0 \quad \text{for } y = 0 \quad \text{and} \int_{0}^{\infty} |\Psi(y,t)|^2 \, \mathrm{d}y = 1 \right\}. \tag{4}$$

In (3) $\dot{l}(t)$ denotes the time derivative of $l(t)$. Below we will denote time derivatives—both ordinary and partial—either by dots or by superscripts in parentheses. Thus, for example, $\Psi^{(n)} \equiv \partial_t^n \Psi$.

2. Exact solutions

Let us write (3) in the following form:

$$\mathrm{i}\partial_t \Psi = \left[\sum_{n=1}^{4} \alpha_i(t) H_i \right] \Psi \tag{5}$$

where

$$H_1 = 1 \qquad H_2 = y \qquad H_3 = \partial_y^2 \qquad H_4 = \mathrm{i}\partial_y$$

and

$$\alpha_1 = gl(t) \qquad \alpha_2 = g \qquad \alpha_3 = -\tfrac{1}{2} \qquad \alpha_4 = \dot{l}(t).$$

The operators $H_i, i = 1 \ldots 4$, generate a four-dimensional Lie algebra K with

$$[H_i, H_j] = \sum_{k=1}^{4} c_{ij}^k H_k$$

where the non-zero structure constants are $c_{23}^4 = 2\mathrm{i}, c_{24}^1 = -\mathrm{i}$. This is a nilpotent algebra with the property

$$[[[K, K], K,], K] = 0.$$

Now it is very tempting to take advantage of the formalism proposed by Wei and Norman [2] and write the solution of (5) in the form

$$\Psi(y,t) = U(t,0)\Psi(y,0) \tag{6}$$

where the unitary time evolution operator $U(t,0)$ is given by

$$U(t,0) = \exp(\beta_1 H_1) \exp(\beta_2 H_2) \exp(\beta_3 H_3) \exp(\beta_4 H_4). \tag{7}$$

Substituting (6) into (5) and taking advantage of the linear independence of H_i one gets the following differential equations for the unknown functions $\beta_i(t)$:

$$\mathrm{i}\dot{\beta}_1 + \beta_2\dot{\beta}_4 + \mathrm{i}\dot{\beta}_3\beta_2^2 = gl$$
$$\mathrm{i}\dot{\beta}_2 = g$$
$$\mathrm{i}\dot{\beta}_3 = -\tfrac{1}{2}$$
$$\mathrm{i}\dot{\beta}_4 - 2\dot{\beta}_3\beta_2 = \dot{l}$$

with the initial conditions

$$\beta_i(0) = 0 \qquad \text{for } i = 1, \ldots, 4.$$

The solution of this nonlinear system of equations is easily obtained and reads

$$\beta_1 = -\mathrm{i}\left[g \int_0^t l(t')\,\mathrm{d}t' + g \int_0^t t'\dot{l}(t')\,\mathrm{d}t' + g^2 t^3/6\right]$$
$$\beta_2 = -\mathrm{i}gt$$
$$\beta_3 = \mathrm{i}t/2$$
$$\beta_4 = -\mathrm{i}[l(t) - l(0) + gt^2/2].$$

If the order of H_i in (7) is denoted by $(1, 2, 3, 4)$ then there are three other distinct forms of such factorized solutions. They have orders $(1, 3, 2, 4)$, $(1, 3, 4, 2)$ and $(1, 4, 2, 3)$. The corresponding functions β_i may also be calculated for each of these cases without any problems. For our nilpotent algebra one may now make an effective use of the celebrated Baker–Hausdorf formula, which in this case reads

$$\exp(\beta_i H_i)\exp(\beta_j H_j) = \exp(\beta_i H_i + \beta_j H_j + \tfrac{1}{2}\beta_i\beta_j[H_i, H_j] + C_{ij} + C_{ji})$$

where

$$C_{ij} = \tfrac{1}{12}\beta_i^2\beta_j[H_i, [H_i, H_j]].$$

Then all four of the distinct factorized forms of $\Psi(y, t)$ lead to the following solution:

$$\Psi(y, t) = \exp\left(\sum_{i=1}^{4} \gamma_i(t) H_i\right)\Psi(y, 0) \tag{8}$$

where

$$\gamma_1 = -\mathrm{i}\left[g \int_0^t l(t')\,\mathrm{d}t' + g \int_0^t t'\dot{l}(t')\,\mathrm{d}t' - \mathrm{i}gt/2(l(t) - l(0))\right] \tag{9}$$
$$\gamma_2 = -\mathrm{i}gt \tag{10}$$
$$\gamma_3 = \mathrm{i}t/2 \tag{11}$$
$$\gamma_4 = -\mathrm{i}[l(t) - l(0)]. \tag{12}$$

The solution given in (8)–(12) can also be written in the following form

$$\Psi(y, t) = \exp\left(-\mathrm{i}\int_0^t \boldsymbol{H}(t')\,\mathrm{d}t' + \tfrac{1}{2}\int_0^t \int_0^{t'} [\boldsymbol{H}(t''), \boldsymbol{H}(t')]\,\mathrm{d}t'\,\mathrm{d}t''\right)\Psi(y, 0)$$

which is known in the literature as the Magnus formula [3].

There are still other forms of Ψ which may be obtained from (8) via the Baker–Hausdorf formula. We mention here the one which appeared in [4]:

$$\Psi(y, t) = \exp(\delta_1 H_1)\exp(-\mathrm{i}\alpha_2 H_2 t - \mathrm{i}\alpha_3 H_3 t)\exp(\delta_4 H_4)\Psi(y, 0) \tag{13}$$

where

$$\delta_1(t) = \mathrm{i}g \int_0^t t' l(t')\,\mathrm{d}t'$$
$$\delta_4(t) = -\mathrm{i}[l(t) - l(0)].$$

We will call the family of equivalent solutions described in this paragraph the Wei–Norman solutions (WNS).

3. The boundary conditions

For an arbitrary $l(t)$ the above exact solutions of the time-dependent Schrödinger equation (WNS) cannot fulfil the boundary conditions given in (4). In what follows it will be demonstrated that the boundary conditions are in general not compatible with the Schrödinger differential equation. If this is the case then the WNS cannot in fact fulfil the boundary conditions.

Let us assume that the function $\Psi(y,t)$ possesses at $t=t_0$ time derivatives of all orders and may be expanded in the Taylor power series in t in an arbitrarily small vicinity Γ_{t_0} of $t=t_0$. Then the initial boundary condition $\Psi(y=0,t_0)=0$ will imply the equality $\Psi(y=0,t)=0$ for $t\in\Gamma_{t_0}$ if

$$\Psi^{(n)}(y,t)|_{t=t_0,y=0}=0 \qquad n=0,1,2,\ldots. \tag{14}$$

In order to simplify the calculations let us perform the gauge transformation that is frequently used while dealing with the bouncer:

$$\Psi(y,t)=\exp(\mathrm{i}\dot{l}(t)H_2)\Phi(y,t).$$

The function Φ fulfils the equation

$$\mathrm{i}\dot{\Phi}=H(t)\Phi \tag{15}$$

with

$$H=(\alpha_1-\tfrac{1}{2}\dot{l}^2)H_1+(\alpha_2+\ddot{l})H_2+\alpha_3H_3 \tag{16}$$

and must obey the boundary condition

$$\forall t:\left\{\Phi(y,t)=0\quad\text{for }y=0\quad\text{and}\quad\int_0^\infty|\Phi(y,t)|^2\,\mathrm{d}y=1\right\}.$$

It may easily be verified that

$$\Psi^{(n)}(y,t)|_{y=0}=\Phi^{(n)}(y,t)|_{y=0}.$$

The hierarchy of conditions given in (14) starts as follows:

$$\Phi_0|_{y=0}=0 \tag{17}$$

$$\dot{\Phi}|_{t=t_0,y=0}=(-\mathrm{i}H_{t=t_0}\Phi_0)|_{y=0}=0 \tag{18}$$

$$\ddot{\Phi}|_{t=t_0,y=0}=((-\mathrm{i})^2H_{t=t_0}^2-\mathrm{i}\dot{H}_{t=t_0})\Phi_0|_{y=0}=0 \tag{19}$$

$$\Phi^{(3)}|_{t=t_0,y=0}=((-\mathrm{i})^3H_{t=t_0}^3+(-\mathrm{i})^2(2\dot{H}H+H\dot{H})_{t=t_0}-\mathrm{i}\ddot{H}_{t=t_0})\Phi_0|_{y=0}=0 \tag{20}$$

...

where $\Phi_0=\Phi(y,t=t_0)$.

It is seen from (16) that

$$H_{t=t_0}^{(n)}=[\alpha_2H_2+\alpha_3H_3]\delta_{n0}+[(\alpha_1-\tfrac{1}{2}\dot{l}^2)_{t=t_0}^{(n)}]H_1+[l_{t=t_0}^{(n+2)}]H_2.$$

Conditions given in (17)–(19) are fulfilled when Φ_0 is of the form

$$\Phi_0(y)=\sum_n c_n\Theta_n(y) \qquad \text{for } y\geqslant 0 \tag{21}$$

where

$$H_{t=t_0}\Theta_n(y)=\Lambda_n\Theta_n(y) \qquad \Theta_n(0)=0$$

Λ_n are eigenvalues and c_n constants. It is well known that a complete orthonormal set of such functions Θ_n exists (it is assumed in this consideration that $g+\ddot{l}_{t=t_0}>0$) and

$$\Theta_n(y)=N_n\mathrm{Ai}([2(g+\ddot{l}_{t=t_0})]^{1/3}y+y_n). \tag{22}$$

Ai is the Airy function, y_n, are zeros of the Airy function, $\mathrm{Ai}(y_n) = 0$, and N_n are normalization factors:

$$\int_0^\infty \Theta_n^2(y)\,\mathrm{d}y = 1.$$

The eigenvalues Λ_n are as follows:

$$\Lambda_n = (\alpha_1 - \tfrac{1}{2}\dot{l}^2)_{t=t_0} - 2^{-1/3}(g + \ddot{l}_{t=t_0})^{2/3} y_n.$$

The condition in (20) now looks as follows

$$\Phi^{(3)}|_{t=t_0,\,y=0} = -\alpha_3 l^{(3)}_{t=t_0} H_3 H_2 \Phi_0|_{y=0} = -\mathrm{i} l^{(3)}_{t=t_0} H_4 \Phi_0|_{y=0}.$$

Since in general $\mathrm{d}\,\mathrm{Ai}(y)/\mathrm{d}y|_{y=y_n} \neq 0$, the vanishing of $\Phi^{(3)}|_{t=t_0,\,y=0}$ requires that $l^{(3)}_{t=t_0} = 0$.

In general $\Phi^{(2+k)}|_{t=t_0,\,y=0} = 0$ for $k = 1, 2, \ldots$ when $l^{(2+i)}_{t=t_0} = 0$ for $i = 1, 2, \ldots, k$.

To sum up the above result: unless the function $l(t)$ has the property $l^{(n)}_{t=t_0} = 0$ for $n \geqslant 3$, solutions of the Schrödinger equation will not vanish at $y = 0$ for $t \in \Gamma_t$ even if they did vanish there for $t = t_0$. Since t_0 is arbitrary, the vanishing of all derivatives of Φ at $y = 0$ is possible only if $l(t)$ is a second-order polynomial.

Let us recall that the condition $\Psi(y, t)|_{y=0} = 0$ is a necessary part of the boundary conditions given in (4). Meanwhile exact solutions which were obtained above via the Wei–Norman method as well as all their mutations, WNS, reached by the application of the Baker–Hausdorf formula were valid for arbitrary $l(t)$. Why is it then that they cannot fulfil the boundary conditions? The reason is as follows. If one adds on the right-hand side of (5) a potential-like term $\alpha_5 H_5$, whose role is to sweep the particle away from the negative semi-axis of y (e.g. $\alpha_5 H_5 = V\theta(-y)$, with $\theta(-y)$ being the step function $\theta(-y) = 0$ for $y > 0, \theta(-y) = 1$ for $y \leqslant 0$ and V is a constant; in the limit $V \to \infty$ this term will guarantee the vanishing of Ψ for $y \leqslant 0$), then the algebra of $H_i, i = 1, 2, \ldots, 5$, is not finite any more and the method of Wei–Norman cannot produce in general an effective solution of the equation. The case $\ddot{l} =$ constant is an exception, however. Although adding the term $\alpha_5 H_5$ to the operator H in (15) ($\alpha_5 H_5$ survives the gauge transformation intact) results also in an infinite algebra of time-indepedent operators, in the case when $\ddot{l}$ is a constant we may write the operator $\bar{H} = H + \alpha_5 H_5$ as

$$\bar{H} = \eta_1 L_1 + \eta_2 L_2$$

where

$$L_1 = H_1 \qquad L_2 = (\alpha_2 + \ddot{l})H_2 + \alpha_3 H_3 + \alpha_5 H_5$$

and

$$\eta_1 = \alpha_1 - \tfrac{1}{2}\dot{l}^2 \qquad \eta_2 = 1.$$

Since time-independent operators L_1 and L_2 form a two-dimensional nilpotent algebra, the problem is in principle solvable. The limit $V \to \infty$ may be legitimately replaced in this case by the boundary conditions

$$\forall t : \left\{ \Phi(0, t) = 0 \text{ and } \int_0^\infty |\Phi(y, t)|^2\,\mathrm{d}y = 1 \right\}$$

imposed on the function

$$\Phi(y, t) = \exp\left(-\mathrm{i} \int_{t_0}^t H(t')\,\mathrm{d}t' \right) \Phi_0(y).$$

It is seen that when the function Φ_0 is taken in the form given in (21) the differential equation (15) is compatible with the boundary conditions. One has

$$\Phi(y,t) = \exp\left(-\mathrm{i}\int_{t_0}^{t}(\alpha_1(t') - \tfrac{1}{2}\dot{l}^2(t'))\,\mathrm{d}t'\right)\sum c_n \exp(\mathrm{i}2^{-1/3}(g+\ddot{l})^{2/3}y_n(t-t_0))\Theta_n(y). \tag{23}$$

The operator $U(t,t_0)$, i.e. the one which transforms Ψ, has in this case the form

$$U(t,t_0) = \exp(\mathrm{i}\dot{l}(t)H_2)\exp\left(-\mathrm{i}\int_{t_0}^{t}H(t')\,\mathrm{d}t'\right)\exp(-\mathrm{i}\dot{l}(t_0)H_2). \tag{24}$$

When the function $l(t)$ is quadratic in t, it is only a matter of tedious algebra to show that the above operator reduces to the one given in (8). It is clear from the derivation of (23) that the operator $U(t,t_0)$ given in (24) must act on functions $\Psi(y,t_0) = \exp(\mathrm{i}\dot{l}(t_0)H_2)\Phi_0(y)$. (The case $\ddot{l} =$ constant has been extensively treated in [5].)

Any solution of (3) which vanishes at $y = 0$ and is normalizable on the positive semi-axis of y may always be expanded as

$$\Psi = \sum b_n(t)\Xi_n \tag{25}$$

on the complete set of orthonormal eigenfunctions $\Xi_n(y)$ of the time-independent operator

$$H_0 = -\tfrac{1}{2}\partial_y^2 + gy = \alpha_3 H_3 + \alpha_2 H_2 \tag{26}$$

$$H_0\Xi_n(y) = E_n^0\Xi_n(y) \qquad \Xi_n(0) = 0 \qquad \int_0^\infty |\Xi_n(y)|^2\,\mathrm{d}y = 1$$

and it follows from (22) that $\Xi_n(y) = N_n\mathrm{Ai}((2g)^{1/3}y + y_n)$. In practice Ψ given by (25) can be obtained if the Schrödinger equation (3) is projected onto the basis Ξ_n and the resulting set of differential equations solved for the functions $b_n(t)$.

The fact that—when $l(t)$ is not a simple parabolic function of t—the WNS do not vanish at $y = 0$ during the evolution is detectable when any of the above mentioned solutions (WNS) is projected onto the basis Ξ_n. The resulting b_n^{WNS} do not satisfy the set of equations that must be satisfied by the expansion coefficients b_n of a correct solution (25). It must be so because an expansion of a solution in the basis Ξ_n implies that the solution vanishes for $y \leqslant 0$ at all instants of time. This in turn means that there is in fact an infinite potential acting on the negative semi-axis of y. We remember that the WNS were obtained by omitting this potential and therefore they cannot be legitimately expanded on such a basis during the evolution. For the solution taken in the form given in (13) this fact was already proved in [6].

4. Concluding remark

We believe that this paper throws some new light on the problem of solving Schrödinger equations in cases when Hamiltonians are time-dependent operators and solutions must be normalized in some subspace Ω of the configurational space. It was explained why in these cases, when the Hamiltonian belongs to a finite nilpotent Lie algebra, the known methods of obtaining closed form solutions which work perfectly well in the infinite configuration space are not applicable in a subspace Ω. Basically, the same type of arguments may be applied to a model of a particle in an infinitely deep potential well with a time-dependent width (recent literature on this model may be found in [7]). In this case, when an infinite potential is disregarded, relevant operators form a solvable algebra (not a nilpotent one) and this is also enough for the Wei–Norman method to generate closed form solutions. Once more, however, these solutions will not obey in general the required boundary conditions.

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