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Exact analytical solutions of the Hamiltonian with a squared tangent potential

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In a very recent article (M.G. Marmorino, J. Math. Chem. 32 (2002) 303), exact ground and first-excited state eigensolutions determined by trial and error have been introduced for the one-dimensional Hamiltonian with a constant multiple of a squared cotangent potential $\nu(\nu-1)\cot^2 x$ on the domain $x \in (0,\pi)$. An explicit formula for the full spectrum was then proposed by the help of numerical experiments. In the present study, the results of Marmorino are mathematically justified and generalized by transforming the problem into an equivalent hypergeometric form.

KEY WORDS: Schrödinger equation, exactly solvable Hamiltonians, cotangent and tangent potentials, hypergeometric functions

1. Introduction

The dimensionless Schrödinger equation for a particle of unit mass moving in a potential $V(x)$

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) - E\right]\Psi(x) = 0, \tag{1}$$

whose exact analytical eigensolutions are expressible in terms of elementary or special functions of mathematical analysis, is of significant importance in quantum mechanics. Many of these potentials can be found by perusing the literature [1].

Most recently, exact solutions for a squared cotangent potential (SCP)

$$V(x) = \nu(\nu-1)\cot^2 x, \quad x \in (0,\pi) \tag{2}$$

have been proposed by Marmorino [2] for the real parameter $\nu \geqslant 1$. To be precise, the lowest two eigenvalues and the corresponding eigenfunctions were determined by trial and error. By means of numerical calculations, the complete spectrum was correctly conjectured to be generated by a recursion relation

$$\Lambda_{k+1} - \Lambda_k = 1 \tag{3a}$$

for the Λ_k, which is the difference between two consecutive eigenvalues λ_{k+1} and λ_k. It is clear that (3a) is a linear, first order, non-homogeneous difference equation with constant coefficients, which can be solved explicitly on using the difference of the first two known eigenvalues as an initial condition. After having determined the Λ_k values, the definition

$$\lambda_{k+1} - \lambda_k = \Lambda_k \tag{3b}$$

is then used to find the desired eigenvalues.

In this work, we give mathematical evidence for the exact solutions of the aforementioned system. First we modify the problem so as to get a symmetric structure by shifting the coordinate axis from x to $x - \pi/2$. Hence we now deal with a Hamiltonian with the squared tangent potential (STP)

$$V(x) = \nu(\nu-1)\tan^2 x, \quad x \in \left(-\frac{1}{2}\pi, \frac{1}{2}\pi\right) \tag{4}$$

on the symmetric domain having an obvious reflection symmetry under the replacement of x by $-x$. Since the STP grows unboundedly at the end points of the interval $(-\pi/2, \pi/2)$, the wave function Ψ should possess an appropriately vanishing behaviour at $x = \pm\pi/2$. Note that the energy eigenvalues E, but not eigenfunctions, of the Hamiltonian with the STP on the symmetric interval $(-\pi/2, \pi/2)$ are precisely the same as those of the Hamiltonian with the SCP on the asymmetric interval $(0, \pi)$ considered by Marmorino in [2].

The plan of this paper is as follows. In section 2, we transform the problem into a hypergeometric form. The anti-symmetric states, in which the eigenfunctions are odd functions of the argument x, are treated in section 3. The last section concludes the paper with further remarks and comments.

2. The hypergeometric form of the problem

Let us consider the Schrödinger equation

$$\left[-\frac{d^2}{dx^2} + \nu(\nu-1)\tan^2 x - E(\nu)\right]\Psi(x;\nu) = 0 \tag{5}$$

subject to the boundary conditions

$$\Psi(x;\nu)\Big|_{x=\pm(1/2)\pi} = 0 \tag{6}$$

for each $\nu \geqslant 1$, describing a well potential problem for which a discrete positive spectrum is sure to exist. The reflection symmetry of the system (5)–(6) suggests that the set of spectral points $\{E_k(\nu)\}$, for $k = 0, 1, \ldots,$ can be decomposed into two subsets $\{E_{2k}(\nu)\}, \{E_{2k+1}(\nu)\}$ in such a way that the eigenfunctions corresponding to the even E_{2k} and odd E_{2k+1} parity energy levels are even and odd functions of x, respectively. These are referred to as the symmetric and anti-symmetric states as well, and may be treated separately without any trouble.

In what follows, introducing the substitution

$$\xi = \sin^2 x, \quad \xi \in [0, 1) \tag{7}$$

which is not one-to-one, we can deal only with the even parity states. With (7), we have the operational equivalences

$$\frac{\mathrm{d}}{\mathrm{d}x} \equiv 2\sqrt{\xi(1-\xi)}\frac{\mathrm{d}}{\mathrm{d}\xi} \tag{8a}$$

and

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2} \equiv 4\xi(1-\xi)\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} + 2(1-2\xi)\frac{\mathrm{d}}{\mathrm{d}\xi} \tag{8b}$$

so that the differential equation takes the form

$$\left\{\xi(1-\xi)\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} + \left(\frac{1}{2} - \xi\right)\frac{\mathrm{d}}{\mathrm{d}\xi} + \Delta(\nu, E) - \frac{1}{4}\frac{\nu(\nu-1)}{1-\xi}\right\}\Psi_{\mathrm{S}}(\xi;\nu) = 0, \tag{9}$$

where

$$\Delta(\nu, E) = \frac{1}{4}\big[\nu(\nu-1) + E(\nu)\big] \tag{10}$$

and $\Psi_{\mathrm{s}}(\xi;\nu)$ denotes an eigenfunction which is even in the original variable x when ξ is replaced by $\sin^2 x$.

Next, the regular singularity at $\xi = 1$ of the differential operator in (9) implies the search for a solution of the type

$$\Psi_{\mathrm{s}}(\xi;\nu) = (1-\xi)^a y(\xi;\nu), \quad a \in \mathbb{R}, \tag{11}$$

which gives the possibility of determining the flexible parameter a so as to get rid of the last term in (9) proportional to $(1-\xi)^{-1}$. Actually, if a is a root of the algebraic equation

$$a^2 - \frac{1}{2}a - \frac{1}{4}\nu(\nu-1) = 0 \tag{12}$$

then the differential equation reduces to a Gauss hypergeometric equation

$$\xi(1-\xi)y'' + \left[\frac{1}{2} - (\alpha+\beta+1)\xi\right]y' - \alpha\beta y = 0 \tag{13}$$

for the new dependent variable y, with the parameters α and β satisfying

$$\alpha + \beta = 2a \tag{14a}$$

and

$$\alpha\beta = a^2 - \Delta(\nu, E), \tag{14b}$$

simultaneously. Clearly, the roots of the quadratic equation (12) are $\nu/2$ and $(1-\nu)/2$. For $a = \nu/2$, the hypergeometric equation (13) admits the pair of linearly independent solutions [3]

$$y_1(\xi;\nu) = {}_2F_1\left(\alpha,\beta;\nu+\frac{1}{2};1-\xi\right) \tag{15a}$$

and

$$y_2(\xi;\nu) = (1-\xi)^{(1/2)-\nu}{}_2F_1\left(\frac{1}{2}-\alpha,\frac{1}{2}-\beta;\frac{3}{2}-\nu;1-\xi\right), \tag{15b}$$

where ${}_2F_1(\alpha,\beta;\gamma;z)$ stands for the Gauss hypergeometric function. Recall that this function has the series expansion about $z=0$

$${}_2F_1(\alpha,\beta;\gamma;z) = \sum_{i=0}^{\infty}\frac{(\alpha)_i(\beta)_i}{(\gamma)_i}\frac{z^i}{i!} = 1+\frac{\alpha\beta}{\gamma}\frac{z}{1!}+\frac{\alpha(\alpha+1)\beta(\beta+1)}{\gamma(\gamma+1)}\frac{z^2}{2!}+\cdots \tag{16a}$$

known as the hypergeometric series [3], in which the notation $(p)_i$ is the Pochhammer's symbol standing for

$$(p)_i = p(p+1)\cdots(p+i-1) \tag{16b}$$

with $(p)_0 = 1$.

It is seen from (14) that the parameters α and β in the solutions (15) are written as

$$\alpha = \frac{1}{2}\nu - \sqrt{\Delta(\nu,E)} \tag{17a}$$

and

$$\beta = \frac{1}{2}\nu + \sqrt{\Delta(\nu,E)} \tag{17b}$$

which depend implicitly on the energy eigenvalues of the system. Thus we have the fundamental solutions for the wave function Ψ_s in (11)

$$\Psi_\mathrm{s}^{(1)}(\xi;\nu) = (1-\xi)^{(1/2)\nu}{}_2F_1\left(\alpha,\beta;\nu+\frac{1}{2};1-\xi\right) \tag{18a}$$

and

$$\Psi_\mathrm{s}^{(2)}(\xi;\nu) = (1-\xi)^{(1/2)(1-\nu)}{}_2F_1\left(\frac{1}{2}-\alpha,\frac{1}{2}-\beta;\frac{3}{2}-\nu;1-\xi\right) \tag{18b}$$

for a prescribed $\nu \geqslant 1$.

On the other hand, the boundary conditions in (6) require that the true wave function must vanish as ξ tends towards one, i.e.,

$$\lim_{\xi\to 1}\Psi(\xi;\nu) = 0 \tag{19}$$

for all $\nu \geqslant 1$. However, from (16) we observe that as $\xi \to 1$

$$\Psi_{\mathrm{s}}^{(2)}(\xi;\nu) = (1-\xi)^{(1/2)(1-\nu)}\bigl[1 + O(1-\xi)\bigr] \tag{20}$$

and that it does not remain bounded at $\xi = 1$, where O is the usual big-O notation. Hence, rejecting the second solution in (18b) we find that the desired solution can possibly be

$$\Psi_{\mathrm{s}}(\xi;\nu) = \Psi_{\mathrm{s}}^{(1)}(\xi;\nu) = \mathcal{A}(\nu)(1-\xi)^{(1/2)\nu}{}_2F_1\left(\alpha,\beta;\nu+\frac{1}{2};1-\xi\right), \tag{21}$$

where $\mathcal{A}$ is some normalization constant.

In like manner, it is not difficult to verify that the second root $a = (1-\nu)/2$ of (12) results exactly in the same solution. Furthermore, it is worth noting that, by the trigonometric transformation in (7), both end points of the original domain $(-\pi/2, \pi/2)$ are taken into the point at $\xi = 1$ on the ξ-axis. As a result, the transformed system obeys only one boundary condition. Nevertheless, we may prove that the hypergeometric series in (21) converges for all $\xi \in [0,1]$ and is analytic in each of α and β parameters and, therefore, does represent the physical solution if and only if it consists of a finite number of terms [4, p. 262]. As a matter of fact, such a series terminates to yield simply polynomials in $1-\xi$ of degree k, for $k = 0, 1, \ldots$, if either α or β is equal to $-k$, due to its symmetric structure in the first two parameters. Thus, assuming such an analiticity condition for the hypergeometric function in question that

$$\alpha = -k, \quad k = 0, 1, \ldots \tag{22}$$

we obtain the eigenfunctions

$$\Psi_{\mathrm{s}}(\xi;\nu) := \Psi_{2k}(\xi;\nu) = \mathcal{A}_k(\nu)(1-\xi)^{(1/2)\nu}{}_2F_1\left(-k,\nu+k;\nu+\frac{1}{2};1-\xi\right) \tag{23}$$

corresponding to the even parity energy levels $E := E_{2k}$. In addition, the significance of (22) is that it can be regarded as a quantization condition to determine the E_{2k} for all k. To be more specific, we deduce from (10) and (17a) that

$$-k = \frac{1}{2}\left[\nu - \sqrt{\nu(\nu-1) + E_{2k}(\nu)}\,\right] \tag{24a}$$

which leads to the explicit formula

$$E_{2k}(\nu) = 4k(\nu+k) + \nu, \quad k = 0, 1, \ldots \tag{24b}$$

for the symmetric state eigenvalues valid for all $\nu \geqslant 1$. Returning back to the original variable x we have the symmetric eigenfunctions

$$\Psi_{2k}(x;\nu) = \mathcal{A}_k(\nu)\cos^{\nu} x\,{}_2F_1\left(-k,\nu+k;\nu+\frac{1}{2};\cos^2 x\right) \tag{25}$$

of the Schrödinger Hamiltonian with the STP in (4).

3. Anti-symmetric states

A careful inspection suggests that the anti-symmetric state eigenfunctions, say $\Psi_{\rm as}$, can be expressed in the form

$$\Psi_{\rm as}(x;\nu) = \sin x\,\Phi(x;\nu), \tag{26}$$

where Φ is necessarily an even function of x. It is straightforward to show that if $\Psi_{\rm as}$ is any solution of the Schrödinger equation in (5), then Φ satisfies the differential equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} - 2\cot x\frac{\mathrm{d}}{\mathrm{d}x} + \nu(\nu-1)\tan^2 x + 1 - E(\nu)\right]\Phi(x;\nu) = 0 \tag{27}$$

which at first sight looks more complicated. However, the evenness of Φ implies that the substitution $\xi = \sin^2 x$ in (7) is again appropriate. Therefore, if we make use of the additional operational equivalence

$$\cot x\frac{\mathrm{d}}{\mathrm{d}x} \equiv 2(1-\xi)\frac{\mathrm{d}}{\mathrm{d}\xi} \tag{28}$$

we arrive at the equation

$$\left\{\xi(1-\xi)\frac{\mathrm{d}^2}{\mathrm{d}\xi^2} + \left(\frac{3}{2} - 2\xi\right)\frac{\mathrm{d}}{\mathrm{d}\xi} + \Delta(\nu,E) - \frac{1}{4} - \frac{1}{4}\frac{\nu(\nu-1)}{1-\xi}\right\}\Phi(\xi;\nu) = 0 \tag{29}$$

in the variable ξ. Tracing a very similar procedure to that of section 2, we see that a transformed dependent variable u, where

$$\Phi(\xi;\nu) = (1-\xi)^{(1/2)\nu}u(\xi;\nu), \tag{30}$$

satisfies the Gauss hypergeometric equation

$$\xi(1-\xi)u'' + \left[\frac{3}{2} - \big(\tilde\alpha + \tilde\beta + 1\big)\xi\right]u' - \tilde\alpha\tilde\beta u = 0 \tag{31}$$

whose parameters $\tilde\alpha$ and $\tilde\beta$ are defined by the relations

$$\tilde\alpha = \frac{1}{2}(\nu+1) - \sqrt{\Delta(\nu,E)} \tag{32a}$$

and

$$\tilde\beta = \frac{1}{2}(\nu+1) + \sqrt{\Delta(\nu,E)}, \tag{32b}$$

respectively. By an argument exactly the same as that used for the symmetric states, we set $\tilde\alpha = -k$ and deduce the formula

$$E_{2k+1}(\nu) = (2k+1)(2\nu+2k+1) + \nu, \quad k = 0,1,\ldots \tag{33}$$

for the odd parity states eigenvalues corresponding to the eigenfunctions

$$\Psi_{2k+1}(\xi;\nu) = \mathcal{B}_k(\nu)\sqrt{\xi}(1-\xi)^{(1/2)\nu}{}_2F_1\left(-k,\nu+k+1;\nu+\frac{1}{2};1-\xi\right), \tag{34}$$

where $\mathcal{B}_k$ is a convenient normalization factor. In terms of the original variable x, the anti-symmetric eigenfunctions are given by

$$\Psi_{2k+1}(x;\nu) = \mathcal{B}_k(\nu)\sin x\cos^\nu x\,{}_2F_1\left(-k,\nu+k+1;\nu+\frac{1}{2};\cos^2 x\right) \tag{35}$$

in which the hypergeometric function is a polynomial of degree k in $\cos^2 x$.

4. Concluding remarks

We have elucidated exact analytical solutions of the quantum mechanical eigenvalue problem in (5)–(6) in the form of finite combinations of trigonometric functions, which are valid for all values of the potential constant $\nu \geqslant 1$. First, it is easily shown that the two separate formulas in (24b) and (33) for the even- and odd-indexed energy levels can be combined in a single expression

$$E_k(\nu) = k(2\nu+k)+\nu, \quad k=0,1,\ldots \tag{36}$$

so as to give the full spectrum, which corroborates the somewhat experimental result of [2]. Note the notational connection

$$E_k(\nu) = 2\lambda_{k+1}(\nu), \quad k=0,1,\ldots \tag{37}$$

between the eigenvalues denoted by λ in [2] and those of this work.

Second, taking advantage of having analytical solutions in terms of the Gauss hypergeometric functions, we may derive alternative such solutions by means of certain familiar relations which exist between them. For instance, it follows from the so-called linear transformation formula,

$$\begin{aligned}{}_2F_1(\alpha,\beta;\gamma;z) = {} & C(\alpha,\beta,\gamma)\,{}_2F_1(\alpha,\beta;\alpha+\beta-\gamma+1;1-z)\\ & + C(\gamma-\alpha,\gamma-\beta,\gamma)(1-z)^{\gamma-\alpha-\beta}\\ & \times {}_2F_1(\gamma-\alpha,\gamma-\beta;\gamma-\alpha-\beta+1;1-z),\end{aligned} \tag{38a}$$

with

$$C(\alpha,\beta,\gamma) = \frac{\Gamma(\gamma)\Gamma(\gamma-\alpha-\beta)}{\Gamma(\gamma-\alpha)\Gamma(\gamma-\beta)} \tag{38b}$$

that the hypergeometric factor in (25) is equivalent to

$${}_2F_1\left(-k,\nu+k;\nu+\frac{1}{2};\cos^2 x\right) = C\left(-k,\nu+k,\nu+\frac{1}{2}\right){}_2F_1\left(-k,\nu+k;\frac{1}{2};\sin^2 x\right) \tag{39}$$

since, in this case, the coefficient of the second term in (38a) containing certain gamma functions becomes zero. Hence we may rewrite the symmetric state eigenfunctions in the form

$$\Psi_{2k}(x;\nu) = \widetilde{\mathcal{A}}_k(\nu)\cos^\nu x\,{}_2F_1\left(-k,\nu+k;\frac{1}{2};\sin^2 x\right) \tag{40}$$

now with a hypergeometric function of argument $\sin^2 x$, where $\widetilde{\mathcal{A}}_k$ is some other normalization constant.

If the variable $x + \pi/2$ is inserted back into our results, we then obtain the eigenfunctions of the Hamiltonian with the SCP on the asymmetric domain $(0, \pi)$. Actually, we see from (25) that the symmetric states become

$$\Psi_{2k}\left(x + \frac{1}{2}\pi; \nu\right) = \sin^\nu x\, {}_2F_1\left(-k, \nu + k; \nu + \frac{1}{2}; \sin^2 x\right) \tag{41}$$

up to an inessential constant. For a particular case in which $\nu = 3$, eigenfunctions of the SCP problem were constructed successfully in [2] by means of symbolic computations on *Mathematica*. In this particular case, we notice the relationship

$$\psi_{2k+1} = \mathcal{N}_k \Psi_{2k}\left(x + \frac{1}{2}\pi; 3\right) = \mathcal{N}_k \sum_{j=0}^{k} \frac{(-k)_j (k+3)_j}{j!(7/2)_j} \sin^{2j+3} x \tag{42}$$

for $k = 0, 1, \ldots$, where the ψ_{2k+1} denote the eigenfunctions of [2], which were referred to as the odd-indexed eigenfunctions there. Further, we perceive that exactly the same eigenfunctions are regenerated if the constant $\mathcal{N}_k$ is taken as

$$\mathcal{N}_k = 4^{k+1} \frac{(7/2)_k}{(k+3)_k} \tag{43}$$

for each k. Note also that exploiting the standard trigonometric relation [5, p. 25]

$$\sin^{2m+3} x = \frac{1}{4^{m+1}} \sum_{j=0}^{m+1} (-1)^{m+1+j} \binom{2m+3}{j} \sin(2m - 2j + 3)x \tag{44}$$

we may express our results in terms of $\sin(2j+1)x$ instead of $\sin^{2j+3} x$. For example, we have

$$\psi_1 = \mathcal{N}_0 \Psi_0\left(x + \frac{1}{2}\pi; 3\right) = 4\sin^3 x = 3\sin x - \sin(3x) \tag{45a}$$

for $k = 0$,

$$\begin{aligned} \psi_3 &= \mathcal{N}_1 \Psi_2\left(x + \frac{1}{2}\pi; 3\right) = 14\sin^3 x\left(1 - \frac{8}{7}\sin^2 x\right) \\ &= \frac{1}{2}\sin x + \frac{3}{2}\sin(3x) - \sin(5x) \end{aligned} \tag{45b}$$

for $k = 1$, and

$$\begin{aligned} \psi_5 &= \mathcal{N}_2 \Psi_4\left(x + \frac{1}{2}\pi; 3\right) = \frac{168}{5}\sin^3 x\left(1 - \frac{20}{7}\sin^2 x + \frac{40}{21}\sin^4 x\right) \\ &= \frac{1}{5}\sin x + \frac{3}{5}\sin(3x) + \sin(5x) - \sin(7x). \end{aligned} \tag{45c}$$

for $k = 2$. Observe once again that the coefficients of $\sin(2j+1)x$ in (45) for $j = 0, 1, \ldots, k+1$, reveal the same pattern as recorded in [2, table 3].

Finally, it is an easy task to verify that our results yield the known eigenvalues and eigenfunctions of the particle-in-a-box Hamiltonian, where

$$V(x) = \begin{cases} 0 & \text{for } x \in \left(-\frac{1}{2}\pi, \frac{1}{2}\pi\right), \\ \infty & \text{for } |x| \geqslant \frac{1}{2}\pi, \end{cases} \tag{46}$$

as the limiting case when $\nu = 1$. More general properties of the exact analytical eigenfunctions will now be investigated and reported in due course.

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