Jacobi polynomials and bound states.

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Abstract

In their recent note [J. Math. Chem. 16 (1994) 211 – 215] Ṣimṣek and Yalçin claim the elementary exact solvability of an s-wave radial Schrödinger equation with a shifted Pöschl-Teller potential. We re-derive and correct their formulae and weaken their conclusions: Their Jacobi polynomial wavefunctions do not comply with a boundary condition in the origin. After its inclusion, at most a triplet of their quasi-exact bound states may survive, and we have to return to non-polynomial hypergeometric wavefunctions $\psi(r)$ in general.

1 Introduction

In applied quantum mechanics, an analysis of complicated systems is usually based on an approximate solution of dynamical equations. A majority of these equations must be solved numerically. The local and central potential models are an exception: Their use enables us to convert the realistic three-dimensional Schrödinger equation (i.e., a partial differential equation

$$-\frac{\hbar^2}{2m}\triangle\Psi(\vec{r})+V(\vec{r})\Psi(\vec{r})=E\Psi(\vec{r}) \tag{1}$$

with $V(\vec{r}) \equiv V(|\vec{r}|)$) into an infinite set of its ordinary differential (so called radial) descendants

$$-\frac{\mathrm{d}^2}{\mathrm{d}r^2}\psi(r)+\frac{\ell(\ell+1)}{r^2}\psi(r)+V(r)\psi(r)=E\psi(r), \quad r\in(0,\infty), \tag{2}$$

numbered by the angular momentum quantum number $\ell = 0, 1, \ldots$.

An exact analytic solvability of the full system (2) is restricted to a few exceptional forces ([1], p. 417). Its truncation to a finite subset ($\ell \leq \ell_{\max}$) facilitates the solution and suffices for the majority of phenomenological purposes. Even the most drastic restriction of eq. (2) to the lowest partial wave (so called s-wave approximation, $\ell = \ell_{\max} = 0$) proves well motivated (cf., e.g., [2]). Recently, Ṣimṣek and Yalçin claimed the exact and elementary solvability of the four-parametric s-wave family

$$-\frac{\mathrm{d}^2}{\mathrm{d}r^2}\psi(r)-\frac{A\exp(-2ar)}{[1+b^2\,\exp(-2ar)]^2}\psi(r)+\frac{B\exp(-2ar)}{[1-b^2\,\exp(-2ar)]^2}\psi(r)=E\,\psi(r) \tag{3}$$

of radial Schrödinger equations for bound states (cf. eq. (17) in ref. [3]). In accord with their construction, energies E_n, $n = 0,\ 1,\ \ldots,\ n_{\max}$ become expressed by a closed formula,

$$E_n=-a^2\,[\beta]^2\,, \qquad \beta=\beta_n=\gamma-\alpha-2n-1, \tag{4}$$

$$\alpha=\frac{1}{2}\sqrt{1+\frac{B}{a^2b^2}}, \qquad \gamma=\frac{1}{2}\sqrt{1+\frac{A}{a^2b^2}}$$

(cf. eq. (21) in ref. [3]), etc. In the present paper, we intend to show that (and why) the Ṣimṣek's and Yalçin's result is incorrect. Marginally, we shall outline how their method might be amended.

2 Bound states in the standard approach

2.1 Hypergeometric solutions

Let us re-define the parameter $b^2 = \exp(-2\delta)$ with $\delta \in (-\infty, \infty)$ and re-write the Șimșek's and Yalçin's s-wave potential in the shifted Pöschl-Teller form

$$V(r) = \frac{e^{2\delta}}{4}\left[-\frac{A}{\cosh^2(ar+\delta)} + \frac{B}{\sinh^2(ar+\delta)}\right], \qquad r \in (0,\infty). \tag{5}$$

For the real and, say, nonnegative b's (i.e., $b = \exp(-\delta)$), this interaction exhibits a strong, impenetrable singularity at $r = -\delta/a$. For the real a's, we may restrict our attention to nonnegative δ's, therefore.

First, we re-scale the coordinates and shift the origin, $r' = ar + \delta$. After such a re-arrangement, wavefunctions remain uninfluenced, $\psi(r) \to \chi'(r')$, but the energy and the couplings change. In the resulting 'primed' differential equation (3),

$$-\frac{d^2}{dr'^2}\chi'(r') - \frac{A'}{\cosh^2 r'}\chi'(r') + \frac{B'}{\sinh^2 r'}\chi'(r') = E'\,\chi'(r'), \quad r' \in (\delta,\infty) \tag{6}$$

with $E' = E/a^2$, $A' = A\exp(2\delta)/4a^2$ and $B' = B\exp(2\delta)/4a^2$, we may put $A' = \gamma^2 - \frac{1}{4} = 4\mu(\mu - \frac{1}{2})$, $B' = \alpha^2 - \frac{1}{4} = 4\nu(\nu - \frac{1}{2})$ and $E' = -4\kappa^2$ (with, say, non-negative μ, ν and κ) and see that our class of interactions forms a three-parametric family in effect, $V(r) = V^{(\alpha,\gamma,\delta)}(r)$.

The second change of variables,

$$y = \cosh^2 r', \quad \chi'(r') = y^\mu (y-1)^\nu \varphi(y) \tag{7}$$

converts eq. (6) into a Gauss' hypergeometric equation

$$y(y-1)\frac{d^2}{dy^2}\varphi(y) + [(2\mu+2\nu+1)y - 2\mu - 1/2]\,\frac{d}{dy}\varphi(y) + [(\mu+\nu)^2 - \kappa^2]\varphi(y) = 0. \tag{8}$$

Hence, the Șimșek's and Yalçin's bound-state problem proves solvable in terms of the hypergeometric power series ${}_2F_1(s,t;c;y)$ with parameters

$$s = \mu+\nu+\kappa, \quad t = \mu+\nu-\kappa, \quad c = 2\mu + \frac{1}{2}. \tag{9}$$

Thus, an explicit general representation of solutions $\varphi(y)$,

$$C_1\ y^{-s}\ {}_2F_1(s,d;e;1-1/y) + C_2\ y^{-f}\ (y-1)^{1-e}\ {}_2F_1(f,1-t;2-e;1-1/y),$$
$$d = s-c+1 = -\mu+\nu+\kappa+1/2,$$
$$e = s+t-c+1 = 2\nu+1/2, \qquad f = c-t = \mu-\nu+\kappa+1/2 \tag{10}$$

(ff. 15.5.11 - 15.5.12 in [4]) is suitable for analysis near $y \approx 1$, while the use of formula

$$\varphi(y) = D_1\ y^{-s}\ {}_2F_1(s,d;2\kappa+1;1/y) + D_2\ y^{-t}\ {}_2F_1(t,1-f;-2\kappa+1;1/y) \tag{11}$$

(cf. [4], ff. 15.5.7 - 15.5.8) may prove more adequate at large distances, $y \to \infty$.

2.2 Boundary conditions

In accord with textbooks, bound states (pertaining to any eq. (2)) may be constructed as superpositions of an arbitrary pair of independent solutions,

$$\psi^{(BS)}(r) = C_1\psi_1(r) + C_2\psi_2(r) \tag{12}$$

(cf., e.g., [5]). The normalizability of these wavefunctions must be required, $\|\psi^{(BS)}\| < \infty$. At $\ell \geq 1$, this normalizability may be shown equivalent to a pair of boundary conditions. Thus, one may use the asymptotic boundary condition

$$\psi(r_\infty) = 0, \qquad r_\infty \to \infty, \tag{13}$$

complemented by its ℓ-dependent threshold counterpart

$$\psi(r_0) \sim r^{\ell+1}, \qquad r_0 \sim 0. \tag{14}$$

Even for sufficiently well-behaved potentials, the situation is slightly different in s-waves where the unphysical solution remains well behaved near the origin, $\psi_{(\text{irregular})}(r_0) \sim r^{-\ell}$, $r_0 \sim 0$. Its elimination (14) has, definitely, nothing to do with normalizability (cf. [1], p. 332, or [5] for a more thorough explanation). This is, presumably, the hidden reason for a complete omission of eq. (14) from the analysis in ref. [3] and, hence, a formal core of our present comment.

In the computations, the pair of restrictions (13) and (14) is rarely used to specify both the coefficients C_i and the binding energy at once. More often, a component (say, $\psi_1(r)$) is chosen as compatible with boundary condition (14) in the origin. Only then, the resulting (so called regular) solution $\psi_{(\text{reg.})}(r)$ is subdued to the second constraint (13). This defines the energies in a way exemplified in sect. 3.1 below.

Alternatively, one may fix the asymptotics (13) and construct the so called Jost solutions $\psi_{(\text{Jost})}(r)$ first. In our present example, the correct asymptotic behaviour pattern

$$\varphi_{(\text{Jost})}(y) \approx y^{-s}, \qquad y \gg 1 \tag{15}$$

will be most easily separated from the unphysical $\varphi_{(\text{unphys.})}(y) \approx y^{-t}$. In the not too singular cases, the pertaining s-wave eigenvalue condition (14) then reads

$$\psi_{(\text{Jost})}(0) = 0, \qquad \ell = 0. \tag{16}$$

Its use has thoroughly been discussed in our older work [6].

The manifestly Jost wavefunctions of Ṣimṣek and Yalçin offer another suitable application area – after all the changes of variables, equation (16) implies that we must postulate

$$\varphi_{(\text{Jost})}(y_0) = 0, \qquad y_0 = \cosh^2 \delta, \qquad \delta > 0 \tag{17}$$

in all the shifted "non-Pöschl-Teller" cases. Incidentally, the Pöschl-Teller limit $\delta \to 0$ induces a strong singularity in eq. (3) itself. A modified boundary condition

$$\varphi_{(\text{Jost})}(y_0) < \infty, \qquad y_0 \to 1, \qquad \nu > 1/4, \qquad \delta = 0 \tag{18}$$

must be employed near the threshold in such a case ([1], p. 392).

3 Bound states as Jacobi polynomials

3.1 The Pöschl-Teller degeneracy, $\delta = 0$

Irrespectively of the value of δ, boundary conditons should be met via a variation of the above general solutions of the differential Schrödinger equation (8). At $\delta = 0$, an undesirable singularity of the general solution (10) in the origin stems from the negative exponent $1 - e < 0$ in its second component. This (i.e., eq. (18)) implies that we must pick up $C_2 = 0$ there.

An analytic-continuation re-arrangement of the function $y^s \varphi_{(\mathrm{reg.})}(y)/C_1$,

$$\frac{\Gamma(e)\Gamma(-2\kappa)}{\Gamma(1-f)\Gamma(t)}\, {}_2F_1(s, d; 2\kappa+1; 1/y) + y^{2\kappa}\frac{\Gamma(e)\Gamma(2\kappa)}{\Gamma(s)\Gamma(d)}\, {}_2F_1(1-f, t; 1-2\kappa; 1/y) \quad (19)$$

([4], f. 15.3.6) describes the correct asympotic behaviour violated by the second component. Its suppression (13) may only be mediated by the choice of a negative argument in a Γ-function in the denominator. There is just one such choice, $d = -n,\ n = 0, 1, \ldots$, and it quantizes the energies precisely in the way prescribed by eq. (4) above. The hypergeometric formula for wavefunctions degenerates to a polynomial,

$$\varphi(y) \sim y^{-s}\, {}_2F_1(2\mu - n - 1/2, -n; 2\kappa+1; 1/y) \sim y^{-s}\, {}_2F_1(s, -n; e; 1 - 1/y) \quad (20)$$

and returns us back to the well known Pöschl-Teller bound states ([2], p. 89).

In a slight modification of the latter construction, we start from the Jost solution (11). Re-arranging the $D_2 = 0$ series as an analytic-continuation superposition

$$\frac{y^s\varphi(y)}{D_1} = \frac{\Gamma(1-e)\Gamma(1+2\kappa)}{\Gamma(f)\Gamma(1-t)}\, {}_2F_1(s, d; e; 1 - 1/y) +$$

$$+ (1 - 1/y)^{1-e}\frac{\Gamma(1-e)\Gamma(2\kappa+1)}{\Gamma(s)\Gamma(d)}\, {}_2F_1(1-t, f; 12 - e; 1 - 1/y) \quad (21)$$

([4], f. 15.3.6), we notice that the second term exhibits an irregular behaviour at $\delta = 0$. Its suppression leads to the same quantization rule as above.

3.2 The shifted Pöschl-Teller potentials, $\delta > 0$

Due to a certain hidden symmetry of hypergeometric functions, **all** the $\delta = 0$ bound states became expressible in terms of elementary Jacobi polynomials. In several independent contexts ranging from analytic considerations up to the formalism of supersymmetric quantum mechanics [7], one would not really expect an extension of such a Jacobi-solvability phenomenon beyond the already known (so called shape invariant [8]) class of potentials. Nevertheless, a partial, incomplete generalization does not seem excluded.

At $\delta > 0$, condition (16) has to be satisfied at $y = \cosh^2 \delta$,

$$ {}_2F_1(s, d; 2\kappa + 1; 1/\cosh^2 \delta) = 0. \tag{22} $$

Both components of eq. (21) may now contribute equally well. Whenever the singularity $\delta^{1-4\nu}$ in the numerator of the second component remains finite, it may be compensated and regularized by a large value of the function $\Gamma(d) = O(1/\triangle)$ with a perturbed integer argument $d = -N + \triangle$ in the denominator. Thus, we encounter the loss of polynomiality and the left hand side remains an infinite series. The roots $\kappa = \kappa(\delta)$ must be determined numerically. At the smallest δ's, the compensation mechanism with $\triangle = O(\delta^{4\nu-1})$ might also be used as a starting point of perturbative constructions.

3.2.1 The "forgotten" boundary condition

Let us accept now the point of view of Ṣimṣek and Yalçin and assume that a certain Jacobi polynomial represents a physical solution at $\delta \neq 0$ as well. Such an assumption need not necessarily contradict our previous perturbative argumentation – we must only fine tune the parameters and preserve the termination condition unchanged, $\triangle = 0$. In such a case, equation (20) extends its validity to shifted potentials and, in the Ṣimṣek's and Yalçin's notation, we just **postulate**

$$ \chi(r) = \mathcal{N} u^{\beta} (1 - u^2)^{(\alpha+1/2)/2} P_n^{(\alpha,\beta)}(2u^2 - 1). \tag{23} $$

Here, P denotes a Jacobi polynomial,

$$P_n^{(\alpha,\beta)}(x) = 2^{-n} \sum_{m=0}^{n} \begin{pmatrix} n+\alpha \\ m \end{pmatrix} \begin{pmatrix} n+\beta \\ n-m \end{pmatrix} (x-1)^{n-m} (x+1)^m \tag{24}$$

(cf. [4], ch. 22) and the range of the new coordinate remains finite,

$$u = u(r) = \frac{2b \exp(-ar)}{1 + b^2 \exp(-2ar)}, \quad b < 1.$$

On the occasion, two typographical errors are revealed in the original elementary formula for wavefunctions as printed, incorrectly, in ref. [3] under the number of eq. (22) [9].

Let us now analyse the condition of polynomiality $\triangle = 0$ in more detail. We have $u(r) \to 0$ near $r \to \infty$ and, since

$$P_n^{(\alpha,\beta)}(2u^2 - 1) \to P_n^{(\alpha,\beta)}(-1) = (-1)^n \begin{pmatrix} n+\beta \\ n \end{pmatrix} \tag{25}$$

we get the correct asymptotic r-dependence (13) of the polynomial $\chi(r)$'s. Near the origin, Jacobi polynomials differ from $\chi(r)$ by an irrelevant nonzero factor,

$$0 < u(0) = 1/\cosh\delta < 1, \quad 1 > 1 - [u(0)]^2 = (\sinh\delta/\cosh\delta)^2 > 0. \tag{26}$$

This reduces the second, threshold boundary condition to the relation

$$P_n^{(\alpha,\beta)}\left(\frac{1 - \sinh^2\delta}{\cosh^2\delta}\right) = 0, \quad \delta > 0 \tag{27}$$

which interrelates, polynomially, parameters $\gamma = \gamma(a, b, A)$, $\alpha = \alpha(a, b, B)$ and $\omega = \sinh^2\delta(b)$ at each particular value of n,

$$\sum_{m=0}^{n} \begin{pmatrix} n+\alpha \\ m \end{pmatrix} \begin{pmatrix} \gamma - \alpha - n - 1 \\ n-m \end{pmatrix} (-\omega)^{n-m} = 0 \tag{28}$$

We may conclude that each Şimşek's and Yalçin's (corrected) elementary solution (23) represents a bound state if and only if the implicit eq. (28) relates its shift parameter $b < 1$ to the couplings A and B and to the scale parameter a in the underlying (in the language of ref. [10], "quasi-exactly solvable") Schrödinger equation (3).

3.2.2 The quasi-exact solutions

At all the nonzero shifts $\delta > 0$, one may insist on the polynomiality of wave-functions at a cost of fixing parameters in the underlying potential. In the literature, such a solvability has been studied quite extensively [10] – in our $V = V^{(\alpha,\gamma,\delta)}(r)$, we shall hardly find more than three separate bound states in the exact Jacobi polynomial form. Seemingly, one must even search for the necessary roots of eq. (28) numerically. In our final remark, let us show that a non-numerical solution of the Jacobi-solvability equations (28) remains feasible, at the first few truncations n at least.

Our first (obvious and negative) observation concerns the absence of any real roots of eq. (28) at $n = 0$: One simply has $P_0^{(\alpha,\beta)}(x) \equiv 1$ identically. In contrast, the subsequent $n > 1$ physical boundary conditions (28),

$$\begin{gathered} 1+\alpha-(\gamma-\alpha-2)\omega=0, \\ (2+\alpha)(1+\alpha)-2(2+\alpha)(\gamma-\alpha-3)\omega+(\gamma-\alpha-3)(\gamma-\alpha-4)\omega^2=0, \\ \ldots \end{gathered} \tag{29}$$

provide the first few "dependent" couplings $\gamma = \gamma_j(\alpha, \omega, n)$, $j = 1, 2, \ldots, n$ in a closed form,

$$\begin{gathered} \gamma_1(\alpha,\omega,1)=2+\alpha+(1+\alpha)/\omega, \\ \gamma_1(\alpha,\omega,2)=7/2+\alpha+(2+\alpha)/\omega-\sqrt{1/4+(2+\alpha)(1/\omega+1/\omega^2)}, \\ \gamma_2(\alpha,\omega,2)=7/2+\alpha+(2+\alpha)/\omega+\sqrt{1/4+(2+\alpha)(1/\omega+1/\omega^2)}, \\ \ldots\,. \end{gathered} \tag{30}$$

They remain real and positive (cf. also their next, $n = 3$ sample in Table 1). This proves the existence of the exceptional Şimşek's and Yalçin's Jacobi-polynomial bound states at $\delta \neq 0$, and illustrates also the last and "missing" details of their construction.

A combination of the first two truncations $n = 1$ and $n = 2$ leads to the coupled system of equations (cf. (29)) and gives a mutual compatibility condition

$$\omega = \frac{1+\alpha}{2}, \qquad n_1 = 1,\ n_2 = 2. \tag{31}$$

The real-number nature of this root proves the existence and illustrates the form of a doublet of the elementary Ṣimṣek's and Yalçin's bound states at the corresponding $\delta = \delta(\omega)$. The problem of doublets acquires a slightly simplified form at the special value of $\omega = \sinh^2 \delta = 1$. Under this choice, a systematic analysis of the pair of equations

$$P_{n_a}^{(\alpha,\beta)}(0) = 0, \qquad P_{n_b}^{(\alpha,\beta)}(0) = 0 \tag{32}$$

enables us to re-write the second row in Table 1 exactly,

$$\gamma_1(\alpha, 1, 3) = 2\alpha + (17 - \sqrt{73 + 24\alpha})/2,$$
$$\gamma_2(\alpha, 1, 3) = 2\alpha + 7, \qquad \gamma_3(\alpha, 1, 3) = 2\alpha + (17 + \sqrt{73 + 24\alpha})/2.$$

The simplest possible triplet choice of $n_1 = 1,\ n_2 = 2$ and $n_3 = 3$ provides, after an analogous algebra, the three non-numerical and real roots $\alpha = -1,\ \alpha = -2$ and $\alpha = -3$. Unfortunately, they are negative and, hence, unacceptable. The existence of triplets remains an open question.

4 Summary

The polynomiality of solutions of Schrödinger-type equations (which is, in itself, formally interesting, e.g., due to its relationship to some underlying Lie-algebraic structures [11]) need not necessarily imply their applicability in quantum mechanics. We have seen that a due care must be paid to the s-wave boundary conditions in the origin. After their proper incorporation, we have shown that only a few Ṣimṣek – Yalçin "exact" solutions survive: For the related potential, certain couplings must be determined as roots of complicated algebraic equations and cease to be arbitrary. Moreover, all the remaining non-exceptional bound states must still be constructed via an appropriate standard infinite Taylor series technique or, at best, in terms of some suitable – here: Gauss hypergeometric – special functions.

Table 1. The triple roots $\gamma = \gamma_{1,2,3}(\alpha, \omega, 3)$ of eq. (28) – a sample.

ω	$\alpha = 0.1$			$\alpha = 1$			$\alpha = 10$		
0.1	8.439	28.71	71.15	13.85	38.71	85.44	83.32	137.9	213.8
1	4.358	7.200	13.04	5.576	9.000	15.42	19.65	27.00	37.35
10	4.102	5.203	6.924	5.007	6.167	8.026	14.18	15.97	18.75

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