The conditionally exactly solvable potentials:  
A misunderstanding

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Abstract

We detect an omission in the paper “Conditionally exactly soluble class of quantum potentials” by A. de Souza Dutra [Phys. Rev. A 47 (1993) R2435]. There, two strongly singular s—wave bound state problems have been claimed completely solvable in closed form. Unfortunately, all the displayed wave functions represented merely asymptotically correct (so called “Jost”) solutions and did not satisfy the appropriate threshold boundary condition. We show that the incorporation of its standard form only leads to a very partial exact solvability at a single energy and for special couplings.
For the two strongly singular $s$–wave potentials given, in the units $\hbar = 2\mu = 1$, by the formulae

$$V_1(r) = \frac{A}{r} + \frac{B}{r^{1/2}} + \frac{G}{r^2}, \quad G = G_0 = -\frac{3}{16},$$

(1)

and

$$V_2(r) = A\frac{r^{2/3}}{r} + \frac{B}{r^{2/3}} + \frac{G}{r^2}, \quad G = g_0 = -\frac{5}{36},$$

(2)

A. de Souza Dutra [1] offered the explicit elementary wave functions as well as closed formulae for all their bound-state energies. One of the three couplings is not free: This entitled him to coin their “conditionally” exactly soluble (CES) status. In what follows we intend to demonstrate that in the sense of the Ushveridze’s monograph [2] both these forces $V_{1,2}(r)$ only remain partially solvable at certain specific values of the energies $E$ and couplings $B$.

Our present main point is that all the solutions presented in ref. [1] still have to satisfy an appropriate and, for reasons to be made understandable here, forgotten boundary condition in the origin. Indeed, it is well known that for a central potential, Schrödinger equation

$$-\nabla^2 \Psi(\vec{r}) + V(|\vec{r}|)\Psi(\vec{r}) = E\Psi(\vec{r}),$$

degenerates to an infinite set of the ordinary (often called radial) decoupled differential equations

$$-\frac{d^2}{dr^2}\psi(r) + \frac{\ell(\ell+1)}{r^2}\psi(r) + V(r)\psi(r) = E\psi(r), \quad \ell = 0, 1, \ldots$$

(3)

for the separate angular-momentum components of the whole original wave function. The Newton’s excellent review [3] summarizes the details. Under the assumption of the analyticity of $V(r)$ in the origin it shows that and why the standard physical requirement of normalizability of bound states $||\Psi(\vec{r})|| < \infty$ is strictly equivalent to the integrability of their partial waves,

$$\psi(r) \in L_2(0, \infty).$$

(4)

For $\ell = 1, 2, \ldots$ the unphysical component $\psi_{irregular}(r) \approx r^{-\ell}$ of the general threshold solution of eq. (3) is manifestly non-integrable near $r \approx 0$. 

In the $s$–wave with $\ell = 0$ a more subtle argumentation is needed [3]. In practice, the subtlety is usually avoided by the replacement of eq. (4) by the boundary condition

$$\lim_{r \to 0} \psi(r) = 0.$$ (5)

Even when we solve the ordinary harmonic oscillator the latter boundary condition in the origin offers a more straightforward recipe for numerical calculations. Let us repeat: for analytic potentials, eqs. (4) and (5) are equivalent but the proof [3] of their equivalence immediately fails for the “very next” non-analytic $V(r) \approx G r^{-2}$, $r \approx 0$, say, in the Kratzer’s solvable phenomenological model [4] with $G \neq 0$ etc. One must re-analyze the whole quantization procedure anew, even for harmonic oscillator at $G \to 0$ [5].

For all the similar singular forces with the finite limit in eq. (3),

$$G = \lim_{r \to 0} r^2 V(r) \neq 0$$

we have to re-define the dominant singularity $\ell(\ell + 1) + G = \mathcal{L}(\mathcal{L} + 1)$. The new parameter $\mathcal{L} = \sqrt{(\ell + \frac{1}{2})^2 + G - \frac{1}{4}}$ enters then the modified threshold solutions $\psi_{\text{regular}}(r) \approx r^{\mathcal{L} + 1}$ and $\psi_{\text{irregular}}(r) \approx r^{-\mathcal{L}}$. The irregular one is eliminated as manifestly violating the normalizability (4) at $\mathcal{L} \geq 1/2$.

The latter bound means $G \geq 3/4$ in $s$–wave with $\ell = 0$. Below such a strength of repulsion the Hamiltonian ceases to be self-adjoint. The conclusion is strongly counter-intuitive. Mathematically, the problem is serious. First spotted and analyzed by Case [6], it means that at $G < 3/4$, the textbook quantization of the Kratzer-like singular models is not unique at all. A more detailed discussion may be found in the literature (cf., e.g., [7] or [8]). In its light, physics community currently accepts a unique way of quantization which is, mathematically speaking, a mere regularization. It is often supported by the various sufficiently robust ad hoc arguments (cf., e.g., [5] on pp. 157 and 167 or ref. [9]).

For our present purposes, in the physical language of textbook [10], the correct recipe may be formulated as follows.
• In the domain of a weak repulsion we distinguish between the physical
\(\psi_{\text{regular}}(r) \approx r^{L+1}\) and unphysical \(\psi_{\text{irregular}}(r) \approx r^{-L}\). As long as both of them remain normalizable, we impose an extra, stronger boundary condition in the origin,

\[
\lim_{r \to 0} \psi(r) = 0, \quad G \in (0, 3/4).
\] (6)

It coincides with (5) but its mathematical meaning of a convenient choice of the most plausible self-adjoint extension is different.

• In the domain of weak attraction, both solutions \(\psi_{\text{regular}}(r) \approx r^{L+1}\) and \(\psi_{\text{irregular}}(r) \approx r^{-L}\) are compatible with eq. (6). In a sensible physical theory which distinguishes between the two, the replacement of eq. (6) by an even stronger artificial constraint is needed,

\[
\lim_{r \to 0} \psi(r)/\sqrt{r} = 0, \quad G \in (-1/4, 0).
\] (7)

• Below the lower bound \(G \leq -1/4\) one cannot prevent the spectrum from collapse by any means. Particles would definitely fall in the origin.

We may summarize: In practice, bound state solutions of the Schrödinger differential eq. (3) may be constructed in two ways, namely,

• [RS] as the regular solutions \(\psi_{\text{regular}}(r)\) constrained by the asymptotic normalizability condition

\[
\psi_{\text{regular}}(R) = 0, \quad R \to \infty;
\]

• [JS] from the so called Jost solutions \(\psi_{\text{Jost}}(r)\), always exhibiting the square-integrable asymptotic decrease by definition.

The former regular-solution approach [RS] proves useful within the framework of the standard Taylor series method [11] and in non-numerical context [12]. Schrödinger equation (3) becomes converted into the exactly solvable two-term recurrences at \(q = 0\) (harmonic oscillator), into the three-term recurrences at
$q = 1$ (sextic forces) etc [13]. Rather unexpectedly, for all the positive integers $q = 1, 2, \ldots$, a few bound states may still appear in an exact polynomial (i.e., terminating Taylor-series) form. An explicit construction of these exceptional elementary states is based on the solution of the Magyari’s nonlinear algebraic equations [14]. They determine a few energy levels exactly and restrict also the free variability of the available couplings.

In the latter context, potentials $V_{1,2}(r)$ exhibit a certain incomplete dynamical symmetry and play an exceptional role as quasi-exactly solvable in a certain narrower sense (cf. ref. [2] for more details). This would make the ambitious conclusions of ref. [1], if they were all true, even more important.

Their analysis must be based on the alternative option [JS] which requires the threshold boundary condition (5), (6) or (7) [7]. This is a core of our present message. For the particular forces (1) and (2) such an approach has already thoroughly been tested numerically in ref. [9]. The Liouvillian [15] change of variables $r \rightarrow x = r^{\text{const}}$ and $\psi(r) \rightarrow x^{\text{const}} \chi(x)$ has been employed there. As long as it leaves the form of the Schrödinger equation unchanged, it reduces all the bound-state problems with forces of the type (1) and (2) to their “canonical” equivalents with polynomial potentials

$$V_T(x) = ar^{-2} + br^2 + cr^4 + \ldots + y r^{4q} + z r^{4q+2}, \quad a > -1/4. \quad (8)$$

On this basis, we may easily deduce the leading-order solutions (near the origin) also for our singular potentials $V_{1,2}(r)$ of eqs. (1) and (2),

$$\psi_{1,\text{regular}}(r) \sim r^{3/4}, \quad \psi_{1,\text{irregular}}(r) \sim r^{1/4},$$
$$\psi_{2,\text{regular}}(r) \sim r^{5/6}, \quad \psi_{2,\text{irregular}}(r) \sim r^{1/6}.$$  
This is to be compared with the Dutra’s wave functions: Say, for potential $V_1(r)$ we may quote equation Nr. (9) from [1],

$$\psi_1^{(D)}(r) = C r^{1/4} \exp \left[ -\frac{1}{2} \beta^2 \left( r^{1/2} - \frac{B}{2E} \right)^2 \right] H_n \left( \beta \left( r^{1/2} - \frac{B}{2E} \right) \right). \quad (9)$$
Its energies $E = -\beta^4/4$ are parametrized by $\beta = \beta_n$ and numbered by an integer $n = 0, 1, \ldots$. The formula also contains a certain normalization constant $C = C_n$ and Hermite polynomials $H_n(x)$. We immediately detect an inconsistency of the latter two equations near the origin.

Similar observation is also made for $\psi_2(r)$ from equation Nr. (13) in [1]: None of the Dutra’s wave functions satisfies the physical boundary condition (7). An explanation of this obvious misunderstanding is in fact not too difficult: The solutions were merely constrained by the too weak (though, in practice, much more frequently encountered) and, hence, inapplicable threshold condition (5). We may summarize that the inconsequent use of the boundary conditions would lead to a physically absurd spectrum covering the whole real line, $E \in (-\infty, \infty)$.

The Dutra’s “non-anonymous” (i.e., Hermite-polynomial) solutions have already evoked a non-negligible response in the current literature. As an example one might quote the paper [16]. Its authors relied on the physical correctness of the Dutra’s argumentation and were misguided in their mathematical appreciation of the role of supersymmetry in the similar problems. Still, the majority of their argument remains valid. Hence, let us show, in the conclusion, how the Dutra’s exceptional solutions could be “saved” for similar applications.

Obviously, one has to incorporate simply the necessary constraint (7). An inspection, say, of our sample eq. (9) reveals that $\psi^{(D)}_1(r)$ satisfies condition (7) if and only if its Hermite-polynomial component acquires an exact nodal zero in the origin. In terms of the known numbers $X = X(n, k)$ (calculated as the $k$–th nontrivial zeros of $H_n(X)$, cf. Table 1) this requirement, unfortunately, fixes the non-Coulombic coupling as a function of the energy $E = -\beta^4/4$,

$$B = \frac{1}{2} X \beta^3 \neq 0.$$

(10)

This makes both these values coupled to the additional (in fact, Magyari’s [14]) constraint. As a cubic equation for the energy $E$ it appears under Nr. (8) in ref. [1]. This algebraic selfconsistency condition must be combined with eq.
(10). The resulting polynomial equation in $\beta$ (of twelfth degree!) is easily factorized in closed form. Its real roots we need are

$$\beta = \beta(n, k) = 2 \sqrt{-A \over 2n + 1 - X^2(n, k)}.$$

They all exist for any $A < 0$. This is an important conclusion: let us note that eq. Nr. (8) of ref. [1] re-appears as equation Nr. (16) in ref. [16], etc.

For illustration, let us finally fix the scale $A = -1$ and display the first few non-numerical specifications of energies $E = -\beta^4$ and their couplings (10) in Table 2. The same parameters are to be used also in the definition (9) of the correct bound-state wave function. *Mutatis mutandis*, the entirely parallel “return to validity” applies also to $\psi^{(D)}_{1,2}(r)$ in [1]. We omit the details here, re-emphasizing only that both the Dutra’s expressions $\psi^{(D)}_{1,2}(r)$ are elementary and still satisfy the Schrödinger differential equation, exhibiting also the correct asymptotic behaviour. Thus, we may return, say, to the paper by Dutt et al [17], originally motivated by ref. [1] as well. In the light of our present notes, the importance of the latter paper increases: Its authors have, involuntarily, found and constructed the first CES example in one dimension!

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Table 1. Non-vanishing zeros $X = X(n, k)$
of the first few Hermite polynomials $H_n(X)$.

| $n$ | 0 | 1 | 2 | 3 | 4 | 5 |
|-----|---|---|---|---|---|---|
| $k$ | 4 | 3 | 2 | 1 | 4 | 5 |

Table 2. Parameters of the first few simplest quasi-exact states in $V_1(r)$.

$M$ counts nodes in $\psi_1(r)$: $M = 0$ means ground state, etc.

| $M$ | $n$ | $k$ | fixed coupling $B' = B/8$ | binding energy $E$ |
|-----|-----|-----|--------------------------|-----------------|
| 0   | 2   | 1   | $\sqrt{1/9^3}$          | $-(4/9)^2$      | $\sim -0.197$ |
|     | 3   | 1   | $\sqrt{3/11^3}$         | $-(4/11)^2$     | $\sim -0.055$ |
|     | 4   | 1   | $\sqrt{(3 + \sqrt{6})/(15 - \sqrt{6})^3}$ | $-[4/(15 + \sqrt{6})]^2$ | $\sim -0.029$ |
|     | 5   | 1   | $\sqrt{(5 + \sqrt{10})/(17 - \sqrt{10})^3}$ | $-[4/(17 + \sqrt{10})]^2$ | $\sim -0.018$ |
| 1   | 2   | 2   | $-\sqrt{1/9^3}$         | $-(4/9)^2$      | $\sim -0.132$ |
|     | 4   | 2   | $\sqrt{(3 - \sqrt{6})/(15 + \sqrt{6})^3}$ | $-[4/(15 - \sqrt{6})]^2$ | $\sim -0.047$ |
|     | 5   | 2   | $\sqrt{(5 - \sqrt{10})/(17 + \sqrt{10})^3}$ | $-[4/(17 - \sqrt{10})]^2$ | $\sim -0.028$ |
| 2   | 3   | 2   | $-\sqrt{3/11^3}$        | $-(4/11)^2$     | $\sim -0.055$ |
|     | 4   | 3   | $-\sqrt{(3 - \sqrt{6})/(15 + \sqrt{6})^3}$ | $-[4/(15 - \sqrt{6})]^2$ | $\sim -0.047$ |
|     | 3   | 4   | $-\sqrt{(3 + \sqrt{6})/(15 - \sqrt{6})^3}$ | $-[4/(15 + \sqrt{6})]^2$ | $\sim -0.029$ |
|     | 5   | 3   | $-\sqrt{(5 - \sqrt{10})/(17 + \sqrt{10})^3}$ | $-[4/(17 - \sqrt{10})]^2$ | $\sim -0.028$ |
| 4   | 5   | 4   | $-\sqrt{(5 + \sqrt{10})/(17 - \sqrt{10})^3}$ | $-[4/(17 + \sqrt{10})]^2$ | $\sim -0.039$ |