Spiked and screened oscillators $V(r) = A\,r^2 + B/r^2 + C/r^4 + D/r^6 + F/(1+G\,r^2)$ and their elementary bound states

Miloslav Znojil† and Rajkumar Roychoudhury‡

†Ústav jaderné fyziky AV ČR, 250 68 Řež, Czech Republic
and
‡Physics and Applied Mathematics Unit, Indian Statistical Institute, Calcutta 700035, India

Abstract

We show that the complicated superpositions $V(r)$ of several important phenomenological forces may still lead to an elementary form of doublets of bound states under transparent algebraic constraints. Constructively, we show how (and when) the constrained couplings preserve compatibility with the physical regularity of wavefunctions.

PACS 03.65.Ge
03.65.Fd 31.15.Md 02.90.+p

1 Introduction

An elementary Ansatz for a particular wavefunction $\psi(r) = \psi_0(r)$ is known to define the related partially solvable phenomenological interaction, say, in laser physics [1]. Often, all the remaining general $\psi_k(r)$ are obtainable via a straightforward generalization of the Ansatz. As an example, one may recall the popular sextic-oscillator example $V(r) = A\,r^2 + B\,r^4 + C\,r^6$ where the Ansatz may be interpreted as a termination of the general power-series solution [2]. Similarly, in the singular models of the type $V(r) = A\,r^2 + B\,r^{-2} + C\,r^{-4} + D\,r^{-6}$, the termination concerns the doubly infinite Laurent series solutions [3].

In such a framework, one may encounter several methodical challenges. The best known one is exemplified by the non-polynomial "screening" anharmonicity in $V(r) = A\,r^2 + F/(1+G\,r^2)$. Its complex poles, obviously, violate the convergence of many simple-minded expansions [4]. At the same time, some of its properties have been shown to share (or only slightly modify) some formal aspects of unperturbed harmonic oscillators [5]. Hence, a crucial test of many methods will be provided by all the "untractable" superpositions of the above-mentioned components. Their "first nontrivial" representative

$$V(r) = A\,r^2 + \frac{B}{r^2} + \frac{C}{r^4} + \frac{D}{r^6} + \frac{F}{1+G\,r^2}, \qquad A > 0, \quad D > 0, \quad G > 0 \tag{1}$$

is also a phenomenologically appealing model. It combines a confinement and strong repulsion with a non-polynomial behaviour and "screening". Mathematically, it still admits an analytic construction of a few elementary bound states [6] but in general, it does not seem to offer any straight or non-numerical understanding of non-exceptional solutions.

One has to resort to perturbative methods. The so called logarithmic perturbation theory [7] seems well suited for such a purpose. In its applications, the importance of partial solvability of similar interactions has repeatedly been emphasized [8]. The formalism is able to combine the merits of partial solvability with the efficiency of computers. The explicit use of the Hilbert space and dual states becomes unnecessary there [9]. Picking up an exceptional elementary solution as a zero order approximant, the prescription circumvents the construction of the so called "unperturbed propagators" [10]. This opens new perspectives.

In the comparatively complicated six-parametric wells of the type (1), the explicit construction of the zero-order bound states seems prohibitively difficult within the standard Lie-algebraic approach to elementary solvability [11]. Fortunately, a combination of the supersymmetric considerations [12] with a Riccati-equation-like re-interpretation of partial solvability [13] throws a new light on these difficulties. This will enable us to complement the older considerations by new constructions here. In particular, we shall see that even the seemingly over-complicated potentials (1) still admit an efficient algebraic construction and analysis of its exceptional Schrödinger bound states.

2 The construction of exceptional solutions

Let us re-write the radial Schrödinger equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{\ell(\ell+1)}{r^2}+V(r)\right]=E\psi(r),\quad \ell=0,1,\ldots\ . \tag{2}$$

as an equation solvable, formally, by its "inversion". Indeed, once we assume a knowledge of a single wavefunction, say,

$$\psi_0(r)=\mathcal{D}(r)\exp[-\mathcal{F}(r)] \tag{3}$$

we may already *define* the corresponding "one-state-solvable" potential via the equation itself, $V(r)=E_0-\frac{\ell(\ell+1)}{r^2}+\psi_0''(r)/\psi_0(r)$ [1]. In this way, with the choice of

$$\mathcal{D}(r)=1+gr^2,\quad \mathcal{F}(r)=ar^2+b\log r+cr^{-2},\quad a,c,g>0 \tag{4}$$

we get an element of our class of potentials (1),

$$V(r)-E_0+\frac{l(l+1)}{r^2}=\mathcal{F}'^2-\mathcal{F}''+\frac{(\mathcal{D}''-2\mathcal{D}'\mathcal{F}')}{\mathcal{D}} \tag{5}$$

Vice versa, our potential (1) acquires the elementary bound state (3) whenever its couplings match the above Ansatz. With $G=G_0=g>0$, this inversion "re-parametrizes" the couplings

$$\begin{array}{c}A=A_0=4a^2,\quad B=B_0=b+b^2+8(g-a)c,\quad C=C_0=-(4b+6)c,\\ D=D_0=4c^2,\quad F=F_0=2g-4bg+8a-8cg^2\end{array} \tag{6}$$

as well as the energy, $E=E_0=2a(5-2b)$.

2.1 The second elementary bound state

The simultaneous existence of the pair of elementary bound states is a less trivial question. In accord with ref. [6], we may employ a careted modification of our Ansatz (3),

$$\widehat{E}=E_0+\varepsilon,\quad \widehat{\mathcal{D}}=\mathcal{D}\,P,\quad \widehat{\mathcal{F}}=\mathcal{F}. \tag{7}$$

It has to satisfy the same Schrödinger equation, i.e., after appropriate insertions, condition $\varepsilon=-2\mathcal{D}'P'/(\mathcal{D}P)+(2P'\mathcal{F}'-P'')/P$ or, more explicitly, equation

$$(1+gr^2)P''(r)+4\mathcal{G}(r)rP'(r)+(1+gr^2)\varepsilon P(r)=0 \tag{8}$$

with an abbreviation $\mathcal{G}(r)=c/r^4+(cg-b/2)/r^2+g-bg/2-a(1+gr^2)$. For all the polynomials $P(r)=\sum_{m=0}^{M}\,d_k\,r^{2k}$, $d_0\neq 0$, $d_M\neq 0$, this differential equation degenerates to the set of recurrences for coefficients d_k,

$$\begin{array}{l}8c(k+2)\,d_{k+2}+2(k+1)(2k+1-2b+4cg)\,d_{k+1}\\ \qquad +[\varepsilon-8ka+2kg(2k+3-2b)]\,d_k+[\varepsilon-8a(k-1)]\,g\,d_{k-1}=0\ .\end{array} \tag{9}$$

At all the subscript values $k \leq -3$ and $k > M+1$, these relations remain trivial. Due to the particular values of our coefficients, we also get just $0 = 0$ at $k = -2$. At the next subscript $k = -1$, one obtains, unexpectedly, a vanishing condition $d_1 = 0$. This is a peculiarity of our system of equations. Another one emerges at the next index $k = 0$ which defines $d_2 = -[\varepsilon/(16c)]\, d_0$. This may be interpreted as a freedom of using either d_0 or d_2 as an arbitrary (nonzero) normalization constant. Here, we shall use it as a definition of d_0 in terms of the normalization $d_2 \neq 0$.

The "last" condition at $k = M+1$ is also trivial and defines the energy $\varepsilon = 8Ma$. The remaining M items with $k = 1, 2, \ldots, M$ become mutually interrelated. They form an overcomplete linear algebraic equation

$$\left(\begin{array}{cccccccc} \beta_2 & \alpha_2 & 0 & \ldots & & & & 0 \\ \gamma_3 & \beta_3 & \alpha_3 & 0 & \ldots & & & 0 \\ \delta_4 & \gamma_4 & \beta_4 & \alpha_4 & 0 & \ldots & & 0 \\ 0 & \delta_5 & \gamma_5 & \beta_5 & \alpha_5 & 0 & \ldots & 0 \\ \vdots & & \ddots & \ddots & \ddots & \ddots & & \vdots \\ 0 & \ldots & 0 & \delta_{M-2} & \gamma_{M-2} & \beta_{M-2} & \alpha_{M-2} & 0 \\ 0 & \ldots & & 0 & \delta_{M-1} & \gamma_{M-1} & \beta_{M-1} & \alpha_{M-1} \\ 0 & \ldots & & & 0 & \delta_M & \gamma_M & \beta_M \\ 0 & \ldots & & & & 0 & \delta_{M+1} & \gamma_{M+1} \end{array} \right) \left(\begin{array}{c} d_2 \\ d_3 \\ \ldots \\ d_M \end{array} \right) = 0\,. \qquad (10)$$

Its $(M-1) \times M-$dimensional four-diagonal matrix has the following elements,

$$\begin{array}{lll} \alpha_k = 8c(k+1), & \beta_k = 4(3-2b), & k = 2, \\ & = 2k(2k-1+4gc-2b), & k \geq 3, \\ \delta_k = 8ag(M-k+2), & \gamma_k = 8a(M-k+1) + 2g(k-1)(2k+1-2b), & \\ & \ k = 2, 3, \ldots, M+1\,. & \end{array} \qquad (11)$$

The solvability and solutions of eq. (10) must be analysed in more detail.

3 Meeting the physical requirements

Whenever the M equations (10) possess a solution, it need not necessarily be compatible with the standard physical requirements [13]. Firstly, due to the unitarity requirements, the couplings must remain real. Secondly, in accord with formula (4), the positivity of the roots $a > 0$, $c > 0$ and $g > 0$ must also be guaranteed: It controls the required regular behaviour of our wavefunctions at $r \to \infty$, at $r \to 0$ and in between these two extremes, respectively.

In the analysis of solutions, one must proceed step-by-step. At the first possible choice of $M = 2$, there exist no solutions at all. The two independent conditions of solvability of our equations (10) read $b = 3/2$ and $b = 7/2$ and contradict each other.

With $M = 3$, the solution is already known [6],

$$\varepsilon = 24a > 0, \qquad c = \frac{2b-3}{4g} > 0, \qquad a = \frac{(2b-9)g}{2} > 0 \tag{12}$$

(notice that eq. (22) of ref. [6] is marred by a misprint). This implies that the "doublet-compatible" $M = 3$ couplings may be defined, say, as functions of arbitrary $g > 0$ and $b > 9/2$. One of these "degrees of freedom" is due to the scaling of coordinates, $r \to const.\, r$, and the solutions depend on a single variable. This is not enough for construction of another, third elementary bound state.

3.1 The first two non-trivial examples: $M = 4$ and $M = 5$

At any $M \geq 3$, our equations (10) admit an easy partial simplification by means of the explicit determinantal formulas

$$d_3 = \frac{d_2}{(-\alpha_2)} \det \left(\begin{array}{c} \beta_2 \end{array} \right)$$

$$d_4 = \frac{d_2}{(-\alpha_2)(-\alpha_3)} \det \left(\begin{array}{cc} \beta_2 & \alpha_2 \\ \gamma_3 & \beta_3 \end{array} \right) \tag{13}$$

an so on. They enable us to eliminate all the arbitrarily normalized coefficients d_k. Alternatively, we might also write

$$d_{M-1} = \frac{d_M}{(-\delta_{M+1})} \det \left(\begin{array}{c} \gamma_{M+1} \end{array} \right)$$

$$d_{M-2} = \frac{d_M}{(-\delta_M)(-\delta_{M+1})} \det \left(\begin{array}{cc} \gamma_M & \beta_M \\ \delta_{M+1} & \gamma_{M+1} \end{array} \right) \tag{14}$$

in a symmetric manner. As a consequence, we are only left with the two "compatibility" or "matching" conditions. They may be written in different forms (cf. the detailed analysis of similar algebraic equations as presented, e.g., in ref. [14]).

For our present purposes, we shall introduce the coupled pair of compatibility equations in the standard secular determinantal form. On the basis of some symbolic manipulation experiments, we may recommend the omission of one of the last two rows in eq. (10). Such a convention seems to offer a maximal simplicity of algebra and leads to the following pair of conditions,

$$\det \left(\begin{array}{cccccccc} \beta_2 & \alpha_2 & 0 & \ldots & & & & 0 \\ \gamma_3 & \beta_3 & \alpha_3 & 0 & \ldots & & & 0 \\ \delta_4 & \gamma_4 & \beta_4 & \alpha_4 & 0 & \ldots & & 0 \\ 0 & \delta_5 & \gamma_5 & \beta_5 & \alpha_5 & 0 & \ldots & 0 \\ \vdots & & \ddots & \ddots & \ddots & \ddots & & \vdots \\ 0 & \ldots & 0 & \delta_{M-2} & \gamma_{M-2} & \beta_{M-2} & \alpha_{M-2} & 0 \\ 0 & \ldots & & 0 & \delta_{M-1} & \gamma_{M-1} & \beta_{M-1} & \alpha_{M-1} \\ 0 & \ldots & & 0 & 0 & 0 & \delta_{M+1} & \gamma_{M+1} \end{array} \right) = 0 \ , \tag{15}$$

$$
\det \begin{pmatrix}
\beta_2 & \alpha_2 & 0 & \dots & & & & 0 \\
\gamma_3 & \beta_3 & \alpha_3 & 0 & \dots & & & 0 \\
\delta_4 & \gamma_4 & \beta_4 & \alpha_4 & 0 & \dots & & 0 \\
0 & \delta_5 & \gamma_5 & \beta_5 & \alpha_5 & 0 & \dots & 0 \\
\vdots & & \ddots & \ddots & \ddots & \ddots & & \vdots \\
0 & \dots & 0 & \delta_{M-2} & \gamma_{M-2} & \beta_{M-2} & \alpha_{M-2} & 0 \\
0 & \dots & & 0 & \delta_{M-1} & \gamma_{M-1} & \beta_{M-1} & \alpha_{M-1} \\
0 & \dots & & 0 & 0 & \delta_M & \gamma_M & \beta_M
\end{pmatrix} = 0\ . \qquad (16)
$$

An elementary transformation of these determinants would enable us to simplify their form. Alternatively, noticing the scaling invariance of the products $a' = ac$, $g' = gc$ and b (cf. also eqs. (1) and (2) for an independent confirmation of this observation), we may achieve the same simplification by the re-scaling – we shall put $c = 1$ from now on. This gives the vanishing pair of the three by three determinants at $M = 4$,

$$
\det \begin{pmatrix}
4\,(3-2\,b) & 24 & 0 \\
16\,a + 4\,(7-2\,b)\,g & 24\,g + 6\,(5-2\,b) & 32 \\
0 & 8\,a\,g & 8\,(11-2\,b)\,g
\end{pmatrix} = 0, \qquad (17)
$$

$$
\det \begin{pmatrix}
4\,(3-2\,b) & 24 & 0 \\
16\,a + 4\,(7-2\,b)\,g & 24\,g + 6\,(5-2\,b) & 32 \\
16\,a\,g & 8\,a + 6\,(9-2\,b)\,g & 32\,g + 8\,(7-2\,b)
\end{pmatrix} = 0 \qquad (18)
$$

etc. In proportion to the growth of M, the dimension of matrices in determinants also increases; at $M = 5$ we must annihilate the determinant of the four by four matrix

$$
\begin{pmatrix}
4\,(3-2\,b) & 24 & 0 & 0 \\
24\,a + 4\,(7-2\,b)\,g & 24\,g + 6\,(5-2\,b) & 32 & 0 \\
24\,a\,g & 16\,a + 6\,(9-2\,b)\,g & 32\,g + 8\,(7-2\,b) & 40 \\
0 & 0 & 8\,a\,g & 10\,(13-2\,b)\,g
\end{pmatrix}, \qquad (19)
$$

as well as of its last-row modification

$$
\begin{pmatrix}
\dots & \dots & \dots & \dots \\
\dots & \dots & \dots & \dots \\
24\,a\,g & 16\,a + 6\,(9-2\,b)\,g & 32\,g + 8\,(7-2\,b) & 40 \\
0 & 16\,a\,g & 8\,a + 8\,(11-2\,b)\,g & 40\,g + 10\,(9-2\,b)
\end{pmatrix} \qquad (20)
$$

etc. *A posteriori*, we notice that the choice of the quantities a and g as independent variables has really led us to the simplest possible form of our coupled polynomial equations parametrized still by the variable b. At $M = 4$ we have

$$
\begin{gathered}
64\,a\,(2\,b-9) + 3\,(11-2\,b)\,(4\,b^2 - 16\,b - 16\,g + 15) = 0, \\
128\,a\,(b-3) - 3\,[8\,b^3 - 60\,b^2 + 2\,b\,(71-32\,g) + 64\,g^2 + 160\,g - 105] = 0,
\end{gathered} \qquad (21)
$$

at $M = 5$ we get

$$\begin{array}{c} 288\,a^2 - 4\,a\,[116\,b^2 - 1024\,b + 3\,(665 - 16\,g)] \\ +3\,(2\,b - 13)\,[8\,b^3 - 60\,b^2 + 2\,b\,(71 - 32\,g) + 64\,g^2 + 160\,g - 105] = 0, \\ 288\,a^2 - 4\,a\,[116\,b^2 - 816\,b + 3\,(465 - 112\,g)] \\ +3\,[16\,b^4 - 192\,b^3 + 8\,b^2\,(103 - 24\,g + 16\,b\,(16\,g^2 + 72\,g - 93) \\ -256\,g^3 - 512\,g^2 - 1680\,g + 945] = 0, \end{array} \tag{22}$$

etc. The method of solving these algebraic equations is standard, based on the use of the so called Groebner bases [15]. In our "teaching by example" approach, once we eliminate a at $M = 4$,

$$a = 3\,\frac{8\,b^3 - 76\,b^2 + 2\,b\,(103 - 16\,g) + 11\,(16\,g - 15)}{64\,(2\,b - 9)} \tag{23}$$

or at $M = 5$,

$$a = 3\,\frac{64\,g^3 - 16\,g^2\,(2\,b + 5) + 4\,g\,(2\,b - 5)\,(2\,b + 5) + (5 - 2\,b)\,(4\,b^2 - 20\,b + 21)}{8\,(36\,g - 26\,b + 75)} \tag{24}$$

we arrive at a single "quasi-secular" or "reduced" polynomial equation for the remaining unknown variable g. The same procedure also applies at the general M.

At $M = 4$, the reduced problem is still an exactly solvable quadratic equation,

$$g^2\,(128\,b - 576) - 32\,g\,(2\,b^2 - 11\,b + 12) + 8\,b^3 - 44\,b^2 + 78\,b - 45 = 0\ . \tag{25}$$

The pair of its roots stays real if an only if $b \leq 4.75$,

$$g_\pm = 3/[4\,(2\,b - 9)] + (b - 1)/4 \pm (2\,b - 3)\,\sqrt{-4\,b + 19}/[8\,(9 - 2\,b)]. \tag{26}$$

An illustrative choice of $b = 4.6$ (with $c = 1$ as above) leads to the positive "weak-coupling" solution $a_+ \approx 0.141$ and $g_+ \approx 1.648$ and to its "strong-coupling" counterpart $a_- \approx 40.661$ and $g_- \approx 7.651$. For $M = 4$, this completes our constructive proof of existence of the solutions of equations (10) which are compatible with all the physical requirements.

In the similar way, at $M = 5$, the elimination of a leads to the sixth-degree polynomial equation for the unknown g,

$$\begin{array}{c} 27648\,g^6 - 13824\,g^5\,(2\,b + 3) - 384\,g^4\,(120\,b^2 - 1754\,b + 4449) \\ +32\,g^3\,(2120\,b^3 - 28996\,b^2 + 115110\,b - 139635) \\ +4\,g^2\,(3 - 2\,b)\,(3160\,b^3 - 40500\,b^2 + 158714\,b - 197835) \\ +8\,g\,(2\,b - 5)\,(2\,b - 3)^2\,(58\,b^2 - 503\,b + 990) + 3\,(7 - 2\,b)\,(2\,b - 5)^2\,(2\,b - 3)^3 = 0 \end{array} \tag{27}$$

The proof of existence of its real and positive (i.e., physical) root(s) is more numerical: With the simple choice of $b = 10$, one finds, i.a., the positive shift $g \approx 1.89059$ and the related coupling $a = 0.375\,(64\,g^3 - 400\,g^2 + 1500\,g - 3315)/(36\,g - 185) \approx 4.73441$.

3.2 Outlook

An analysis of the further, $M > 5$ cases, if needed, could proceed precisely along the same lines, giving already quite complicated quasi-secular eighth-order equation for g at $M = 6$,

$$33554432\, g^8\, (2\, b - 9)\, (b^2 - 12\, b + 36) - \ldots - 196210350\, b + 40186125 = 0 \qquad (28)$$

etc. We may summarize: The present class of interactions (1), chosen on phenomenological grounds, combines the asymptotic confinement and short range repulsion with a simple complex-pole term. We have seen that even these forces, constrained by their elementary solvability, exhibit still a pleasant flexibility. The variability of their free parameter b proved important – it helped us to guarantee the regularity of solutions $\psi(r)$ in the origin and near infinity. Simultaneously, the specification of b also enabled us to eliminate any undesirable imaginary component and/or real-axis singularity of the interaction $V(r)$ itself.

Acknowledgements

Discussions with many people (and, in particular, with Pinaki Roy from ISI Calcutta) were vital for our inspiration and motivation. One of us (M.Z.) appreciates the partial support of this work by the grants Nr. A 104 860 2 (GA AV ČR) and 202/96/0218 (GA ČR). R.R. is grateful to Czech Academy of Sciences, INSA and Indian Statistical Institute in Calcutta for financial support.

References

[1] H. Risken and H. Vollmer, Z. Phys. 201, 323 (1967);

H. Haken, Laser Theory, in Enc. of Phys., Vol. XXV/2c (Van Nostrand, Princeton, 1970).

[2] V. Singh, S. N. Biswas and K. Datta, Phys. Rev. D 18, 1901 (1978);

R. Roychoudhury, Y. P. Varshni and M. Sengupta, Phys Rev A 42, 184 (1990).

[3] M. Znojil, J. Phys. A: Math. Gen. 15, 2111 (1982) and J. Math. Phys. 31, 108 (1990).

[4] A. K. Mitra, J. Math. Phys. 19, 2018 (1978);

S. K. Kaushal, J. Phys. A: Math. Gen 12, 1253 (1979);

F. M. Fernández, Phys. Lett.. A 160, 116 (1991).

[5] R. R. Whitehead, A. Watt, G. P. Flessas and M. A. Nagarajan, J. Phys. A: Math. Gen. 15, 1217 (1982);

B. Roy, R. Roychoudhury and P. Roy, J. Phys. A: Math. Gen. 21, 1579 (1988);

A. Lakhtakia, J Phys A: Math. Gen. 22, 1701 (1989);

G. Vanden Berghe and H. E. De Meyer, ibid., p. 1705.

[6] M. Znojil and P. G. L. Leach, J. Math. Phys. 33, 2785 (1992).

[7] R. Sternheimer, Phys. Rev. 84, 244 (1951);

Y. Aharonov and C. K. Au, Phys. Rev. Lett. 42, 1582 (1979) and references listed therein.

[8] A. V. Turbiner and A. G. Ushveridze, J. Math. Phys. 29, 2053 (1988).

[9] L. Skála and J. Čížek, J. Phys. A: Math. Gen. 29, L129 and 6467 (1996);

M. Znojil, ibid., p. 5253;

R. Guardiola and J. Ros, ibid., p. 6461.

[10] A. Messiah, Quantum Mechanics (North Holland, Amsterdam, 1961).

[11] A. V. Turbiner, Comm. Math. Phys. 118, 467 (1987);

P. Roy, B. Roy and R. Roychoudhury, Phys. Lett. A 144, 55 (1990).

[12] P. Roy and R. Roychoudhury, Phys. Lett. A 122, 275 (1987);

R. Adhikari, R. Dutt and Y. P. Varshni, J. Math. Phys. 32, 441 (1991);

F. Cooper, A. Khare and U. Sukhatme, Phys. Rep. 251, 267 (1995).

[13] A. G. Ushveridze, Quasi-exactly solvable models in quantum mechanics (IOPP, Bristol, 1994).

[14] M. Znojil, J. Phys. A: Math. Gen. 27, 4945 and 7491 (1994).

[15] W. W. Adams and P. Loustaunau, An Introduction to Gröbner Bases (AMS, Providence, 1994).