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Bound states in the Kratzer plus polynomial potentials and the new form of perturbation theory

Miloslav Znojil

OTF, Ústav jaderné fyziky AV ČR, 250 68 Řež, Czech Republic

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The Schrödinger equation with potentials of the Kratzer plus polynomial type (say, quartic $V(r) = Ar^4 + Br^3 + Cr^2 + Dr + F/r + G/r^2$ etc.) is considered and a new method of exact construction of some of its bound states is presented. Our approach is made feasible via a combination of the traditional use of the infinite series $\psi(r)$ (terminated *rigorously* after $N+1$ terms at certain specific couplings and energies) with several new ideas. We proceed in two steps. Firstly, in the strong coupling regime with $G \to \infty$, we find the exact, complete and compact unperturbed solution of our $N+2$ coupled and *nonlinear* algebraic conditions of the termination. Secondly, we adapt the current Rayleigh–Schrödinger perturbation theory to our nonlinear equations and define the general $G < \infty$ bound states via an innovated, *triple* perturbation series. In its tests we show how all the corrections appear in integer arithmetics and remain, therefore, exact.

1. Introduction

Bound states in the Coulomb or, after a slight generalization, Kratzer's [31] potential

$$V_{\{0\}}(r) = F/r + G/r^2$$

played an important role in the history of quantum mechanics [23] as well as in the various methodical studies of its limitations [11,12,21,42]. In applications the potential offered one of the most important exactly solvable models of atomic and molecular physics and quantum chemistry. The model is extremely transparent, its spectrum of energies E is numbered by integers $N = 0, 1, \ldots$ and its wave functions are proportional to Laguerre polynomials of degree N [20]. Almost 30 years ago Hautot noticed [24] that the exact solvability of the Kratzer's potential survives, in a way, its immersion in the shifted harmonic confining well,

$$V_{\{1\}}(r) = Cr^2 + Dr + F/r + G/r^2.$$

For *any integer* $N = 0, 1, \ldots$ one may construct $N+1$ different "Sturmian" exact wave functions proportional to polynomials of degree N. In contrast to the Kratzer's

model the Hautot's elementary bound states do not form a complete set. In literature the solutions of this type are called quasi-exact [48].

The two classes of forces $V_{\{0\}}(r)$ and $V_{\{1\}}(r)$ are usually considered exceptional. This attitude finds a deeper mathematical foundation in the representation theory of Lie algebras [10,45]. Still, certain remnants of their elementary solvability may be detected in all their further polynomial extensions. This has been first noticed by Magyari [34] who generalized the Hautot's method to all the polynomial forces

$$V_{\{m\}}(r) = Ar^{2m} + Br^{2m-1} + \cdots + F/r + G/r^2. \tag{1}$$

The generalized construction with degree $m \geqslant 2$ did not inspire, unfortunately, too many applications. Basically, this was due to its numerous practical shortcomings. In introduction, let us only mention that Magyari replaced the *linear* Schrödinger equation by a *nonlinear* algebraic system. The solution of these equations seems only feasible for the first two choices of indices $m = 0$ and $m = 1$, with nonlinearity more or less kept under control. In the present paper we intend to demonstrate that such a constraint and *a priori* scepticism about the feasibility of solution of the Magyari's equations are undeserved, for the important [2,4,5,14,15,28,30,32,38,39,46,50] choice of $m = 2$ at least.

The paper is inspired by certain unpublished numerical experiments with Magyari equations ([56], also section 2). In the first step of a new development we show in section 3 that certain unsolvable interactions (1) with $m = 2$ and with a strong repulsive core $G \to \infty$ *leave the Magyari's equations exactly solvable at any dimension* N. This is our key result.

In the equally important second step we demonstrate how one can deal with the corrections for finite $G < \infty$. Section 4 offers a new perturbation method of construction of their sequence in closed form. The method emphasizes several close parallels between our nonlinear algebraic problem and its simpler linear analogues. Technical details of our Rayleigh–Schrödinger-like new perturbation theory are illustrated on our quartic example $V_{\{2\}}(r)$ in full detail. Section 5 adds a few concluding remarks.

2. Matrix form of the Schrödinger equation

An overall methodical background of the Magyari's treatment of the ordinary radial Schrödinger equation

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

with angular momentum $\ell = 0, 1, \ldots$ lies somewhere in between the variational and nonvariational approaches. While one usually expands wave functions in an appropriate orthonormalized basis, Magyari uses the mere Taylor series. His recipe weakens the current emphasis upon methodical universality and numerical efficiency. It favors, instead, an enhanced simplicity, analyticity and closed, non-numerical form of

his quasi-exact bound states in a way which is regaining a new credit in recent literature [3,8,9,40,47,57].

At the very beginning of our considerations let us note that all the asymptotically polynomial forces (1) with $m \geqslant 1$ imply the same asymptotically exponential form of their bound-state wave functions,

$$\psi(r) = \exp\left\{-\sqrt{A}\left[r^{m+1}/(m+1) + Br^m/2A + \mathcal{O}\left(r^{m-1}\right)\right]\right\}.$$

This is an important information. Once we restrict our attention to the mere quartic $m = 2$ potential for the sake of definiteness and brevity,

$$V_{\{2\}}(r) = Ar^4 + Br^3 + Cr^2 + Dr + Fr^{-1} + Gr^{-2}, \tag{3}$$

we may try to write down the polynomial ansatz

$$\psi_{\{2\}}(r) = \exp\left(-\frac{1}{3}\alpha r^3 - \frac{1}{2}\beta r^2 - \gamma r\right) \sum_{n=0}^{N} \omega_n r^{n+l+1}. \tag{4}$$

At an arbitrary finite integer $N \geqslant 0$ the requirement of its asymptotically correct behaviour fixes the parameters $\alpha = \sqrt{A} > 0$, $\beta = B/2\alpha$ and $\gamma = (C - \beta^2)/2\alpha$. The next order of asympotic analysis also reveals the uniqueness of the N-dependent "termination-admitting" value of the coupling constant $D = D(N) = -2\alpha(N + l + 2) + 2\beta\gamma$. This parallels the Hautot's observations made at $m = 1$ [24].

Near the origin the ansatz (4) combines the angular momentum $\ell = 0, 1, \ldots$ with the centrifugal-like coupling $G > -1/4$ into a new quantity $l = l(G)$ such that $G + \ell(\ell + 1) = l(l + 1)$. After the removal of a sign ambiguity in $l = -1/2 + \sqrt{G + (\ell + 1/2)^2} > -1/2$ we may insert our ansatz in equation (2) with potential (3). This transforms the differential Schrödinger equation into equivalent recurrences for Taylor coefficients ω_j,

$$R_k\omega_{k-2} + T_k\omega_{k-1} + S_k\omega_k + P_k\omega_{k+1} = 0 \tag{5}$$

with $k = 0, 1, \ldots, N + 1$, and coefficients

$$R_n = 2\alpha(N + 2 - n), \qquad T_m = E + \gamma^2 - \beta(2m + 2l + 1)$$

(abbreviated as $T_m \equiv 2T - 2(m - 1)\beta$) and

$$S_m = -2\gamma(m + l + 1) - F, \qquad P_m = (m + 1)(m + 2l + 2)$$

(with abbreviations $S_m \equiv 2S - 2\gamma m$ and $l + 1 \equiv \Omega$). These equations form an over-determined linear system of equations for parameters ω_j with asymmetric and nonsquare four-diagonal matrix $N + 2$ by $N + 1$,

$$\left(\begin{array}{ccccccc} S & \Omega & & & & & \\ T & S-\gamma & 2\Omega+1 & & & & \\ N\alpha & T-\beta & S-2\gamma & 3\Omega+3 & & & \\ & (N-1)\alpha & T-2\beta & \ddots & \ddots & & \\ & & \ddots & \ddots & S-(N-1)\gamma & N\Omega+\binom{N}{2} & \\ & & & 2\alpha & T-(N-1)\beta & S-N\gamma & \\ & & & & \alpha & T-N\beta & \end{array} \right).$$

Within the approach based on the latter equations one only works with a few exceptional bound states. They are elementary and preserve a strong formal similarity to the popular harmonic oscillators. Unfortunately, this parallel seems to weaken with the growth of N since the explicit solution of our nonlinear problem (5) quickly becomes more and more complicated.

We intend to simplify the equations in question at a cost of their perturbative rearrangement. Such an attempt is motivated by the possibility of a suppression of the most quickly growing (binomial) matrix elements at large $\Omega \equiv l(G) + 1 \sim G^{1/2} \gg 1$, i.e., under the presence of a strong repulsive core in potential (3). A routine rescaling of coordinates $r \to \mu r$ in equation (2) and of the related coefficients $\omega_n \to u_n = \omega_n \mu^n$ in equation (4) leads to a modified and more transparent matrix form $Q\boldsymbol{u} = 0$ of the Magyari's equation (5),

$$\left(\begin{array}{cccc} S & \Omega/\mu & & \\ T\mu & S-\gamma & 2\Omega/\mu+1/\mu & \\ \alpha N\mu^2 & (T-\beta)\mu & S-2\gamma & \ddots \\ & \ddots & \ddots & \ddots \\ & & \alpha\mu^2 & (T-N\beta)\mu \end{array} \right) \left(\begin{array}{c} u_0 \\ u_1 \\ \vdots \\ u_N \end{array} \right) = 0. \qquad (6)$$

In the repulsive $\Omega \gg N$ regime we notice that $|S| \gg N|\gamma|$ and $|T| \gg N|\beta|$. The two main diagonals of Q become approximately constant.

With the energy E proportional to the new parameter $T = T(E)$ and with the Coulomb coupling F contained in $S = S(F)$ a "symmetry" of Q may be enhanced by the choice of the value of the scaling parameter μ in such a way that the magnitude of its uppermost and lowest diagonals is balanced. For example, with $\alpha\mu^2 = \Omega/\mu = \tau$ we fix the unique values of $\mu = (\Omega/\alpha)^{1/3}$ and $\tau = (\Omega^2\alpha)^{1/3}$. Then we may abbreviate $s = S/\tau$ and $t = \mu T/\tau$ and premultiply and split our pseudo-Hamiltonian into a sum

of matrices $Q = Q^{(0)} + \lambda Q^{(1)}$. Its first component

$$Q^{(0)} = Q^{(0)}(s,t) = \begin{pmatrix} s & 1 & & & & \\ t & s & 2 & & & \\ N & t & s & 3 & & \\ & \ddots & \ddots & \ddots & \ddots & \\ & & 3 & t & s & N \\ & & & 2 & t & s \\ & & & & 1 & t \end{pmatrix}$$

will play the role of our unperturbed Magyari–Schrödinger pseudo-Hamiltonian. In the strong-core limit $G \to \infty$ our zero-order Magyari equation reads

$$Q^{(0)}(s,t) \begin{pmatrix} u_0^{(0)} \\ u_1^{(0)} \\ \vdots \\ u_N^{(0)} \end{pmatrix} = 0. \tag{7}$$

It has the form of an over-complete system of $N+2$ equations which should determine all the $N+1$ Taylor coefficients $u_n^{(0)}$ plus the two spectral-like parameters $s = s^{(0)}$ and $t = t^{(0)}$. In the purely mathematical setting, the difficulties represented by nonsquare form of their pseudo-Hamiltonian $Q^{(0)}(s,t)$ are quite new and rarely encountered in the mainly linear formalism of the traditional quantum mechanics. Of course, the solvability of equation (7) with $m \geqslant 2$ loses a natural Lie-algebraic background and interpretation of its quasi-exact predecessors with $m \leqslant 1$ [10,45].

3. Unperturbed solutions

At an arbitrary N, let us introduce the two nonsquare quasi-unit matrices $\mathcal{I}$ and $\mathcal{K}$ such that $Q^{(0)}(s,t) = Q^{(0)}(0,0) + s\mathcal{I} + t\mathcal{K}$. Denoting their transposition by a superscript $^{\mathrm{T}}$ it is easy to imagine that the products $\mathcal{I}^{\mathrm{T}}Q^{(0)}(s,t)$ and $\mathcal{K}^{\mathrm{T}}Q^{(0)}(s,t)$ are square matrices. In such a notation the necessary and sufficient condition of the nontrivial solvability of equation (7) may be formulated as a simultaneous disappearance of the two independent secular determinants, say,

$$\det\left[\mathcal{I}^{\mathrm{T}}Q^{(0)}(0,t) + sI\right] = 0, \qquad \det\left[\mathcal{K}^{\mathrm{T}}Q^{(0)}(s,0) + tI\right] = 0. \tag{8}$$

Our two free unperturbed parameters $s = s^{(0)}$ and $t = t^{(0)}$ will be fixed and determined by these two coupled polynomial equations at any N in principle.

Due to symmetries of our generalized, coupled eigenvalue problem (8) the pairs of its (in general, complex) solutions will always remain complex conjugate, $s^{(0)} = [t^{(0)}]^*$. For physical reasons we must ask whether at least some of these solutions remain real, $s^{(0)} = t^{(0)}$. The answer may be found by their explicit evaluation.

At $N = 0$ the solution of equation (8) is unique. From the natural normalization $u_N^{(0)} = 1$ we only get the trivial $s = t = 0$. At $N = 1$ the same normalization implies

Table 1
The key to our nonlinear problem (8): its roots $s^{(0)}=t^{(0)}$ for the first few $N\neq 0$.

N	1		2				3					
2 Re $s^{(0)}$	2	-1	4	1	-2	-2	6	3	0	0	-3	-3
2 Im $s^{(0)}/\sqrt{3}$	0	± 1	0	± 1	0	± 2	0	± 1	0	± 2	± 1	± 3

N	4								
2 Re $s^{(0)}$	8	5	2	2	-1	-1	-4	-4	-4
2 Im $s^{(0)}/\sqrt{3}$	0	± 1	0	± 2	± 1	± 3	0	± 2	± 4

N	5											
2 Re $s^{(0)}$	10	7	4	4	1	1	-2	-2	-2	-5	-5	-5
2 Im $s^{(0)}/\sqrt{3}$	0	± 1	0	± 2	± 1	± 3	0	± 2	± 4	± 1	± 3	± 5

that $u_0^{(0)}=-1/s$ (e.g., via the first row of equation (7)). The second row defines $t=s^2$ and our set degenerates to the single cubic equation $s^3=1$. Out of its three different complex roots only one is real and we have the unique physical solution $s=t=1$. At the next dimension $N=2$ an alternative, intermediate normalization $u_1^{(0)}=1$ helps us to eliminate $u_0^{(0)}=-1/s$ and $u_2^{(0)}=-1/t$ via the respective first and last row of equation (7). This gives $s^3=t^3$ and linear relation $t=a\,s$ with the three possible complex constants a such that $a^3=1$. One ends up with a triplet of alternative quadratic equations for the unknown s. Similarly, one proceeds at the higher integers N.

The resulting sets of the roots s are sampled in table 1. The general pattern of their N-dependence is obvious. Once we pay attention to the real solutions only, we arrive at the general formula

$$s=t=s^{(0)}_{[n+1]}(N)=t^{(0)}_{[n+1]}(N)=N-3n,\quad n=0,1,\ldots,[N/2]. \tag{9}$$

We see that in the limit $G\to\infty$ our double eigenvalue problem (8) is solvable in closed form at any $N=0,1,2,\ldots$.

3.1. Pascal-like triangle for the Taylor coefficients

Taylor coefficients $u^{(0)}_{[n+1],k}(N)$, $k=0,1,\ldots,N$, define the exact wave functions $\psi^{(0)}_{[n]}(r)$ (4) at each physical root (9). Via a suitable N-dependent normalization one may calculate these coefficients in integer arithmetics (i.e., exactly). This is illustrated in table 2. At the maximal real roots $s=s_{[1]}(N)=N$ we have

$$u^{(0)}_{[1],n}(N)=(-1)^{N+n}\binom{N}{n},$$

and our recurrences degenerate to the Pascal triangle for binomial coefficients,

$$\binom{N}{n}=\binom{N-1}{n}+\binom{N-1}{n-1}. \tag{10}$$

Table 2
Real eigenvectors of our pseudo-Hamiltonians $Q^{(0)}$.

N	$s^{(0)}$	$u_0^{(0)}$	$u_1^{(0)}$	$u_2^{(0)}$	$u_3^{(0)}$	$u_4^{(0)}$	$u_5^{(0)}$	$u_6^{(0)}$
0	0	1	–	–	–	–	–	–
1	1	1	−1	–	–	–	–	–
2	2	1	−2	1	–	–	–	–
	−1	1	1	1	–	–	–	–
3	3	1	−3	3	−1	–	–	–
	0	1	0	0	−1	–	–	–
4	4	1	−4	6	−4	1	–	–
	1	1	−1	0	−1	1	–	–
	−2	1	2	3	2	1	–	–
5	5	1	−5	10	−10	5	−1	–
	2	1	−2	1	−1	2	−1	–
	−1	1	1	1	−1	−1	−1	–
6	6	1	−6	15	−20	15	−6	1
	3	1	−3	3	−2	3	−3	1
	0	1	0	0	−2	0	0	1
	−3	1	3	6	7	6	3	1

This implies the elementary form $\psi(r) = \psi_{[1]}(r) \sim (1 - r/\mu)^N$ of the related exact wave functions. One detects the presence of a degenerate nodal zero of multiplicity N at $r = r_z = \mu$. A transition to the next, smaller real root $s = s_{[2]}(N) = N - 3$ makes the multiplicity of the mode in $\psi(r) = \psi_{[2]}(r)$ lowered by two. The phenomenon survives iterations in the bracketed subscripts. Our closed formula (9) for the roots may be complemented by the similar rule $N - 2n$ for the nodal multiplicities. With the odd integer $N = 2J + 1$ the iterations end at the real spectral root $s_{[J+1]}(2J + 1) = 1 - J$. A simple, nondegenerate zero appears in the related wave function $\psi^{(0)}_{[J+1]}(r)$. This characterizes the first excitation. At even $N = 2K$ the final choice of the minimal $s_{[K+1]}(2K) = -K$ produces the nodeless wave function $\psi^{(0)}_{[K+1]}(r)$. It describes the ground state.

A closer inspection of the numerical values of the Taylor coefficients reveals the presence of certain nonbinomial cases. Most quickly this "anomaly" is spotted in the ground-state coefficients $u^{(0)}_{[K+1],k}(2K)$, $k = 0, 1, \ldots, 2K$. The same pattern reappears in the first excitations $u^{(0)}_{[J+1],j}(2J + 1)$, $j = 0, 1, \ldots, 2J + 1$, at the higher J for odd $N = 2J + 1$, etc. Thus, the ground-state set is most fundamental and a few more values $u^{(0)}_{[K+1],k}(2K)$ are displayed in table 3. It definitely confirms a surprise. Each of the coefficients proves to be a *sum of its **three** closest upper neighbors*,

$$u^{(0)}_{[K+1],k}(2K) = u^{(0)}_{[K],k}(2K - 2) + u^{(0)}_{[K],k-1}(2K - 2) + u^{(0)}_{[K],k-2}(2K - 2).$$

In an unexpected parallel of the above two-term rule (10) our table 3 forms a new Pascal-like triangle. For ground states with different K we have $\psi^{(0)}_{[1]}(r) = 1$, $\psi^{(0)}_{[2]}(r) =$

Table 3
Generalized Pascal triangle (ground states: $N = 2K, s_{[K+1]} = -K$).

K	...	$u^{(0)}_{K-4}$	$u^{(0)}_{K-3}$	$u^{(0)}_{K-2}$	$u^{(0)}_{K-1}$	$u^{(0)}_{K}$	$u^{(0)}_{K+1}$	$u^{(0)}_{K+2}$	$u^{(0)}_{K+3}$	$u^{(0)}_{K+4}$	...
0	...	0	0	0	0	1	0	0	0	0	...
1	...	0	0	0	1	1	1	0	0	0	...
2	...	0	0	1	2	3	2	1	0	0	...
3	...	0	1	3	6	7	6	3	1	0	...
4	...	1	4	10	16	19	16	10	4	1	...
5	...	5	15	30	45	51	45	30	15	5	...
6	...	21	50	90	126	141	126	90	50	21	...
⋮						...					

$1 + r/\mu + r^2/\mu^2$, $\psi^{(0)}_{[3]}(r) = (1 + r/\mu + r^2/\mu^2)^2$ and so on. We may generalize this result also to all the wave functions $\psi^{(0)}_{[n+1]}(r)$ which correspond to the same (even or odd) integer $N = 0, 1, \ldots,$

$$\psi^{(0)}_{[n+1]}(r) = (1 - r/\mu)^{N-2n}\big(1 + r/\mu + r^2/\mu^2\big)^n, \quad n = 0, 1, \ldots, \left[\frac{N}{2}\right]. \tag{11}$$

This formula is valid, by induction, for all the bracketed subscripts.

3.2. *Interesting special cases*

The multiple, seemingly degenerate nodal zeros of solutions (11) require a "magnification" of their vicinity by an appropriate inclusion of a few higher-order corrections $\mathcal{O}(1/\Omega)$, $\mathcal{O}(1/\Omega^2), \ldots$. The only exceptions are the particular minimal-root ground states

$$\psi^{(0)}_{[K+1]}(r) = \big(1 + r/\mu + r^2/\mu^2\big)^K, \qquad N = 2K, \qquad s = t = -K,$$

and the first excitations

$$\psi^{(0)}_{[J+1]}(r) = (1 - r/\mu)\big(1 + r/\mu + r^2/\mu^2\big)^J, \qquad N = 2J + 1, \qquad s = t = 1 - J$$

without multiple zeros. In the strong-core phenomenological regime they may prove useful for immediate applications in principle. In such a context even the most simplified schematic example $V(r) = Ar^4 + G/r^2$ with $G \gg A$ indicates that the forces with large $G \gg 1$ need not necessarily lose a reasonable physical interpretation. A minimum of this function lies at a point $r_0 = (G/2A)^{1/6}$ which only slowly moves with G. Whenever necessary, this motion may further be slowed down by a simultaneous increase of the coupling A.

In order to get a feeling for the subtleties of structure of the systems with large G let us pick up our ground-state solution with $N = 4$ and $s = t = -K = -2$ in s-wave ($\ell = 0$). For simplicity let us assume the absence of the Coulombic and cubic terms in our potential $V_{\{2\}}(r)$. This means $F = B = 0$ and fixes the values of $\beta = 0$ and

$\gamma = C/2\alpha$ with $C = 4(A^2/\Omega)^{1/3}$. At the ground-state energy $E = -\gamma^2 - 4(A\Omega)^{1/3}$ our special example

$$V_{\{2\}}(r) = \alpha^2 r^4 + 4\left(\alpha^4/\Omega\right)^{1/3} r^2 - 2\alpha(\Omega+5)r + \Omega(\Omega-1)/r^2 \qquad (12)$$

is still only solvable in the limit $\Omega \to \infty$. Nevertheless, due to our explicit knowledge of the wave function, we may now invert the procedure easily. All the higher-order deviations from solvability may already be added to equation (12) in an explicit form produced, say, via the insertion of our elementary ground state formula for $\psi_{[2]}(r)$ in the original, differential Schrödinger equation (2).

For definiteness of our illustration let us choose the unit spring-constant coefficient $C = 1$ at r^2 in $V_{\{2\}}(r)$. We get, as a consequence, a strong quartic confinement $\alpha^2 = A = \sqrt{\Omega}/8$ combined with the repulsive linear force possessing an even stronger, $\mathcal{O}(\Omega^{5/4})$ coupling $D = -\Omega^{1/4}(\Omega+5)/\sqrt{2}$. We may rescale the coordinate $r \to r\Omega^{1/4}$ in our radial differential Schrödinger equation (2) with force (12). In the leading-order $1 + \mathcal{O}(1/\Omega)$ approximation this leads to the zero-energy problem with the dominant three-term interaction $V_{\{2\}}(r) = \text{const}\, r^4 - \text{const}' r - \text{const}''/r^2$. All its coupling constants are of the same order of magnitude $\mathcal{O}(1)$. It is known [55] that the solutions of such a problem may also be elementary and proportional to Laguerre polynomials.

We may conclude that in the limit $\Omega \to \infty$ the whole picture and scheme of elementary solvability is nicely self-consistent. We also see the usefulness of our present generalized construction. It leads to a richer class of polynomial solutions $\psi(r)$ in a fairly nontrivial though still feasible and manageable way. What remains for us is to extend the same pattern of self-consistency to all the higher-order (i.e., presumably, $1/\Omega^k$) corrections.

4. Corrections

At the finite values of the coupling G the strength of the perturbation $\lambda Q^{(1)} = Q - Q^{(0)}$ is measured by the parameter $\lambda = 1/(\mu\tau) = 1/\Omega$. Its smallness is strictly equivalent to our above assumption $\Omega \gg N$. In a perturbative treatment of our bound-state problem $Q\boldsymbol{u} = 0$ we have to avoid the following two most serious obstacles.

Firstly, our pseudo-Hamiltonian $Q(s,t)$ of equation (6) and its unperturbed simplification $Q^{(0)}(s,t)$ as well as their three-diagonal difference

$$Q^{(1)} = \begin{pmatrix} 0 & 0 & & & & \\ 0 & -\gamma\mu & 1 & & & \\ & -\beta\mu^2 & -2\gamma\mu & 3 & & \\ & & -2\beta\mu^2 & -3\gamma\mu & \ddots & \\ & & & -3\beta\mu^2 & \ddots & \frac{N(N-1)}{2} \\ & & & & \ddots & -N\gamma\mu \\ & & & & & -N\beta\mu^2 \end{pmatrix}$$

are nonsquare matrices. This means nonlinearity, not tractable by the standard perturbation formalisms. Secondly, our zero-order pseudo-Hamiltonian itself is a four-diagonal matrix. This would cause difficulties even in the linear case, with an unclear idea how one could construct an unperturbed propagator. Fortunately, the apparently unavoidable methodical pessimism is not in place. With certain care one can proceed in an almost complete analogy with the traditional Rayleigh–Schrödinger textbook prescription,

- choosing an arbitrary integer $N \geqslant 0$,
- picking up a real root $s^{(0)} = t^{(0)}$ as given by equation (9),
- postulating, in nonstandard manner, the *two* different expansions

$$s = s^{(0)} + \lambda s^{(1)} + \lambda^2 s^{(2)} + \cdots,$$

$$t = t^{(0)} + \lambda t^{(1)} + \lambda^2 t^{(2)} + \cdots,$$

  plus, more traditionally,

$$\begin{pmatrix} u_0 \\ u_1 \\ \vdots \\ u_N \end{pmatrix} = \begin{pmatrix} u_0^{(0)} \\ u_1^{(0)} \\ \vdots \\ u_N^{(0)} \end{pmatrix} + \lambda \begin{pmatrix} u_0^{(1)} \\ u_1^{(1)} \\ \vdots \\ u_N^{(1)} \end{pmatrix} + \lambda^2 \begin{pmatrix} u_0^{(2)} \\ u_1^{(2)} \\ \vdots \\ u_N^{(2)} \end{pmatrix} + \cdots,$$

- combining all these expansions with input $Q = Q^{(0)} + \lambda Q^{(1)}$.

As a net result we get the hierarchy of equations for corrections. On all the subsequent levels of precision $\mathcal{O}(\lambda^k)$, i.e., in the kth perturbation order with $k = 1, 2, \ldots$, these equations will play the role of implicit definitions of the "charge", "energy" and "wave function" corrections $s^{(k)}$, $t^{(k)}$ and $\boldsymbol{u}^{(k)}$, respectively. The set will be initiated by the above zero-order problem (7). All the subsequent new equations will have the same nonsquare and nonhomogeneous common matrix form

$$\begin{aligned} &\left[Q^{(0)}(0,0) + s^{(0)}\mathcal{I} + t^{(0)}\mathcal{K}\right]\boldsymbol{u}^{(k)} + \left[Q^{(1)}(0,0) + s^{(1)}\mathcal{I} + t^{(1)}\mathcal{K}\right]\boldsymbol{u}^{(k-1)} \\ &\quad + \left(s^{(2)}\mathcal{I} + t^{(2)}\mathcal{K}\right)\boldsymbol{u}^{(k-2)} + \cdots + \left(s^{(k)}\mathcal{I} + t^{(k)}\mathcal{K}\right)\boldsymbol{u}^{(0)} = 0. \end{aligned} \tag{13}$$

Mutatis mutandis, we may parallel the standard textbook perturbation theory of the Rayleigh–Schrödinger type [36].

4.1. Perturbations of the charges and energies

Our first important observation is that equation (7) and properties of our zero-order pseudo-Hamiltonians $Q^{(0)}(s^{(0)}, t^{(0)}) = Q^{(0)}(0,0) + s^{(0)}\mathcal{I} + t^{(0)}\mathcal{K}$ imply that these nonsquare and $(N+2) \times (N+1)$-dimensional matrices always possess the *pairs of independent left eigenvectors*. Their explicit sample $[\boldsymbol{v}^{[s]}]^{\mathrm{T}}$ and $[\boldsymbol{v}^{[a]}]^{\mathrm{T}}$ is displayed in the first part of table 4. We normalized these vectors of dimension $N+2$ in the symmetric and antisymmetric manner, respectively. Wherever necessary, the Dirac's

Table 4
Pairs of independent left eigenvectors of $Q^{(0)}(s,s)$.

		Sym. and antisym. v_k						Shortened σ_k and θ_k					Overlaps
N	$k=s$	0	1	2	3	4	5	0	1	2	3	4	$\langle v\|(\mathcal{I}\boldsymbol{u}^{(0)})\rangle$
0	0	1	1	–	–	–	–	1	–	–	–	–	1
		1	−1	–	–	–	–	1	–	–	–	–	1
1	1	1	−2	1	–	–	–	1	−1	–	–	–	3
		1	0	−1	–	–	–	−1	1	–	–	–	1
2	2	2	−1	−1	2	–	–	0	1	−1	–	–	3
		0	1	−1	0	–	–	–	–	–	–	–	−3
	−1	1	1	1	1	–	–	3	1	2	–	–	3
		3	−1	1	−3	–	–	2	1	3	–	–	3
3	3	1	1	−2	1	1	–	1	0	−1	1	–	−9
		1	−1	0	1	−1	–	1	−1	0	1	–	3
	0	2	−1	0	−1	2	–	2	0	0	−1	–	3
		2	1	0	−1	−2	–	−1	0	0	2	–	3
4	4	1	−2	1	1	−2	1	1	−1	0	1	−1	9
		1	0	−1	1	0	−1	−1	1	0	−1	1	−9
	1	7	1	−2	−2	1	7	7	−3	−1	−1	4	9
		1	−1	0	0	1	−1	4	−1	−1	−3	7	3
	−2	1	1	1	1	1	1	3	1	2	1	2	9
		3	−1	1	−1	1	−3	2	1	2	1	3	3

symbols will be used to denote the similar "longer" columns as "kets" (e.g., $\boldsymbol{v}^{[s]} \equiv |v^{[s]}\rangle$) and the rows as "bras" (say, $[\boldsymbol{v}^{[s]}]^{\rm T} \equiv \langle v^{[s]}|$ etc.).

Marginally, let us admit that there exist alternative possibilities of normalization. The requirement of disappearance of the first or last matrix element in a suitable linear superposition of $\langle v^{[s/a]}|$ may be used to define the "compactified" left eigenvectors $\langle w_\star| \equiv \boldsymbol{\sigma}^{\rm T}\mathcal{I}^{\rm T}$ and $\langle w^\star| \equiv \boldsymbol{\theta}^{\rm T}\mathcal{K}^{\rm T}$. The study of their properties discouraged us from their use in computations since the new doublets do not always remain linearly independent. This is exemplified at $N=2$ and $s^{(0)}=2$ in the second part of table 4.

The left action of a left auxiliary eigenbra $\langle v^{[s/a]}|$ completely eliminates the vector $\boldsymbol{u}^{(k)}$ from equation (13). We abbreviate

$$\begin{aligned}\big|\Xi^{(k-1)}\big\rangle = &-\big[Q^{(1)}(0,0) + s^{(1)}\mathcal{I} + t^{(1)}\mathcal{K}\big]\boldsymbol{u}^{(k-1)} \\ &-\big(s^{(2)}\mathcal{I} + t^{(2)}\mathcal{K}\big)\boldsymbol{u}^{(k-2)} - \cdots - \big(s^{(k-1)}\mathcal{I} + t^{(k-1)}\mathcal{K}\big)\boldsymbol{u}^{(1)}\end{aligned}$$

and arrive at the two independent equations

$$\big\langle v^{[s]}\big|\big(\mathcal{I}\boldsymbol{u}^{(0)}\big)\big\rangle s^{(k)} + \big\langle v^{[s]}\big|\big(\mathcal{K}\boldsymbol{u}^{(0)}\big)\big\rangle t^{(k)} = \big\langle v^{[s]}\big|\Xi^{(k-1)}\big\rangle,$$

$$\big\langle v^{[a]}\big|\big(\mathcal{I}\boldsymbol{u}^{(0)}\big)\big\rangle s^{(k)} + \big\langle v^{[a]}\big|\big(\mathcal{K}\boldsymbol{u}^{(0)}\big)\big\rangle t^{(k)} = \big\langle v^{[a]}\big|\Xi^{(k-1)}\big\rangle.$$

They may be interpreted as a two-by-two matrix inversion. The symmetric and anti-symmetric normalization of our auxiliary eigenvectors implies that

$$\left\langle v^{[s]}\right|\left(\mathcal{I}\boldsymbol{u}^{(0)}\right)\rangle = \left\langle v^{[s]}\right|\left(\mathcal{K}\boldsymbol{u}^{(0)}\right)\rangle \quad \text{and} \quad \left\langle v^{[a]}\right|\left(\mathcal{I}\boldsymbol{u}^{(0)}\right)\rangle = -\left\langle v^{[a]}\right|\left(\mathcal{K}\boldsymbol{u}^{(0)}\right)\rangle.$$

This enables us to invert the left-hand-side matrix in an explicit manner,

$$\begin{pmatrix} s^{(k)} \\ t^{(k)} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1/\left\langle v^{[s]}\right|\left(\mathcal{I}\boldsymbol{u}^{(0)}\right)\rangle & 1/\left\langle v^{[a]}\right|\left(\mathcal{I}\boldsymbol{u}^{(0)}\right)\rangle \\ 1/\left\langle v^{[s]}\right|\left(\mathcal{K}\boldsymbol{u}^{(0)}\right)\rangle & 1/\left\langle v^{[a]}\right|\left(\mathcal{K}\boldsymbol{u}^{(0)}\right)\rangle \end{pmatrix}\begin{pmatrix} \left\langle v^{[s]}\right|\left.\Xi^{(k-1)}\right\rangle \\ \left\langle v^{[a]}\right|\left.\Xi^{(k-1)}\right\rangle \end{pmatrix}.$$

This is our first final closed formula for corrections $s^{(k)}$ and $t^{(k)}$, an extended nonlinear parallel to the usual Rayleigh–Schrödinger definition of energies.

4.2. Perturbations of the wave functions

The column vector of corrections $\boldsymbol{u}^{(k)}$ is characterized by its renormalization ambiguity $\boldsymbol{u}^{(k)} \to \boldsymbol{u}^{(k)} + \text{const} \times \boldsymbol{u}^{(0)}$. This follows from the very definition (13) and implies that, say, the first component of $\boldsymbol{u}^{(k)}$ may be chosen as vanishing. Let us indicate such an option by a superscript * in $\boldsymbol{u}^{(k)} = \boldsymbol{u}^{\star(k)}$ with $u_0^{\star(k)} = 0$ for $k > 0$. In our definition (13) this choice of normalization makes the pseudo-Hamiltonian matrix $Q^{(0)}(s^{(0)}, t^{(0)})$, in effect, lower triangular. In the same equation all the known terms may be collected in the single ket

$$\left|\tau^{(k-1)}\right\rangle = \left|\Xi^{(k-1)}\right\rangle - s^{(k)}\mathcal{I}\boldsymbol{u}^{(0)} - t^{(k)}\mathcal{K}\boldsymbol{u}^{(0)}$$

entering the right-hand side of our set of relations $Q^{(0)}(s^{(0)}, t^{(0)})\boldsymbol{u}^{\star(k)} = |\tau^{(k-1)}\rangle$. Two of its rows (or, more precisely, the two linear combinations of all these rows) have already been used for the determination of the quantities $s^{(k)}$ and $t^{(k)}$. We are left with the N independent equations. In the second decisive step of our method we recommend their choice which drops the last two lines and offers the relations

$$R^\star\begin{pmatrix} u_1^{\star(k)} \\ u_2^{\star(k)} \\ \vdots \\ u_N^{\star(k)} \end{pmatrix} = \begin{pmatrix} \tau_0^{\star(k-1)} \\ \tau_1^{\star(k-1)} \\ \vdots \\ \tau_{N-1}^{\star(k-1)} \end{pmatrix}$$

with

$$R^\star = \begin{pmatrix} 1 & & & & & \\ s^{(0)} & 2 & & & & \\ t^{(0)} & s^{(0)} & 3 & & & \\ N-1 & t^{(0)} & s^{(0)} & 4 & & \\ & \ddots & \ddots & \ddots & \ddots & \\ & & 3 & t^{(0)} & s^{(0)} & N \end{pmatrix},$$

i.e., an N-dimensional linear matrix equation which defines all the remaining unknown quantities. Computationally, it just offers the highly economical evaluation

of the higher-order corrections $\boldsymbol{u}^{(k)}$ via the downwards-running and finite four-term recurrences.

An important merit of our proposal is that the main diagonal of our lower triangular (and finite-dimensional) matrix $R^\star$ is safely nonzero. Hence, the matrix itself is regular, $\det R^\star = N! \neq 0$. Its lower triangular inversion $(R^\star)^{-1}$ exists and may be interpreted as the present analogue of the current Rayleigh–Schrödinger unperturbed propagator.

The direction of our recurrences is an inessential consequence of the choice of normalization. After its alternative specification $\boldsymbol{u}^{(k)} = \boldsymbol{u}_\star^{(k)}$ with $(u_\star^{(k)})_N = 0$ in all the orders $k > 0$ we annihilate the last column of $Q^{(0)}(s^{(0)}, t^{(0)})$. Naturally, one omits now the first two rows. Thus, we cut the N-dimensional and upper triangular submatrix $R_\star$ out of $Q^{(0)}(s^{(0)}, t^{(0)})$ and define the alternative unperturbed propagator by inversion,

$$\begin{pmatrix} u_{\star 1}^{(k)} \\ u_{\star 2}^{(k)} \\ \vdots \\ u_{\star N}^{(k)} \end{pmatrix} = (R_\star)^{-1} \begin{pmatrix} \tau_{\star 0}^{(k-1)} \\ \tau_{\star 1}^{(k-1)} \\ \vdots \\ \tau_{\star N-1}^{(k-1)} \end{pmatrix}.$$

Computationally, of course, the higher-order corrections $\boldsymbol{u}_\star^{(k)}$ are again much more easily evaluated directly, via the upwards-running four-term recurrences.

5. Conclusions

The core of our present paper may be seen in the progress we achieved in the non-numerical Magyari-like constructions. By means of their decisive perturbative simplification we were able to offer new solutions of certain "next-to-solvable" models.

In the first step we analyzed the limit $G \to \infty$ of quartic forces $V_{\{2\}}(r)$ and were able to find an exact and complete solution of the underlying nonlinear algebraic equations. This demonstrates that far beyond the "safe" territory of the exact and quasi-exact solutions one may still get closed formulas much more easily than expected before.

Another pleasant surprise appeared during our study of corrections $\mathcal{O}(1/\Omega)$. For many years we felt deterred by the strong N-dependence of their traditional numerical analyses as well as by the quick increase of complexity of their explicit description with $m \geqslant 2$ and dimensions N beyond, say, $N = 0$ of $N = 1$ [19]. In this context, the simple form of our present quasi-linear and N-independent perturbative formalism opens a new direction of development towards many practical (say, phenomenological) applications yet to be constructed and appreciated.

We have demonstrated that the traditional Taylor-series approach [17,27,33] to the differential Schrödinger equation may still offer new surprises. Its main merit lies in its ability of combination of the correct threshold behaviour with the correct physical asymptotics of $\psi(r)$ for a broad class of elementary potentials. As a consequence,

many simple models in quantum mechanics may efficiently be clarified by means of the related "most natural" power series ansatzs:

- in place of the differential equation one gets a (sometimes more transparent) set of recurrences,
- their unique solution may often be written in a closed (often called Hill-determinant [54]) form at any trial energy E,
- the truncated power-series wave functions remain fairly precise in a finite (i.e., most relevant) interval of coordinates even after a rough energy guess.

The transparency of the recipe is often marred by its various practical disadvantages. For example, the efficiency of the Hill-determinant algorithms often lags behind the universal variational approaches [7,16,26,53]. Also the domains of their applicability may be much more constrained, the unpleasant phenomenon which leads to many nontrivial misunderstandings [13,25,29,37,44]. Difficulties emerge even in numerical implementations of these algorithms: In the fixed-precision computer arithmetics one has to avoid the potential instability of recurrences etc. [6,22,43]. In such a context the most reliable remedy lies, obviously, in an *exact* termination of the infinite series.

In our paper we emphasized that the disadvantages connected with the latter strategy are often overestimated in applications. We succeeded in showing that the merits of using the algebraic Magyari-like equations may often be preserved at a reasonable price. Proceeding in a consequently constructive way we have shown that their nonlinearity has, in a way, a "weak" form which admits a certain "quasi-linear" treatment.

This attitude is, of course, trivial for the models of the Coulomb, Kratzer or harmonic oscillator type. For all of them the power series method is able to generate *all* their exact bound-state solutions as terminating. Their exact solvability involves all the angular momenta ℓ and physical energies E. Similarly, under weaker assumptions, the same polynomial ansatzs also succeed in offering the "quasi-exact" [48] multiplets of bound states of a finite size N.

The *freedom* of choosing the multiplicity N has been significantly extended here. Having noticed that the latter two "solvable" categories mean mostly the two- and three-term character of the underlying recurrences, we paid thorough attention to their very next, four-term generalization. In the context of an enormous interest in quartic oscillators [1,6,18,35,41,49,51,52] we imagined that one need not always perceive the comparatively short four-term recurrences as prohibitively complicated. At the same time, for many phenomenological applications, they offer a partially non-numerical insight into the new class of interactions which is already fairly rich.

In the light of our present results, the nonlinearity of the underlying algebra need not represent a serious technical obstacle. This is our main message. Via a detailed analysis of our present quartic polynomial examples we have shown that the explicit solution of the related Schrödinger and Magyari equations remains feasible in an almost complete parallel with their quadratic predecessors.

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