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A generalized Morse asymmetric potential and multiplets of its non-numerical exact bound states

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Abstract. The solvable Morse model with its asymmetric phenomenological potential $V(r) = A\{1 - \exp[-\mu(r - r_\alpha)]\}^2$ is generalized: via a computer-assisted algebraic construction, we show that for certain three-component phenomenological potentials

$$V(r) = A\{1 - \exp[-\mu(r - r_\alpha)]\}^2 + B\{1 - \exp[-\mu(r - r_\beta)]\}^3 + C\{1 - \exp[-\mu(r - r_\gamma)]\}^4$$

the closed and exact bound states may exist not only in singlets, but also in doublets and triplets.

1. Introduction and summary

The one-dimensional Schrödinger equation

$$\left[-\frac{d^2}{dr^2} + V(r)\right]\psi(r) = E\psi(r) \qquad r \in (-\infty, \infty) \tag{1}$$

with the so-called Morse potential

$$V(r) = A\{1 - \exp[-\mu(r - r_\alpha)]\}^2 \qquad A > 0 \qquad \mu > 0 \tag{2}$$

is well known and exactly solvable in terms of Laguerre polynomials. The specific shape of potential (2) also explains its immediate phenomenological appeal in molecular physics and quantum chemistry [1].

In the latter setting, a 'more realistic' re-interpretation of our equation (1) is usually preferred, with a three-dimensional s-wave choice of the range of coordinates $r \in (0, \infty)$. During this transition to an unsolvable equation, the related errors are usually made negligible by an *ad hoc* assumption of a very large value for the parameter $r_\alpha \gg 1$ [2].

In contemporary molecular phenomenology, the solvable (or, in three dimensions, 'almost solvable') Morse model represents a highly schematic zero-order approximation (say, to the—often *ab initio*—calculated energy surfaces [3]). Hence, naturally, one may try to introduce corrections and contemplate the next three-term interaction

$$V(r) = A\left(1 - e^{-\mu(r-r_\alpha)}\right)^2 + B\left(1 - e^{-\mu(r-r_\beta)}\right)^3 + C\left(1 - e^{-\mu(r-r_\gamma)}\right)^4 \tag{3}$$

with $C > 0$ for, say, a more reliable prediction of a vibrational molecular spectrum [4].

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Methodically, the simplicity and seemingly 'next-to-solvable' character makes our generalized potential (3) even more challenging. One might study its relationship to the very similar Morse-like interaction terms which emerge in the so-called Toda systems on a lattice [5]. In particular, our Schrödinger-like equation may appear during the stability analysis of their solitons [6] or, in a way proposed by one of the referees, one might immediately identify equations (1) and (3) with some linear differential equations which emerge in the related inverse-scattering formalism [7, p 629].

In accordance with Turbiner [8], another independent motivation for our study stems from the possible existence of certain underlying 'quasidynamical' Lie algebras. Whenever they exist, these algebras (plus the standard theory of their representations) offer a simple *explanation for the existence of a broad class of partially solvable* (the so-called *quasi*-exactly solvable (QES)) systems (cf, e.g., our recent review [9] for more details).

In what follows, we shall see that equations (1) and (3) may easily be identified with one of the known QES systems. Unfortunately, its Lie-algebraic treatment will be shown to offer just a single isolated QES eigenvalue. From the point of view of several important applications (the Hill-determinant [10] and perturbative [11] methods, to name just two), this is not sufficient. In the present paper, we intend to show that in our Schrödinger bound-state problem (1), the exact one-dimensional solvability of the Morse model may still be preserved for forces of the more flexible form (3) and, let us re-emphasize, *at several different energy levels*.

A priori, the possible existence of multiple QES solutions was not clear. Empirically, we have even succeeded in showing that, as a rule, the simplest possibilities regularly fail to reveal any multiplets at all. During our research, such a phenomenon proved extremely discouraging. Only the strong (mostly phenomenological and quantum-chemical [2, 7]) practical relevance of the generalized Morse potentials, as well as the theoretical importance and possible algebraic background of the existence of multiplets [9], kept us moving towards the more complicated situations and, finally, to affirmative answers.

Our presentation of results will start by a concise introduction to the general QES problem (section 2). We shall study in detail the suitable choice of variables (subsection 2.1) and the structure of the underlying (namely, coupled and nonlinear) 'simultaneous solvability' algebraic equations (subsection 2.2). Next, we shall find and describe some of their explicit solutions which form the elementary bound-state doublets (section 3). For clarity, we shall distinguish between the trivial (subsection 3.1) and next-to-trivial (subsection 3.2) cases. Similarly, in section 4, we shall demonstrate the existence of triplets.

The contemporary progress in symbolic manipulations on computers [12] was of significant importance and crucial help. With their assistance, the search for solutions finally proved successful, in spite of the unpleasant fact of life that there are no obvious theorems which would guarantee the simultaneous existence of several bound states 'globally', in a way parallelling some other QES examples [13, 14].

Our results were obtained by the extensive use of computer algebra. Our first seven triplet solutions (namely, the four roots in subsection 4.1 and the three results of subsection 4.2) involve the 'elementary' doublets of subsection 3.1. Together, with the first 'less elementary' closed solution obtained in subsection 4.3, all the first eight constructions remain fully non-numerical. The other possible (and, presumably, numerical) triplet solutions are also sampled here as our ninth solution in subsection 4.3.

Our construction demonstrates the usefulness of the generalization (3) of Morse forces. The complexity of its multiplets is not prohibitive—up to a single exception, all our closed triplet solutions (see later) were purely non-numerical. The elementary character of these triplets resulted from the (unexpected) numerous simplifications encountered in the underlying algebra. An analysis of the deeper reasons for this (as well as of some further open questions, e.g. the conjectured absence of the 'neighbouring' doublets etc) seems to be of less immediate physical appeal and interest. It might deserve a more mathematically oriented study in the future.

2. Elementary bound states

2.1. The Liouvillean change of variables

Let us first re-scale the coordinate $r \to \rho r$ in such a way that $\mu = 2$ in our one-dimensional potentials. The change of variables

$$r \to R = R(r) \equiv \exp(-r) \in (0, \infty) \qquad \psi(r) \to \phi(R) = R^{1/2}\psi(r) \tag{4}$$

may then be performed in accordance with Liouville [15]. This transforms equation (1) into another equivalent radial Schrödinger equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}R^2} + \frac{L(L+1)}{R^2} + V^{(\mathrm{Liouv})}(R)\right]\phi(R) = \varepsilon\phi(R) \tag{5}$$

with the formal Lth wave potential

$$\begin{aligned} V^{(\mathrm{Liouv})}(R) &= g_2R^2 + g_4R^4 + g_6R^6 \\ g_2 &= A\exp(4r_\alpha) + 3B\exp(4r_\beta) + 6C\exp(4r_\gamma) \\ g_4 &= -B\exp(6r_\beta) - 4C\exp(6r_\gamma) \\ g_6 &= C\exp(8r_\gamma) > 0. \end{aligned} \tag{6}$$

We see that our generalized Morse model must share at least some of the distinctive features of the QES sextic oscillators. Even the ordinary Morse potential (with $B = C = 0$) may be understood as being equivalent to the exactly and completely solvable harmonic oscillator itself in this language.

In the 'quasi-realistic' s-wave problem (the approximative half-axis domain is not studied in any detail in what follows), our new 'Liouvillean' system and forces (6) become confined to a box with infinitely high walls at a finite radius $R \in (0, 1)$. Under certain circumstances, this might have high numerical merit [16]. Here, we intend to proceed purely non-numerically.

One of the most attractive properties of sextic oscillators (6) lies in their QES property. The corresponding multiplets of the exact solutions of equations (5) and (6) (with an elementary harmonic-oscillator-like structure of wavefunctions) were originally derived, without any use of Lie algebras, in a detailed paper by Singh *et al* [13]. This publication was preceded by a virtually unnoticed discovery of this possibility by Hautot [17], approximately ten years earlier. Both these studies, not often cited, have inspired a boom of similar constructions during the last fifteen years (cf, for example, their short review [9] as well as a randomly chosen sample [18] of their recurrent rediscoveries).

In contrast to the QES sextic example, the Liouvillean change of variables will assign each element of Singh's multiplet of wavefunctions to a different generalized Morse potential

(3). The explanation is easy. Transformation (4) replaces the original energy E by a new parameter of an 'angular momentum'

$$L = -\tfrac{1}{2} + \sqrt{A+B+C-E} > -\tfrac{1}{2}. \tag{7}$$

Thus, we may write

$$E = A + B + C - Z^2 \qquad Z = L + \tfrac{1}{2} > 0. \tag{8}$$

Alternatively, the 'new energy' ε can be abbreviated to

$$\varepsilon = 2A\exp(2r_\alpha) + 3B\exp(2r_\beta) + 4C\exp(2r_\gamma) \tag{9}$$

and remains fixed by potential (3). As a consequence, a straightforward translation of Singh's construction generates a set of the so-called Sturmians [14] rather than a multiplet of bound states belonging to the same potential.

The feasibility of constructing a genuine multiplet of elementary bound states (so useful, for example, in perturbation theory [19]) remains an open question in the present generalized Morse setting. This inspired our paper which pays attention to the difficult problem of multiplets.

2.2. *The algebraic* QES *conditions*

Morse [1] derives his potential via an elementary special-function ansatz. Here, a more general result will be achieved via a polynomial ansatz

$$\phi^{(\text{elementary})}(R) = e^{-G(R)} R^{L+1} \sum_{n=0}^{N} h_n R^{2n} \qquad L > -\tfrac{1}{2}. \tag{10}$$

Without any further specification of its coefficients and with an arbitary integer $N < \infty$ and a WKB-compatible exponent

$$G(R) = \tfrac{1}{4}\lambda R^4 + \tfrac{1}{2}\xi R^2 \qquad \lambda = \sqrt{C}\exp(4r_\gamma) > 0 \qquad \xi = g_4/(2\lambda) \tag{11}$$

our normalizable (i.e. physical and correct) bound-state ansatz transforms differential equation (1), with a generalized Morse potential, into its algebraic realization

$$\begin{aligned}
&B_n h_{n+1} = C_n^{(0)} h_n + C_n^{(1)} h_{n-1} \\
&B_n = 4(n+1)(n+Z+1) \qquad Z \equiv L + \tfrac{1}{2} \\
&C_n^{(0)} = 2\xi(2n+Z+1) - \varepsilon \\
&C_n^{(1)} = 2\lambda(2n+Z) - \xi^2 + g_2 \qquad n = 0, 1, \ldots \\
&h_0 \neq 0 \qquad h_N \neq 0 \qquad h_{N+1} = h_{N+2} = \cdots = 0.
\end{aligned} \tag{12}$$

At an arbitrary energy (either the 'new' ε or 'old' E), the latter form of Schrödinger's equation happens to be exactly solvable

$$h_{n+1} = \frac{h_0}{\prod_{k=1}^{n} B_k} \det H^{[n]} \qquad n = 0, 1, \ldots$$

$$H^{[n]} = \begin{pmatrix} C_0^{(0)} & -B_0 & & & \\ C_1^{(1)} & C_1^{(0)} & -B_1 & & \\ 0 & C_2^{(1)} & C_2^{(0)} & -B_2 & \\ & & & \ldots & \\ & \ldots & 0 & C_n^{(1)} & C_n^{(0)} \end{pmatrix}. \tag{13}$$

The existence of our closed bound-state solutions proves formally equivalent to the validity of the only two remaining termination or 'self-consistency' conditions

$$C_{N+1}^{(1)}(= 2\lambda(2N + Z + 2) - \xi^2 + g_2) = 0 \tag{14}$$

(cf $h_{N+1} = h_{N+2} = 0$ and $h_N \neq 0$) and

$$\det H^{[N]} = 0 \tag{15}$$

(the requirement $h_{N+1} = 0$ in the language of determinantal equation (13)).

After a short inspection of the former constraint (14), we notice that whenever we fix all the couplings in our generalized Morse potential (3), the only possible source of variation in the 'new angular momentum' parameters L or Z is the dimension N itself

$$Z = Z(N) = (g_4)^2/(2\lambda)^3 - g_2/(2\lambda) - 2N - 2 > 0 \qquad N = 0, 1, \ldots . \tag{16}$$

In ascending order, all the 'solvable' energy levels (if any) become numerated by this N in accordance with equation (8)

$$\begin{aligned} &E_N^{(\text{solvable})} = -4N^2 + 4Nz + A + B + C - z^2 \\ &N = 0, 1, \ldots, N_{\max} \qquad N_{\max} = -\,\text{entier}[-z/2] \\ &z(\equiv Z(0)) = (g_4)^2/(2\lambda)^3 - g_2/(2\lambda) - 2. \end{aligned} \tag{17}$$

Vice versa, at a fixed N, equation (16) enables us to eliminate, say, g_2 as a function of $z = Z(0)$. This reduces the whole set of five free constants in Schrödinger equation (5) to a mere quadruplet.

A re-scaling of the R's enables us to assign any numerical value to r_γ, g_6 or λ. This means that on the r-line, the $r \to -r$ asymmetry of our forces $V(r)$ leaves the position of the origin virtually undetermined. After we take $\lambda = \frac{1}{2}$ for definiteness, we are left with three independent free parameters, say x $(= \varepsilon)$, y $(= -2g_4 \equiv -g_4/\lambda)$ and z $(= Z(0) > 2N \geqslant 0)$.

The proof of the existence of at least one elementary bound-state energy level now has to be based on an analysis of our last constraint (15). One of the available three free parameters must be eliminated by this constraint. With relation (14) taken into account, the constraint reads

$$\det Q^{[N]}(x, y, z) = 0. \tag{18}$$

Here, $Q^{[N]}(x, y, z)$ denotes the $(N + 1)$-dimensional tridiagonal matrix

$$\begin{pmatrix} x + y(Z+1) & 4+4Z & & & \\ 2N & x + y(Z+3) & 16+8Z & & \\ & \cdots & & & \\ & 4 & x + y(Z+2N-1) & 4N^2+4NZ \\ & & 2 & x + y(Z+2N+1) \end{pmatrix} \tag{19}$$

i.e. matrix $H^{[N]}$ with $Z = Z(N) = z - 2N > 0$. Mathematically speaking, we now only have to show that the roots of equation (18) are real. This is not difficult: due to the positivity of all the off-diagonal matrix elements in equation (19), the tridiagonal matrix $Q^{[N]}(x, y, z)$ may easily be symmetrized. Then, algebraic equation (18) may be visualized as a diagonalization of a real and symmetric matrix. Up to a possible degeneracy [20], this always gives an $(N + 1)$-plet of 'Sturmian' real eigenvalues x or y.

3. The construction of doublets

In the study of pairs of elementary bound-state solutions, a necessary condition for their existence

$$\begin{aligned} &\det Q^{[N]}(x,y,z)=0 \qquad N\geqslant 0\\ &\det Q^{[M]}(x,y,z)=0 \qquad M>N \end{aligned} \tag{20}$$

has to be understood as a coupled pair of polynomial equations (18) in two variables, say, x and y. Their choice from a menu

$$\begin{aligned} &x+y(z+1)=0 \qquad N=0\\ &x^2+2yzx+y^2(z^2-1)+8(1-z)=0 \qquad N,M=1\\ &x^3+yx^2(3z-3)+x[y^2(3z^2-6z-1)+16(5-2z)]\\ &\qquad +y(z-3)[y^2(z^2-1)+16(1-2z)]=0 \qquad N,M=2\\ &x^4+yx^3(4z-8)+x^2[y^2(6z^2-24z+14)+80(4-z)]\\ &\qquad +4yx[y^2(z^3-6z^2+7z+2)-8(5z^2-30z+34)]\\ &\qquad +(z-5)[y^4(z-3)(z^2-1)-16y^2(5z^2-15z+4)+576(z-3)]=0\\ &\ldots \qquad\qquad N,M=3 \end{aligned} \tag{21}$$

is instructive in showing the mathematical difficulty of the problem: doublets will be defined as a solution of a coupled pair (20) of nonlinear algebraic equations (21).

3.1. The simplest choice, $N=0$

At $N=0$, the linear item in (21) leads to the unique and real root $x=-y(z+1)$. The positivity of $Z(M)=z-2M>0$ is to be demanded as equivalent to the correct $r\to\infty$ asymptotics (and finite norm) of the wavefunctions. *A priori*, the simplest doublets of elementary bound states might then result from an insertion of x $(=\varepsilon(0))$ in the rest of our menu. We get a new sequence of restrictions

$$\begin{aligned} &8(1-z)=0 \qquad M=1 \qquad z>2\\ &64y(z-2)=0 \qquad M=2 \qquad z>4\\ &576(3-z)[y^2-(z-5)]=0 \qquad M=3 \qquad z>6\\ &2048y(z-4)[3y^2-2(4z-25)]=0 \qquad M=4 \qquad z>8\\ &12\,800(5-z)[6y^4+y^2(217-29z)+9(z-9)(z-7)]=0 \qquad M=5 \qquad z>10\\ &221\,184y(z-6)[5y^4+y^2(322-37z)+4(8z^2-148z+675)]=0\\ &\qquad M=6 \qquad z>12\\ &\ldots \end{aligned} \tag{22}$$

imposed upon y and z.

The simplest choice of degrees $(N, M) = (0, 1)$ implies that $Z(M) = -1$ remains negative and, hence, unacceptable. The related $M = 1$ wavefunction (10) does not behave properly at $R = 0$, i.e. at $r \gg 1$. The choice of larger M's is more rewarding and leads to the following abundance of real and acceptable roots $y = y_m(M, z)$:

$$
\begin{aligned}
&y_1(2, z) = 0 \\
&y_{1,2}(3, z) = \pm\sqrt{z-5} \\
&3y_{1,2}(4, z) = \pm\sqrt{24z - 150} \\
&6y_{1,2,3,4}(5, z) = \pm\sqrt{87z - 651 \pm 3\sqrt{625z^2 - 9130z + 33\,481}} \\
&y_{1,2,3,4}(6, z) = \pm\sqrt{\pm\sqrt{729z^2 - 11\,988z + 49\,684} + 37z - 322}/\sqrt{10} \\
&\ldots.
\end{aligned}
\tag{23}
$$

All these doublet roots stay real under the automatically satisfied conditions $z > c(M)$ with $c(3) = 5$, $c(4) = 6.25$, $c(5) = 9$, $c(6) = 10.34$, etc.

3.2. *The next case, $N = 1$*

At $N = 1$, the quadratic polynomial (21) possesses a pair of real roots

$$
\varepsilon(1) = x_{1,2} = -yz \pm \sqrt{y^2 + 8z - 8} \tag{24}
$$

which define the two different potentials (3). Each of the roots remains real in a non-empty domain $8z + y^2 \geqslant 8$ $(z \geqslant 1)$ which again incorporates all the physical z's, $Z(M) = z - 2M \in (1 - 2M, \infty)$.

The elimination of $\varepsilon(1)$ generates the new hierarchy of equations

$$
\begin{aligned}
&8(3-z)\left(3\sqrt{y^2 + 8z - 8} - y\right) = 0 \qquad M = 2 \\
&128(z-4)\left(2y\sqrt{y^2 + 8z - 8} - y^2 - 12\right) = 0 \qquad M = 3 \\
&\ldots.
\end{aligned}
\tag{25}
$$

An unacceptable imaginary solution emerges at $M = 2$, but the next steps of the search with $M \geqslant 3$ are successful and yield the physical parameters $y^2 = y_j^2(M, z)$ as real roots of polynomials of degree $M - 1$:

$$
\begin{aligned}
\sqrt{3}y_{1,2}(3, z) &= \pm 2\sqrt{2\sqrt{4z^2 - 14z + 19} - 4z + 7} \\
&= \pm 2\sqrt{2\sqrt{4a^2 + 34a + 79} - 4a - 17} \qquad a = z - 6 > 0 \\
&\ldots.
\end{aligned}
\tag{26}
$$

4. The triplets of elementary bound states

Both equations (22) and (25) and their elementary-doublet solutions (23) and (26) depend on the last free parameter z. We may try to fix its value by an additional constraint

$$\begin{aligned} &\det Q^{[N]}(x, y, z) = 0 \qquad N \geqslant 0 \\ &\det Q^{[M]}(x, y, z) = 0 \qquad M > N \\ &\det Q^{[K]}(x, y, z) = 0 \qquad K > M \end{aligned} \tag{27}$$

in combination with the appropriate boundary-condition formula

$$Z(K) = z - 2K > 0. \tag{28}$$

This would guarantee the existence of triplets of elementary bound-state wavefunctions (10) in the given generalized Morse potential (3).

In the light of our preceding results, the absence of doublets implies the absence of triplets at any $(N, M, K) = (0, 1, K)$ and $(N, M, K) = (1, 2, K)$ (and, we feel tempted to conjecture, at any $(N, M, K) = (N, N+1, K)$). We may also eliminate $(N, M, 2k+1) = (0, 2, 2k+1)$ with $k = 1, 2, \ldots$ since all the related solutions read $z = z_i(N, M, K) = z_i(0, 2, 2k+1) = 2k + 2i + 1$, $i = 0, 1, \ldots, k$ and contradict equation (28). Finally, in the case of $(N, M, K) = (0, 2, 2t)$ with $t = 2, 3, \ldots$, with 'quasi-trivial' solutions $x = y = 0$ and with *arbitrary* z's, it is easy to demonstrate that all the related potentials (3) degenerate back to the ordinary Morse force after a re-scaling $\mu \to \mu/2$. Within our present formalism, the quasi-trivial equations (12) with disappearing h_{2k+1}'s degenerate to recurrences for $q_k \equiv h_{2k}$'s:

$$q_1 = -4tq_0/(16 + 8Z) \qquad q_2 = -(4t - 4)q_1/(64 + 16Z), \ldots. \tag{29}$$

These equations are solvable and their solution

$$q_k (\equiv h_{2k}) = (-1)^k 4^{-k} \binom{t}{k} \frac{\Gamma(1 + Z/2)}{\Gamma(k + 1 + Z/2)} q_0 \qquad k = 0, 1, \ldots, t \tag{30}$$

may easily be recognized as a definition of Laguerre polynomials. In this way, the consistency of our approach becomes confirmed *a posteriori*.

For the next few non-trivial (N, M, K)'s, let us now perform a (computer-assisted) search for non-trivial triplets of terminating bound states (10).

4.1. A systematic study of $(N, M, K) = (0, 3, K)$

In the light of equation (28), all the common roots $z_0(N, 3, K) = 3$ and their K-dependent partners $z_1(0, 3, K) = K + 3$ may be ignored as unphysical. An inspection of equation (22) and an elimination of $y^2 = z - 5$ via its third row shows that $K = 4$ and $K = 6$ offer no other real roots, while $K = 5$ gives a just too small (= 'unphysical') root $z_2 = 23/7 \approx 3.29 \ll 10$. The first success is only encountered at $K = 7$. Via a quadratic equation, and in addition to an unphysical $z_2 \approx 3.66$, we get our first physical solution

$$z^{(1)} = z_3(0, 3, 7) = \left(126 + \sqrt{7417}\right)/11 \approx 19.283\,818\,77 \ (> 14). \tag{31}$$

Similarly, $K = 8$ gives the unphysical $z_2 \approx -4.72$ and our second acceptable solution

$$z^{(2)} = z_3(0, 3, 8) = \left(563 + 18\sqrt{3039}\right)/91 \approx 17.091\,079\,83 \; (> 16). \tag{32}$$

In the same manner, the forthcoming sequence of equations

$$\begin{aligned}
&81z^2 - 1694z + 5325 = 0 \qquad K = 9 \\
&374z^3 - 20\,441z^2 + 229\,555z + 245\,840 = 0 \qquad K = 10 \\
&1729z^4 - 55\,730z^3 - 470\,604z^2 + 2\,058\,0178z - 71\,914\,325 = 0 \qquad K = 11 \\
&\ldots
\end{aligned} \tag{33}$$

has to be solved step-by-step. This leads to the unphysical $K = 9$ pair of roots $z_{2,3} = (847 \pm 2\sqrt{71\,521})/81 \approx \{17.06, 3.85\}$ followed by the three $K = 10$ solutions, etc. In the latter case, the unphysical pair $z_{2,3} \approx \{17.55, -0.98\}$ is accompanied by our third physical root

$$\begin{aligned}
z^{(3)} &= z_4(0, 3, 10) = \sqrt{160\,273\,771}\sin[(\theta + \pi)/3]/561 + 20441/1122 \\
&\approx 38.0864 > 20 \\
\tan\theta &= 8\frac{\sqrt{726\,279\,854\,616\,578\,142\,691\,575\,099\,403\,044\,347\,355}}{2\,427\,112\,467\,348\,350\,355\,585}.
\end{aligned} \tag{34}$$

This is to be complemented by the four real roots $z_{2,3,4,5}$ at $K = 11$. Besides the unphysical subset $z_{2,3,4} \approx \{-19.35, 4.02, 18.25\}$, our fourth well behaved solution is

$$z^{(4)} = z_5(0, 3, 11) = \cdots \approx 29.319\,614 > 22. \tag{35}$$

In principle, this is still a non-numerical result [20], but study of the higher K's already seems to require an alternative purely numerical approach to the corresponding polynomial equations (33).

4.2. The case of $(N, M, K) = (0, 4, K)$

The common root $z_0(N, 4, K) = 4$, the less trivial and K-dependent integer $z_1(0, 4, K) = K + 4 < 2K$, the fractional and unique solutions of linear equations $z_2(0, 4, 5) = 461/77 \approx 5.99$, $z_2(0, 4, 6) = 115/28 \approx 4.11$ and $z_2(0, 4, 8) = 1433/320 \approx 4.48$ at $K = 5$, 6 and $K = 8$ as well as, finally, the two $K = 7$ roots $z_{2,3}(0, 4, 7) = (197 \pm 6\sqrt{33\,829})/221 \approx \{5.88, 4.10\}$ of the underlying quadratic equation may be ignored. All of them violate normalizability condition (28). Only the subsequent $M = 4$ counterparts of equation (33), namely

$$\begin{aligned}
&33\,649z^3 - 1\,432\,887z^2 + 8\,607\,483z - 7\,813\,045 = 0 \qquad K = 9 \\
&16\,016z^3 - 399\,768z^2 - 1\,531\,515z + 14\,532\,070 = 0 \qquad K = 10 \\
&96\,135z^4 + 45\,620z^3 - 87\,827\,630z^2 + 696\,931\,300z - 1\,172\,415\,169 = 0 \qquad K = 11 \\
&\ldots
\end{aligned} \tag{36}$$

become productive. At $K = 9$ they give the (still non-numerical) unphysical solutions $z_2(0, 4, 9) \approx 5.90$, $z_3(0, 4, 9) \approx 1.11$ plus our fifth satisfactory root

$$\begin{aligned} z^{[5]} &= z_2(0, 4, 9) \\ &= 8\sqrt{8\,224\,066\,447}\sin[(\phi + \pi)/3]/33\,649 + 477\,629/33\,649 \approx 35.576\,62 \\ \tan\phi &= 5\frac{\sqrt{16\,431\,691\,081\,236\,520\,032\,956\,144\,866\,990\,550\,350\,030\,008\,502}}{260\,640\,269\,959\,315\,432\,063\,878}. \end{aligned} \tag{37}$$

Similarly, the unphysical pair $z_2(0, 4, 10) \approx -7.03$ and $z_3(0, 4, 10) \approx 4.74$ is complemented by the physical

$$\begin{aligned} z^{[6]} &= z_4(0, 4, 10) \\ &= \sqrt{1\,620\,838\,101}\sin[(\psi + \pi)/3]/2002 + 16\,657/2002 \approx 27.247\,85 \\ \tan\psi &= 26\,217\frac{\sqrt{1\,744\,721\,478\,818\,204\,141\,179\,114\,862\,880\,068\,355}}{58\,154\,543\,543\,305\,571\,091\,730}. \end{aligned} \tag{38}$$

The list of non-numerical possibilities seems completed by a biquadratic equation (36) at $K = 11$. The unacceptable triplet of its too small roots $z_2(0, 4, 11) \approx -33.97$, $z_3(0, 4, 11) \approx 2.41$, $z_4(0, 4, 11) \approx 5.93$ is accompanied by our last $N = 0$ acceptable solution

$$z^{[7]} = z_5(0, 4, 11) = \cdots \approx 25.153\,897 > 22\ldots. \tag{39}$$

Again, the latter root is non-numerical [20] but its explicit non-numerical form proves impractical for virtually any purpose.

4.3. The more complicated series $(N, M, K) = (1, 3, K)$

At $N = 1$, we have to expand the even powers of the square root $v = \sqrt{64(4z^2 - 14z + 19)/9}$ in terms of z's. This is a clumsy but straightforward procedure—we obtain equations which are linear in v and of the $(K-1)$th order in the second variable z:

$$\begin{aligned} &7075z^3 - 15z^2(80v + 5739) + 15z(796v + 19\,651) - 24\,780v - 271\,915 = 0 \qquad K = 4 \\ &\ldots. \end{aligned} \tag{40}$$

The elimination of v and its squaring leads to another series of equations

$$\begin{aligned} &13\,475z^4 - 196\,000z^3 + 725\,114z^2 - 659\,040z - 272\,925 = 0 \qquad K = 4 \\ &560z^3 - 8351z^2 + 33\,096z - 33\,260 = 0 \qquad K = 5 \\ &\ldots. \end{aligned} \tag{41}$$

Their K-dependence ceases to be trivial—we obtain a polynomial of the eighth degree at $K = 6$, etc. We may omit the redundant details now. In addition to the unphysical $z_2(1, 3, 4) = -0.304$, $z_3(1, 3, 4) = 15/7 \approx 2.14$ and $z_4(1, 3, 4) \approx 3.31$, we get our final non-numerical physical $K = 4$ solution

$$z^{[8]} = z_2(1, 3, 4) = \cdots \approx 9.397\,468\,8 > 8. \tag{42}$$

Indeed, the next equation produces just unacceptable roots $z_2(1, 3, 5) = 9.18$, $z_3(1, 3, 5) = 4.19$, $z_4(1, 3, 5) = 1.54$ while, as already mentioned, the subsequent $K = 6$ item in equation (41) would already require a purely numerical treatment.

Finally, it should be noted that the specialized numerical algorithms proved to be extremely efficient in practice. Their careful use even enabled us to prove the existence of the physical solutions of the type

$$z^{[9]} = z_2(1, 3, 6) = \cdots \approx 15.078\,82 > 12 \tag{43}$$

i.e. roots and bound states without a consequently non-numerical character.

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