Bound state method with elementary-product wavefunctions: J. Phys. A 28 (1995) 6265-76

M. Znojil

Ústav jaderné fyziky AV ČR, 250 68 Řež u Prahy, Czech Republic

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Abstract

We propose a new version of multipoint Padé technique to solve Schrödinger equations in their first-order Riccati form. Our compact product representation of wavefunctions interpolates or "matches" available approximants at several points. The mechanism of "matching" determines the energies and eliminates spurious solutions. On $V(x) = \mu^2 x^2 + \lambda x^2/(1 + g x^2)$, its efficiency is illustrated numerically.

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1 Introduction

In the applied quantum mechanics, realistic calculations often rely on the sophisticated variational constructions with non-orthogonal bases $\{|n\rangle\}$. One-dimensional and/or central-symmetric models and Hamiltonians $H = -\frac{\hbar^2}{2m}\triangle + V(\vec{r})$ with power-series wavefunctions

$$|\Psi\rangle = \sum_{n=n_0}^{\infty} a_n\,|n\rangle, \qquad \langle r|n\rangle = r^n\,\exp[-\omega(r)] \tag{1}$$

are being recalled as a methodical guide. With a suitable $\omega(r)$, they do not only reproduce the well known special-function solutions [1] but they also remain applicable to the majority of the "next-to-solvable" polynomial interactions

$$V(r) = a + b\,r^2 + c\,r^4 + \ldots + z\,r^{2p}. \tag{2}$$

The lack of orthogonality of $|n\rangle$'s (1) makes the direct calculation of the physical bound-state energies E a little bit tedious. One may employ a purely numerical matching of Ansatz $\Psi(r)$ to its correct asymptotics [2] (physics remains clearly represented by the standard boundary conditions) as well as a more algebraic Hill determinant method [3]. Unfortunately, serious difficulties may arise for the very next, non-polynomially generalized class of forces (2),

$$V(r) = \frac{a + b\,r^2 + c\,r^4 + \ldots + z\,r^{2p}}{A + B\,r^2 + C\,r^4 + \ldots + Z\,r^{2P}} \tag{3}$$

due to the influence of the complex poles on the analytic properties of $\Psi(r)$'s [4]. At the same time, the choice of exponents $\omega(r)$ in $|n\rangle$'s remains virtually arbitrary and plays just an auxiliary role [5].

An improvement of $\omega(r)$'s [6] or even a full replacement of wavefunctions $\Psi(r)$ by their (negative) logarithmic derivatives $F(r) = -\Psi'(r)/\Psi(r)$ (well motivated numerically: [7]) seems to be a promising methodical alternative. In a way suggested recently by Fernández et al [8], the particularly useful form of transition $\Psi(r) \to F(x)$ may be based on, or combined with, the standard Padé approximation [9]. Numerically, such an approach (Riccati-Padé method, RPM) proved fully capable to compete with the other and specialized numerical algorithms [10]. In a non-numerical setting, the direct use of $F(r)$'s simplifies, e.g., the analysis and constructions of particular (so called quasi-exact) elementary bound-state solutions (cf. [11]) as well as of perturbation expansions (cf. ref. [12] for a nice illustration). Here, we shall study and develop the RPM idea further on.

In sections 2 and 3, we shall emphasize non-numerical aspects of the RPM constructions and restrict our attention to wavefunctions. Energy E will be treated there as a mere external parameter. Having the general class of forces (3) in mind, section 2 will pay attention to the transition from the ordinary linear Schrödinger equation for $\Psi(r)$'s to its equivalent nonlinear Riccati re-arrangement for $F(r)$'s and vice versa. The closed-formula character of these transformations will be stressed, assigning a product form to wavefunction $\Psi(r)$ in a way which reflects the partial-fraction re-summation of the functions $F(r)$.

Section 3 will develop the construction of $\Psi(r)$'s in more detail. "Teaching by" the simplest $p = 2$ and $P = 1$ example, it will display the recurrent power-series structure of $F(r)$'s. Next, it will re-recommend (cf. [10]) the two-point Padé interpolation between the threshold and asymptotic WKB-like approximations. Finally, it will also introduce a brand new idea of matching the (easily determined) complex-plane singularities (if any) via a (in practice: simpler!) multi-point Padé fit.

The consistent numerical determination of energies will be studied in the second part of the paper (section 4). In subsection 4.1, we re-derive the old (one-point, extrapolative – cf. [8] – and two-point, interpolative – cf. [10]) RPM recipes, and describe their new, multi-point (explicitly: three-point) Padé descendants. The (rather extensive family of) possible secular equations will be numbered by their dimension, by the number of the incorporated "boundary conditions" and, finally, by an auxiliary set of "weights" of the separate "boundary conditions" (here: an integer parameter J).

As long as one of the main obstacles of a broader applicability of the (otherwise: fairly universal and marvelously convergent) older numerical RPM prescriptions [8, 12] seems related to occurrence of numerous redundant energy approximants, subsections 4.2 and 4.3 will pay more attention to their elimination. We conjecture and test a new algorithm which employs the variability of J (in practice, from -1 up to cca half of its maximal permissible value) for such a purpose. The key importance of the resulting suppression of ambiguities and selection of the optimal and reliable approximants is re-emphasized in the summary (Section 5).

2 Wavefunctions

In accord with the numerous studies initiated by the old work by Darboux [13], a switch from wavefunctions $\Psi(r)$ to their negative logarithmic derivatives $F(r) = -\Psi'(r)/\Psi(r)$ proves useful for a coordinate-dependent analysis of scattering [14], as a complement of the textbook Rayleigh-Schrödinger perturbation theory [15] and also in the supersymmetric quantum mechanics [16]. Here, we intend to describe several further merits of the related exponential-plus-integral re-parametrization

$$\Psi(r) = \exp\left[-\int_{r_{ini}}^{r} F(x)dx\right] \tag{4}$$

of the bound-state wavefunctions.

2.1 The descriptive properties of $F(r)$'s

The emergence of a nodal zero in the wavefunction $\Psi(r) = (r - r_z)\Psi_0(r)$ at a real r_z induces a pole in the logarithmic derivative, $-F(r) = -F_0(r) + 1/(r - r_z)$. Near this pole, the return from $F(r)$ to $\Psi(r)$ must be performed carefully: At $r > r_z$, the term $1/(r-r_z)$ emerges as the first derivative of $\ln(r-r_z)$, but the same term is also equal to the first derivative of $\ln(r_z - r)$ at $r < r_z$. With integration (4) defined in the sense of Cauchy principal value, an incorrect wavefunction would result, $\Psi(r) = |(r-r_z)|\Psi_0(r)$. Vice versa, we obtain a correct wavefunctions once we fix, say, $r_{ini} > r_z$, shift r_z slightly off the real axis, $r_z \to r_z - i\varepsilon$, and use the definition

$$(r - r_z) \times \Psi_0(r) = \exp\left[\int_{r_{ini}}^{r} \left(-F_0(x) + \frac{1}{x - r_z + i\varepsilon}\right) dx\right] \tag{5}$$

in the limit $\varepsilon \to 0^+$ (cf. ref. [1], p. 177, eq. (7.7)).

The feasibility of the closed-form integration is an important merit of such a construction. It extends to all the Padé approximated $F(r)$'s and reconstructed $\Psi(r)$'s. Indeed, whenever we expand

$$F(r) \approx F^{\{M_1,\, M_2\}}(r) = \frac{f_{0,0} + f_{0,1}\, r + \ldots + f_{0,M_1} r^{M_1}}{f_{1,0} + f_{1,1} r + \ldots + f_{1,M_2} r^{M_2}}, \quad M_1 + M_2 \gg 1. \tag{6}$$

in the sum of partial elementary fractions (plus powers if any),

$$\begin{aligned} F^{\{M_1,\, M_2\}}(r) &= z\, r^{M_1 - M_2} + y\, r^{M_1 - M_2 - 1} + \ldots \\ &+ \sum_k \left[\frac{c_{k,1}}{(r - r_k)} + \frac{c_{k,2}}{(r - r_k)^2} + \ldots + \frac{c_{k,m(k)}}{(r - r_k)^{m(k)}}\right] \end{aligned} \tag{7}$$

([17], sec. 1.7-4), all the integrals in (4) remain expressible in closed form. Besides the trivial integrations of powers r^n and of the above-mentioned $m(k) = 1$ case, the rule

$$\int^{r} \frac{\mathrm{d}x}{(x - r_k)^m} = const - \frac{1}{(m-1)(r - r_k)^{m-1}}, \quad m > 1 \tag{8}$$

applies in general ([17], sec. 4.6-6). Finally, having the exponent $F(r)$ defined in the form of a sum (of logarithms and the like), it makes sense to simplify and re-write wavefunction $\Psi(r)$ as a product. In the exact limit $M_1 \to \infty$, $M_2 \to \infty$, both the partial fraction sums in $F(r)$ and products in $\Psi(r)$ become infinite.

2.2 The threshold and asymptotic approximations

Assume that $V(r)$'s are not too singular (i.e., whenever $\lim_{r\to 0} r^2\, V(r) > -1/4$) and replace angular momenta $l = 0, 1, \ldots$, by the real parameters $\ell = \ell(l)$ defined by the quadratic equation

$$\ell(\ell+1) = l(l+1) + \lim_{r\to 0} r^2\, V(r), \quad \mathcal{R}e(\ell) > -1/2. \tag{9}$$

Then, we may postulate the threshold boundary condition in the simple form [1]

$$\Psi(r_0) \approx r_0^{\ell+1}, \qquad |r_0| \ll 1. \tag{10}$$

Among all the corresponding regular $\Psi(r)$'s, correct physical bound states become selected by the second, asymptotic boundary condition. We may write it in the explicit form

$$\Psi(r_\infty) \approx \exp\left(-\frac{\mu}{s} r_\infty^s\right), \qquad |r_\infty| \gg 1 \tag{11}$$

whenever $\lim_{r\to\infty} r^{2-2s}\, V(r) = \mu^2 < \infty$ at some suitable s.

In accord with standard textbooks [2], Schrödinger equation

$$-\Psi''(r) + \frac{\ell(\ell+1)}{r^2}\Psi(r) + V(r)\Psi(r) = E\Psi(r), \quad r(\equiv |\vec{r}|) \in (0,\infty) \tag{12}$$

may be re-written as an equivalent nonlinear, first-order Riccati differential equation

$$F'(r) - F^2(r) + \frac{\ell(\ell+1)}{r^2} + V(r) - E = 0. \tag{13}$$

Expanding the denominator of $V(r)$ (3) in a geometric series, we may recall the standard power-series philosophy and postulate, near the threshold,

$$F(r) = \sum_{j=j_0}^{\infty} F_j r^j . \tag{14}$$

In the zeroth-order approximation, the regularity of $V(r)$ leads just to the quadratic algebraic selfconsistency condition which fixes $j_0 = -1$ and defines a pair of the eligible leading-order coefficients $F_{-1}^{(+)} = \ell$ and $F_{-1}^{(-)} = -\ell - 1$. Recurrently, they would generate the two sequences of coefficients $\{F_j^{(\pm)}\}$ and, subsequently, the pair of independent $\Psi(r)$'s, as they should. Vice versa, the physical (= regular) solutions (compatible with eq. (10)) possess $F_{-1} = F_{-1}^{(-)} = -\ell - 1$, and we may discard the plus-superscripted solutions $F_j^{(+)}$ as redundant and unphysical.

A parallel natural asymptotic series assumption based on eq. (11) reads

$$F(r) \sim \sum_{k=1-s}^{\infty} G_k r^{-k}, \quad r \gg 1 \tag{15}$$

and implies the unique and physical $G_{-1} = \mu$ and G_k's.

3 An anharmonic oscillator illustration

For each particular interaction $V(r)$, it remains for us to derive the proper form of $F(r) \approx F^{\{M_1, M_2\}}(r)$ from the available input F_j's and G_k's. Let us illustrate this procedure on a simple though nontrivial example

$$V_{(\mu,\lambda,g)}(x) = \mu\, x^2 + \lambda\, x^2/(1 + g\, x^2), \qquad g > 0 \tag{16}$$

which seems extremely suitable for such a purpose. A phenomenological appeal makes the family of interactions (16) frequently encountered in the current literature (cf., e.g., its extensive list in [4]).

Methodically, our choice is, first of all, dictated by its non-polynomiality (3). In accord with preceding section, nonlinear recurrences

$$(2\ell+k+3)F_{k+1} - \sum_{n=0}^{k} F_n F_{k-n} - E\delta_{k,0} + (\mu^2+\lambda)\delta_{k,2} - \lambda g \delta_{k,4} + \lambda g^2 \delta_{k,6} - \ldots = 0,$$
$$k = -1, 0, 1, \ldots \qquad (17)$$

result from eq. (14) and assign zeros to all the even coefficients, $F_0 = F_2 = \ldots = 0$. After we modify our notation accordingly,

$$F(r) \approx F^{[K]\,(\mathrm{regular})}(r) = \frac{f_0}{r} + \sum_{n=1}^{K} f_n r^{2n-1} + O(r^{2K+1}) \qquad (18)$$

we may generate the explicit $f_0 \equiv F_{-1} = -\ell - 1$, $f_1 \equiv F_1 = E/(2\ell+3)$, $f_2 \equiv F_3 = [E^2/(2\ell+3)^2 - \mu^2 - \lambda]/(2\ell+5)$ etc. Similarly, equation (15) implies the second set of recurrences

$$-\sum_{n=-1}^{k+1} G_n G_{k-n} - (k-1)G_{k-1} + (-E+\lambda/g)\delta_{k,0} + [\ell(\ell+1) - \lambda/g^2]\delta_{k,2} + \lambda/g^3 \delta_{k,4} - \ldots = 0,$$
$$k = -1, 0, 1, \ldots \qquad (19)$$

with disappearing $G_0 = G_2 = \ldots = 0$. The shortened formula

$$F(r) \approx F^{[J]\,(\mathrm{Jost})}(r) = g_0\, r + \sum_{m=1}^{J} g_m r^{-(2m-1)} + O(r^{-(2J+1)}) \qquad (20)$$

may, *mutatis mutandis*, be assigned $g_0 \equiv G_{-1} = \mu$, $g_1 \equiv G_1 = (s - E + \lambda/g)/2\mu$ etc.

3.1 Integration

An overall requirement of compatibility of our universal Padé formula (6) with the particular regular expansion (18) and with its Jost-type counterpart (20), i.e., the respective prescriptions

$$F^{\{M_1,\, M_2\}}(r) = F^{[K]\,(\mathrm{regular})}(r) + O(r^{2K+1}), \quad |r| \ll 1 \qquad (21)$$

and

$$F^{\{M_1,\,M_2\}}(r) = F^{[J]\,(\mathrm{Jost})}(r) + O(r^{-(2J+1)}), \quad |r| \gg 1 \tag{22}$$

constraint the full freedom of eq. (6),

$$F^{\{M_1,\,M_2\}}(r) \equiv F^{[N]}(r) = \frac{a_0 + a_1\, r^2 + a_2 r^4 + \ldots + a_{N+1} r^{2N+2}}{b_1 r + b_2 r^3 + \ldots + b_{N+1} r^{2N+1}}. \tag{23}$$

Any denominator in such a function may be given the factorized form,

$$F^{[N]}(r) = \frac{a_0 + a_1\, r^2 + a_2 r^4 + \ldots + a_{N+1} r^{2N+2}}{c_1 r\,(1+g_0\, r^2)(1+g_1\, r^2)\ldots(1+g_{N-1}\, r^2)} \tag{24}$$

so that we may generate and integrate the partial-fraction expansion,

$$\int^r F^{[N]}(x)\,\mathrm{d}x \equiv \int^r \left[\frac{\alpha}{x} + \left(\sum_j \frac{2\,g_j\,\beta_j\,x}{1+g_j\,x^2}\right) + \gamma\,x\right]\,\mathrm{d}x$$

$$= \alpha\,\ln r + \left(\sum_j \beta_j\, \ln(1+g_j\, r^2)\right) + \frac{1}{2}\gamma\, r^2 \tag{25}$$

where the coefficients $\beta_j = \beta_j^{[N]}$ read

$$\beta_0^{[1]} = \frac{-a_0\, g_0^2 + a_1\, g_0 - a_2}{2\, g_0^2}, \tag{26}$$

$$\beta_0^{[2]} = \frac{a_0\, g_0^3 - a_1\, g_0^2 + a_2\, g_0 - a_3}{2\, g_0^2\,(g_1 - g_0)}, \quad \beta_1^{[2]} = \frac{a_0\, g_1^3 - a_1\, g_1^2 + a_2\, g_1 - a_3}{2\, g_1^2\,(g_0 - g_1)} \tag{27}$$

or

$$\beta_0^{[3]} = -\frac{a_0\, g_0^4 - a_1\, g_0^3 + a_2\, g_0^2 - a_3\, g_0 + a_4}{2\, g_0^2\,(g_0^2 - g_0\,(g_1+g_2) + g_1\, g_2)}, \quad \beta_1^{[3]} = \frac{a_0\, g_1^4 - a_1\, g_1^3 + a_2\, g_1^2 - a_3\, g_1 + a_4}{2\, g_1^2\,(g_0 - g_1)\,(g_1 - g_2)},$$

$$\beta_2^{[3]} = \frac{a_0\, g_2^4 - a_1\, g_2^3 + a_2\, g_2^2 - a_3\, g_2 + a_4}{2\, g_2^2\,(g_0 - g_2)\,(g_2 - g_1)} \tag{28}$$

etc. As long as $\alpha = -\ell - 1$ and $\gamma = \mu$, this defines the wavefunctions $\Psi(r)$ non-numerically,

$$\Psi(r) = r^{\ell+1} \exp\left(-\frac{\mu}{2}\, r^2\right)\, (1+g_0\, r^2)^{\beta_0}(1+g_1\, r^2)^{\beta_1} \ldots (1+g_{N-1}\, r^2)^{\beta_{N-1}}. \tag{29}$$

At $N = 0$, the nodeless exact ground-state structure of the $\lambda = 0$ harmonic oscillator is reproduced. At all the finite $N < \infty$, the generalized elementary form of eq. (29) makes the scheme attractive for variational purposes. We skip *this* idea here.

3.2 Padé coefficients

3.2.1 One-point scheme.

The explicit determination of coefficients in the fundamental eq. (23) remains routine [9]. At some fixed and finite K we re-write eq. (21) as a set of $K+1$ algebraic equations

$$a_k = f_k b_1 + f_{k-1} b_2 + \ldots + f_0 b_{k+1}, \quad k = 0, 1, \ldots, K, \tag{30}$$

understanding that $a_{N+2} = a_{N+3} = \ldots = 0$ and $b_{N+2} = b_{N+3} = \ldots = 0$. Without any additional requirement, we may already perform a transition to eq. (23) provided only that the number of the new parameters remains the same, $2N+2 = K+1$. Indeed, the first $N+2$ lines of eq. (30) form an explicit linear matrix definition of the numerator (coefficients a_i),

$$a_k = f_k b_1 + f_{k-1} b_2 + \ldots + f_0 b_{k+1}, \quad k = 0, 1, \ldots, N+1. \tag{31}$$

The remaining N items

$$-f_k b_1 = f_{k-1} b_2 + \ldots + f_{k-N} b_{N+1}, \quad k = N+2, N+3, \ldots, 2N+1 \tag{32}$$

is another matrix-inversion definition of the $N+1$ coefficients b_j, one of which (say, $b_1 \equiv 1$) was chosen, in advance, as a normalization.

3.2.2 Two-point scheme.

After we complement eq. (21) by its asymptotic-estimate counterpart (22) or, order-by-order in r,

$$a_{N+1-j} = g_j b_{N+1} + g_{j-1} b_N + \ldots + g_0 b_{N+1-j}, \quad j = 0, 1, \ldots, J, \tag{33}$$

we may concatenate both the systems (30) and (33) and solve them as $K+J+2$ non-homogeneous linear algebraic equations for the $2N+2$ unknown coefficients a_i and b_j.

The resulting Padé formula (often called a two-point Padé approximant $F^{[N]}(r)$ – cf. the book [9], p. 100, for more details) with a normalization $b_1 = 1$ or $b_{N+1} = 1$ may easily be constructed in the same routine manner as above.

3.2.3 The simplified three-point scheme

In the $N \to \infty$ limit, Padé formulae for $F(r)$ and/or $\Psi(r)$ may develop a singularity near each pole of $V(r)$. Knowing their positions ($r_{\text{pole}} = \pm i/\sqrt{g}$ in our example), we may simulate the presence of a singularity in advance. In particular, postulating $g_0 \equiv g$, i.e.,

$$F^{[N]}(r) = \frac{a_0 + a_1 r^2 + a_2 r^4 + \ldots + a_{N+1} r^{2N+2}}{(1 + g\, r^2)(c_1 r + c_2 r^3 + \ldots + c_N r^{2N-1})} \tag{34}$$

at any finite N, we have just re-defined the b's,

$$b_1 = c_1,\ b_2 = g\, c_1 + c_2,\ \ldots, b_N = g\, c_{N-1} + c_N,\ b_{N+1} = g\, c_N. \tag{35}$$

The new (multi-point – here: four- or rather three-point) Padé formulae will only contain less unknown coefficients, $2N + 1 = K + J + 2$.

4 Energies

4.1 Secular equations

Up to now, the physical bound-state energy E was a free parameter. In the spirit of the extrapolative philosophy of the Riccat-Padé method of ref. [8] and/or of its interpolative modification [10], we shall fix the energy via one more row

$$f_{K+1} = [a_{K+1} - (f_K b_2 + \ldots + f_0 b_{K+2})]/b_1. \tag{36}$$

added to eq. (30) or, alternatively, via an additional item

$$g_{J+1} = [a_{N-J} - (g_J b_N + \ldots + g_0 b_{N-J})]/b_{N+1} \tag{37}$$

written in the spirit of eq. (33).

4.1.1 $J = -1$ and the old one-point RPM extrapolation

Without any explicit information about asymptotics (i.e., after having fixed $J = -1$ in the above one- or two-point Padé schemes), one retains the old elimination (31) of a_j's and complements the remaining N equations (30) for the N unknown (normalized) b_j's by the additional equation (36). In the other words, we just convert the old non-homogeneous set of N equations into the homogeneous linear set of $N+1$ equations. It possesses a nontrivial solution if and only if its secular determinant disappears,

$$\det \|f_{N+i-j+2}\|_{i,j=1}^{N+1} = 0, \quad J = -1 \tag{38}$$

More details may be found elsewhere [8].

4.1.2 $J \geq 0$ and the old two-point RPM interpolations

The energy-determining RPM incorporation of the one-line equation (36) or (37) may be re-interpreted as a one-unit increase of the integer K or J, respectively. With $K + J = 2N + 1$ in an extended two-point scheme, nontrivial combinations of equations (30) and (33) start at $J = 0$. With the same definition (31) of a_j's as above, a sequence of the homogeneous linear sets of $N+1$ equations for b_j's is obtained. The Toeplitz-determinant conditions of their nontrivial solvability remain similar to eq. (38),

$$\left| \begin{array}{ccccc} f_{N+1} & f_N & \cdots & f_2 & (f_1 - g_0) \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ f_{2N+1} & f_{2N} & \cdots & f_{N+2} & f_{N+1} \end{array} \right| = 0, \quad J = 0, \tag{39}$$

$$\begin{vmatrix} f_N & \cdots & f_2 & (f_1-g_0) & (f_0-g_1) \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ f_{2N} & \cdots & f_{N+2} & f_{N+1} & f_N \end{vmatrix} = 0, \quad J=1, \tag{40}$$

etc (cf. ref. [10] for more details).

4.1.3 The new, three-point RPM secular equations

With the $N+1$ two-point coefficients b_j replaced, in accord with eq. (35), by the N three-point coefficients c_k, we may fit the $K+1$ plus $J+1$ input coefficients f_k and g_k to the $2N+1$ output arbitrarily normalized Padé parameters a_i and c_j plus one energy E, i.e., $K+J+2=2N+2$. After the same elimination of a_j's as above, we get secular determinants again. Their three-point series starts from the exceptional

$$\begin{vmatrix} f_{N+2}+gf_{N+1} & f_{N+1}+gf_N & \cdots & f_3+gf_2 \\ f_{N+3}+gf_{N+2} & f_{N+2}+gf_{N+1} & \cdots & f_4+gf_3 \\ \cdots & \cdots & \cdots & \cdots \\ f_{2N+1}+gf_{2N} & f_{2N}+gf_{2N-1} & \cdots & f_{N+2}+gf_{N+1} \end{vmatrix} = 0, \quad J=-1 \tag{41}$$

which matches just the incomplete doublet of “boundary conditions” at $r=0$ and at $r^2=-1/g$. The further, regular three-point equations form a sequence

$$\begin{vmatrix} f_{N+1}+gf_N & f_N+gf_{N-1} & \cdots & f_2+g(f_1-g_0) \\ f_{N+2}+gf_{N+1} & f_{N+1}+gf_N & \cdots & f_3+gf_2 \\ \cdots & \cdots & \cdots & \cdots \\ f_{2N}+gf_{2N-1} & f_{2N-1}+gf_{2N-2} & \cdots & f_{N+1}+gf_N \end{vmatrix} = 0, \quad J=0, \tag{42}$$

$$
\begin{vmatrix}
f_N + g f_{N-1} & f_{N-1} + g f_{N-2} & \cdots & f_1 - g_0 + g(f_0 - g_1) \\
f_{N+1} + g f_N & f_N + g f_{N-1} & \cdots & f_2 + g(f_1 - g_0) \\
\cdots & \cdots & \cdots & \cdots \\
f_{2N-1} + g f_{2N-2} & f_{2N-2} + g f_{2N-3} & \cdots & f_N + g f_{N-1}
\end{vmatrix} = 0, \quad J = 1 \qquad (43)
$$

etc., which ends, formally, at the $K = 0$ item

$$
\begin{vmatrix}
-(g_N + g\, g_{N+1}) & -(g_{N+1} + g\, g_{N+2}) & \cdots & -(g_{2N-1} + g\, g_{2N}) \\
\cdots & \cdots & \cdots & \cdots \\
-(g_2 + g\, g_3) & -(g_3 + g\, g_4) & \cdots & -(g_{N+1} + g\, g_{N+2}) \\
f_0 - (g_1 + g\, g_2) & -(g_2 + g\, g_3) & \cdots & -(g_N + g\, g_{N+1})
\end{vmatrix} = 0, \quad J = 2N. \qquad (44)
$$

Let us notice that the dimensions of determinants are smaller, namely, equal to N now.

4.2 Variable matching J as a new methodical freedom

For the simplest numerical illustration of efficiency of the old as well as new RPM schemes we restricted our attention just to the single set of couplings $\mu = 1$, $\lambda = 1$ and $g = 1$. The results presented in Table 1 indicate the quick growth of precision with the growing sum of weights K and J of the respective threshold and asympotic input information.

One may notice that the exact numerical values of energies ($E_{\text{exact}} = 1.232\ 350\ 723$ for ground state [18], etc) seem bracketed by their separate RPM estimates at different J's. If confirmed by the further numerical and/or analytic work, the latter bracketing phenomenon might facilitate a standard numerical acceleration of convergence [19].

The precision seems to remain the same or comparable for (at least the first few) different J's at a fixed N. The use of the large $J > N$ should be discouraged, in full accord with our older experience [10].

At the smallest dimensions (cf. Table 2), the identification of the unique physical energy root is not difficult once it proceeds, in agreement with the standard RPM recommendations, via the tentative N-independence criterion (cf. also [12]). Indeed, the total number of roots (denoted here as $\mathcal{N} \equiv \mathcal{N}(K, J)$) is still very small. The closest left and right neighbours of the correct energy root remain strongly N-dependent (if applicable, we listed a real part of the closest complex root in parentheses, indicating its auxiliary character).

In accord with Tables 1 and 2, an overall pattern of the $K + J \to \infty$ convergence seems uninfluenced by technical differences between our old (two-point) and new (three-point) RPM schemes. Even at a fixed N, the precision remains solely controlled by the amount of the input information $K + J$ itself, remaining almost constant at several different J's. It is just of a marginal technical interest to notice that in fact, the new three-point scheme (characterized by the even $K + J$) is slightly more efficient (than its two-point alternative with odd $K + J$) as it works with matrices of the slightly smaller dimension.

What is more exciting is the observation that at a (still comparatively small) dimension 6, Table 1 already offers cca eight correct significant digits in the ground state energy. In accord with Table 3, also the precision of the excited-state energies decreases much less than you would expect in the light of the smallness of the dimension. The last row offers the best estimates provided by the simple J-averaging which, for example, leads to the nine-digit precision in the resulting ground state energy.

4.3 Spurious roots at large N

At a fixed level of precision, the necessary RPM secular matrix dimensions are, purely empirically, much smaller than in the other methods available in the current literature [4, 18]). Hence, RPM may seem suitable for high-precision computations. Unfortunately, its current versions cannot be considered absolutely superior in this area. The reason lies in the observation that the growth of N leads to an accumulation of many spurious roots near the exact one. This makes the standard numerical RPM high-precision algorithms ambiguous [12].

The free variability of J seems to bring a new hope. Indeed, besides the expected N-oscillations, Table 2 indicates also a presence of a strong oscillatory J-dependence of all the spurious solutions. In comparison, correct roots only exhibited a much less pronounced J-dependence. A simpler and more straightforward rule and criterion of optimality may be conjectured: Discard all the roots which oscillate too quickly with the change of J.

At the higher N's, our conjecture is, for the present particular example at least, well confirmed by our final Table 4 empirically. Its large, $O(10^{-3})$ oscillations of spurious ground states contrast sharply with the strongly suppressed $O(10^{-7})$ oscillations of the correct roots (explicitly, the differences $E^{\text{correct}}_{\text{ground state}} - E_{\text{exact}}$ also appear in the third column of Table 1). Similar observation concerns also the excited states (compare with Table 3). Hence, on the basis of our tests, we may recommend a combined variation of N and J as a source of reliability in the practical high-precision computations.

5 Summary

Our present methodical conjecture was inspired by an observation that exponential Ansätze play a nonnegligible role in the complicated realistic manybody calculations [20]. In the present, not entirely unrelated RPM context, bound states also seem surprisingly well represented by the similar *infinite-product-like* wavefunctions: Their approximate wavefunctions possess a nonstandard though still elementary and transparent closed form.

Our main attention was paid to a particular anharmonic oscillator example. This restriction was independently motivated by the popularity and use of this model in the theory of lasers, chemistry, field theory as well as in perturbation theory and in some further, purely methodical analyses (cf. ref. [4] which contains an extensive list of further references). Our results on this "ill-behaved force" support the current expectations that the efficiency of the universal Riccati-Padé strategy may prove, up to a big extent at least, independent of the detailed structure of $V(r)$'s.

In the older RPM studies, the underlying Padé-type re-arrangement of Riccatian wavefunctions has led to several unsettling methodical challenges:

- With a bad quality of the input information (exemplified here by the expansion of $F(r)$ which diverges beyond the finite radius $r_{(max)} = 1/\sqrt{g}$), a suspicion might concern the reliability of the high-precision results.
- Among all the increasingly many energy roots (which accumulate closer and closer to the correct physical energy), the choice of correct approximants is more and more ambiguous at the higher N's.

In our paper we tried to avoid both these inconsistencies. We found that the first problem finds a natural solution in the consequent transition to the multi-point Padé interpolation. We have shown that such a formal tool enables us to compactify all the available information about the position of (complex) singularities.

We have found that the new, characteristic J dependence of the energy roots is of a fundamental importance and that its destabilization-of-spuriosities effect might become a key to the final resolution of the second puzzle.

On the basis of our numerical tests, we may preliminarily conclude that in spite of the fact that only the limit $N \to \infty$ defines the exact wavefunctions and energies, the very first $N = O(1)$ prescriptions may already supply several significant digits correctly.

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Table 1. The RPM convergence of the two- and three-point ground-state-energies.

	$(E - E_{\text{exact}}) \times 10^8$			
	dimension = 4		dimension = 6	
	two − point	three − point	two − point	three − point
	$N = 3$	$N = 4$	$N = 5$	$N = 6$
J	$K + J = 7$	$K + J = 8$	$K + J = 11$	$K + J = 12$
0	−325	−84	−7	−2
1	+334	+82	+7	+2
2	−432	−97	−6	−2
3	+7189	+145	+9	+3
4	−1554	−269	−	−4

Table 2. J-independence of the correct RPM roots.

energies :			spurious	physical	spurious
roots :			left neighbour	correct	right neighbour
K	J	$\mathcal{N}$			
2	0	2	-4.2	1.193	∞
1	1	1	$-\infty$	1.333	∞
0	2	2	$-\infty$	(1.0)	∞
3	0	4	-1.75	1.227	(3.3)
2	1	3	0.25	1.241	6.51
1	2	3	$-\infty$	1.20	(3.9)
0	3	4	$-\infty$	1.47	(2.5)
4	0	6	-1.4	1.2313	1.61
3	1	4	0.95	1.2340	5.78
2	2	4	-9.5	1.2285	1.87
1	3	4	$-\infty$	1.249	2.18
0	4	6	-3.8	0.87	(2.4)
5	0	9	-0.9	1.23215	1.30
4	1	7	1.18	1.23261	5.62
3	2	6	-0.66	1.23187	1.31
2	3	6	1.01	1.2337	(3.1)
1	4	7	$-\infty$	1.226	2.24
0	5	9	$-\infty$	1.32	(2.4)

Table 3. The RPM spectrum at $K + J = 11$.

	ground state	the second excitation	the fourth excitation
J	$E - 1.232350$	$E - 5.5897$	$E - 9.68$
0	0.651×10^{-6}	0.695×10^{-4}	0.191×10^{-2}
1	0.788×10^{-6}	0.847×10^{-4}	0.489×10^{-2}
2	0.655×10^{-6}	0.745×10^{-4}	0.362×10^{-2}
3	0.811×10^{-6}	0.831×10^{-4}	0.430×10^{-2}
average	0.726×10^{-6}	0.780×10^{-4}	0.368×10^{-2}

Table 4. Spurious roots at $K + J = 11$.

	ground state		the second excited state	
J	$E_{\text{left}}^{\text{spurious}} - E_{\text{exact}}$	$E_{\text{right}}^{\text{spurious}} - E_{\text{exact}}$	$E_{\text{left}}^{\text{spurious}} - E_{\text{exact}}$	$E_{\text{right}}^{\text{spurious}} - E_{\text{exact}}$
0	-0.07	$+0.00003$	(-1.9)	$+0.008$
1	-0.00002	$+0.003$	-0.003	$(+2.1)$
2	-0.02	$+0.00002$	-0.5	$+0.002$
3	-0.00002	$+0.002$	-0.001	$+0.2$