Accurate eigenvalues of the Schrödinger equation with the potential $V(r) = V_0 r^\alpha$

Francisco M Fernández

INIFTA, División Química Teórica, Blvd. 113 y 64 (S/N), Sucursal 4, Casilla de Correo 16, 1900 La Plata, Argentina

E-mail: fernande@quimica.unlp.edu.ar

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Abstract
We calculate accurate eigenvalues of the Schrödinger equation with the potential $V(r) = V_0 r^\alpha$, $\alpha \geq -1$, $V_0 > 0$. We resort to the Riccati-Padé method that is based on a rational approximation to the logarithmic derivative of the wavefunction. This approach applies when $\alpha$ is a rational number.

Keywords: Schrödinger equation, exponential potential, Riccati-Padé method, accurate eigenvalues

(Some figures may appear in colour only in the online journal)

1. Introduction
The Schrödinger equation can be solved exactly only for some particular models. Two of them, relevant for present paper, are the harmonic oscillator and the hydrogen atom [1]. In most cases of physical interest one has to resort to approximate methods. Perturbation and variational approaches are known since long ago and have been applied to a wide variety of problems [2]. In addition to these general methods there are others that apply to particular models [3] (and references therein). From time to time a researcher proposes a new approximate method for the treatment of a class of particular problems [3] (and references therein). New methods are commonly tested against exact or accurate approximate results [3]. For this reason there is considerable interest in reliable benchmark eigenvalues, eigenfunctions, matrix elements, etc.

Some time ago Fernández et al [4] proposed a modification of the Riccati-Padé method (RPM) [5, 6] for the calculation of the eigenvalues of the Schrödinger equation with the potential $V(r) = gr^\alpha$, where $\alpha > -2$ is a rational exponent and $g_0 > 0$. As an illustrative example they applied the standard RPM to the case $\alpha = -1/2$ and obtained the ground-state energy quite accurately [4]. Such class of interaction potentials has been of interest in the study of the bound states of a heavy quark and antiquark [7]. Note that the cases $\alpha = -1$ (hydrogen atom) and $\alpha = 2$ (harmonic oscillator) are exactly solvable [1].

In a recent paper Li and Dai [8] showed that the Schrödinger equation with the potential $V(r) = -\alpha r^{-1/2}$, $\alpha > 0$, can be solved exactly in terms of Heun biconfluent functions. They obtained the eigenvalues $E_{\nu,l}$ for $\nu$, $l = 0$, 1, ..., 5, where $\nu$ and $l$ are the well known radial and angular-momentum quantum numbers, respectively. However, the resulting quantization condition, given in terms of such functions, does not seem to be quite amenable for the accurate calculation of the eigenvalues. Their estimate $E_{00} = -0.4380$ is considerably less accurate that the RPM result $E_{00} = -0.438041241942506$ obtained many years earlier [4]. Therefore, the latter approach seems to be more convenient for the calculation of benchmark eigenvalues.

We are not aware of accurate calculations of the eigenvalues of the potential $V(r) = gr^\alpha$ for non-integer values of $\alpha$ except for the slightly accurate ones in the paper mentioned above for $\alpha = -1/2$ [8]. The modified RPM just mentioned [4] appears to be unnecessarily complicated and the authors only obtained the ground state for the case $\alpha = -1/2$. The purpose of this paper is to show that the standard (and much more straightforward) RPM [5, 6] (see also [9] for more details and references) is a suitable tool for the accurate calculation of the eigenvalues of the potential $V(r) = V_0 r^\alpha$, where $\alpha \geq -1$ is a rational number and $V_0 > 0$.

In section 2 we outline the approach. In section 3 we apply the RPM to selected examples with several values of $\alpha$ and discuss the accuracy of the results. Finally, in section 4 we summarize the main results and draw conclusions.
2. The Riccati-Padé method

The Schrödinger equation for the present central-field model is

\[ H\psi = E\psi, \]

\[ H = -\frac{\hbar^2}{2m} \nabla^2 + V_0 r^\alpha, \quad \alpha V_0 > 0. \]  \hspace{1cm} (1)

On choosing the units of length \( r_0 = [\hbar^2/(2mV_0)]^{1/(\alpha+2)} \) and energy \( e_0 = [\hbar^2 V_0^{\beta/(\alpha+1)}/(2m)]^{(\alpha+1)/(\alpha+2)} \) the resulting dimensionless Hamiltonian becomes

\[ H = -\nabla^2 + \sigma r^\alpha, \quad \sigma = \frac{\alpha}{|\alpha|} \left\frac{V_0}{|V_0|} \right. \]  \hspace{1cm} (2)

The solutions are of the form \( \psi(r, \theta, \phi) = R(r)Y^m(\theta, \phi) \), where \( Y^m(\theta, \phi) \) are the spherical harmonics with angular-momentum quantum numbers \( l = 0, 1, \ldots \) and \( m = 0, \pm 1, \ldots, \pm l \). The radial part of the solution satisfies the eigenvalue equation

\[ -u''(r) + \left[ \frac{l(l+1)}{r^2} + \sigma r^\alpha \right]u(r) = \epsilon u(r), \]  \hspace{1cm} (3)

where \( u(r) = rR(r) \) and \( \epsilon = E/e_0 \) is the dimensionless energy.

The modified logarithmic derivative

\[ f(r) = \frac{l+1}{r} - u'(r)/u(r), \]  \hspace{1cm} (4)

satisfies the Riccati equation

\[ f'(r) = f(r)^2 - \frac{2(l+1)}{r}f(r) + \epsilon - \sigma r^\alpha. \]  \hspace{1cm} (5)

In order to apply the RPM we define the new independent and dependent variables \( z = r^\beta \) and \( g(z) = f(rz) \), respectively; the latter satisfies the Riccati equation

\[ \beta z g' + 2(l+1)g(z) = z^{1/\beta}g(z)^2 + \epsilon z^{1/\beta} - \sigma z^{(\alpha+1)/\beta}. \]  \hspace{1cm} (6)

If \( \alpha = p/q \), where \( p \) and \( q \) are integers, we choose \( \beta = 1/q \) so that the Riccati equation (6) becomes

\[ \frac{1}{q} z g' + 2(l+1)g(z) = z^{q}g(z)^2 + \epsilon z^{q} - \sigma z^{p+q}. \]  \hspace{1cm} (7)

If \( q > 0 \) and \( p + q \geq 0 \) (which lead to \( \alpha \geq -1 \)) we can expand the solution of (7) in a Taylor series about \( z = 0 \)

\[ g(z) = \sum_{j=0}^{\infty} a_j z^j, \]  \hspace{1cm} (8)

where the coefficients \( a_j \) are polynomial functions of \( \epsilon \). They can be obtained from the recurrence relation

\[ a_n = \frac{1}{2l + \frac{\beta}{q} + 2} \left[ w(n - q) \sum_{j=0}^{n-q} a_j a_{n-j} - \epsilon \sigma a_{n-q} \right], \quad n = 0, 1, \ldots, \]  \hspace{1cm} (9)

where \( w(x) \) is the Heaviside function \( (w(x) = 0 \text{ if } x < 0 \text{ and } w(x) = 1 \text{ otherwise}) \).

No transformation is required when \( \alpha \) is an integer \( (\beta = 1, z = r) \) and the RPM yields the exact eigenvalues for the exactly-solvable cases \( \alpha = -1 \) and \( \alpha = 2 \) (see, for example, reference [9]).

If we look for a rational approximation to the solution of (7) of the form

\[ [M, N](z) = \frac{\sum_{j=0}^{M} \alpha_{j} z^j}{1 + \sum_{k=0}^{N} b_k z^k} = \sum_{k=0}^{M+N+1} g_k z^k + O(z^{M+N+2}), \]  \hspace{1cm} (10)

then the approximate eigenvalue \( \epsilon \) should be a root of the Hankel determinant \( H^D_{\gamma}(\epsilon) = 0 \), where \( D = N + 1 \) and \( d = M - N \). The matrix elements of this determinant are \( g_{i+j+d-1}, i, j = 1, 2, \ldots, D \). Earlier applications of the RPM showed that there are sequences of roots \( \epsilon^{(D,d)} \), \( D = 2, 3, \ldots \) that converge towards the actual eigenvalues of the problem [5, 6] (in particular, see [9] and references therein). Typically, the rate of convergence exhibits exponential behaviour \( \epsilon^{(D+1,d)} - \epsilon^{(D,d)} = Ae^{-Bd} \), \( A, B > 0 \), for sufficiently large \( D \).

When both \( q \) and \( p + q \) are odd, then \( g(z) \) is an odd function of \( z \) and \( g_{2k} = 0, k = 0, 1, \ldots \). Although both equation (9) and the procedure just outlined are still valid under these conditions it only makes sense to construct the sequences of roots with either \( D \) even or \( D \) odd or, which is more convenient from a practical point of view, to construct the Hankel determinants directly from the nonzero expansion coefficients \( a_{2k+1} \) instead of \( g_k \). Note that the actual expansion variable in this case is \( z^2 \) instead of \( z \).

The version of the RPM outlined in this section is considerably simpler than the one discussed earlier [4] that takes into account the asymptotic behaviour of \( g(z) \) explicitly. In what follows we will show that such condition is not necessary for the application of the method and will test its rate of convergence on several quantum-mechanical models that were not considered before.

3. Examples

As indicated above, the Schrödinger equation (1) has been proposed as one of the simplest phenomenological models for the study of the bound states of a heavy quark and antiquark [7]. Disregarding which are the most suitable model parameters for each particular application (for example, \( \alpha > 0 \) in the one just mentioned) in this section we apply the RPM to several examples in order to show that the approach is sufficiently general. We calculate the expansion coefficients \( g_j \) and the Hankel determinants \( H^D_{\gamma}(\epsilon) \) analytically as polynomial functions of \( \epsilon \) and then obtain the roots of \( H^D_{\gamma}(\epsilon) = 0 \) numerically. Note that in this way there will be no round-off errors, except in the last step. Most computer algebra software available today allow an almost unlimited precision which enables one to obtain results of striking accuracy. Although the rate of convergence may slightly vary with the chosen value of \( d \) we restrict ourselves to the case \( d = 2 \) for concreteness. The analytical calculation of the Hankel determinants is time consuming but here we are mainly interested in testing the rate of convergence of their roots. The reader...
more interested in a faster strategy may have a look at recent calculations of the resonances of the Stark effect in hydrogen and the most accurate eigenvalues ever calculated for such a problem. It is well known that the RPM yields the actual eigenvalues of the polynomial equation \( H_0^{(l)}(\nu) = 0 \). In what follows we label the dimensionless energies as \( \epsilon_{\nu, l} \), where \( l, \nu = 0, 1, 2, 3, 4 \) are the angular-momentum and radial quantum numbers, respectively.

The first example is given by the exponent \( \alpha = -1/2 \) that was treated earlier by means of the RPM [4] and has recently been proved to lead to a Schrödinger equation that is exactly solvable in terms of Heun biconfluent functions [8].

Here we apply the standard RPM outlined in section 2 with \( p = -1 \) and \( q = 2 \).

Table 1. Some eigenvalues for the potential \( V(r) = -r^{-1/2} \).

| \( l, \nu \) | \( \epsilon_{\nu, l} \) |
|---|---|
| (0, 0) | \(-0.438 041 241 942 505 887 099 625 301 211 018 073 928 496 394 488 \) |
| (0, 1) | \(-0.263 203 069 697 075 806 981 126 460 451 511 573 625 086 \) |
| (0, 2) | \(-0.197 558 399 925 620 717 777 064 487 394 853 997 \) |
| (0, 3) | \(-0.161 704 966 236 690 197 808 417 848 856 83 \) |
| (0, 4) | \(-0.138 637 391 239 231 884 846 885 804 \) |
| (0, 5) | \(-0.122 345 763 853 304 593 157 67 \) |
| (1, 0) | \(-0.286 610 968 720 162 690 813 624 325 199 674 233 362 664 4870 \) |
| (1, 1) | \(-0.209 800 146 853 345 733 733 456 545 715 93 \) |
| (1, 2) | \(-0.169 415 987 748 241 969 345 733 456 545 715 93 \) |
| (1, 3) | \(-0.144 018 998 103 941 636 732 449 264 637 \) |
| (1, 4) | \(-0.126 354 291 248 013 627 171 152 87 \) |
| (1, 5) | \(-0.113 245 984 197 889 268 322 2 \) |
| (2, 0) | \(-0.221 505 876 391 467 564 736 613 765 005 165 746 2702 \) |
| (2, 1) | \(-0.176 817 135 425 491 197 207 487 464 178 593 035 496 \) |
| (2, 2) | \(-0.149 198 085 273 071 908 219 344 017 212 7977 \) |
| (2, 3) | \(-0.130 219 955 532 154 314 232 404 909 998 \) |
| (2, 4) | \(-0.116 263 146 867 944 596 282 685 95 \) |
| (2, 5) | \(-0.105 030 282 242 143 48 3474 \) |
| (3, 0) | \(-0.184 005 130 322 370 703 515 087 127 728 860 236 129 1698 \) |
| (3, 1) | \(-0.154 238 772 239 809 683 597 305 239 264 557 854 75 \) |
| (3, 2) | \(-0.133 988 137 631 347 323 419 903 542 822 5626 \) |
| (3, 3) | \(-0.119 207 770 503 498 684 928 014 243 98 \) |
| (3, 4) | \(-0.107 880 266 541 301 867 535 0206 \) |
| (3, 5) | \(-0.098 882 179 268 629 446 7534 \) |

Table 2. Some eigenvalues for the potential \( V(r) = -r^{-1/3} \).

| \( l, \nu \) | \( \epsilon_{\nu, l} \) |
|---|---|
| (0, 0) | \(-0.549 744 967 939 855 368 082 139 3889 \) |
| (0, 1) | \(-0.402 464 971 075 782 307 9445 \) |
| (0, 2) | \(-0.338 155 834 585 944 0423 \) |
| (1, 0) | \(-0.428 711 664 253 722 958 404 048 87 \) |
| (1, 1) | \(-0.353 300 738 105 266 076 4965 \) |
| (1, 2) | \(-0.309 831 060 165 466 52 \) |
| (2, 0) | \(-0.368 082 183 733 761 766 618 413 29 \) |
| (2, 1) | \(-0.287 939 568 477 979 73 \) |
| (3, 0) | \(-0.329 645 913 475 774 067 101 662 \) |
| (3, 1) | \(-0.270 499 310 496 2070 \) |

Figure 1. Logarithmic error \( L_D \) for the eigenvalues of \( V(r) = -r^{-1/2} \) with \( l = 0 \) and \( \nu = 0, 1, 2, 3, 4, 5 \) (from left to right).
Table 3. Some eigenvalues for the potential $V(r) = -r^{-2/3}$.

| $(l, \nu)$ | $\epsilon_l\nu$ |
|-----------|-----------------|
| (0, 0)    | 0.355 382 696 084 542 752 796 309 404 564 396 775 756 607 112 120 147 898 660 287 302 944 9984 |
| (0, 1)    | 0.168 683 258 081 531 519 601 545 532 829 809 724 986 671 444 440 803 569 221 040 21 |
| (0, 2)    | 0.110 383 658 989 434 848 246 212 984 001 459 684 755 450 082 989 166 388 97 |
| (0, 3)    | 0.081 999 526 908 911 404 704 158 808 703 005 121 437 968 376 047 937 |
| (0, 4)    | 0.065 218 099 314 362 849 986 654 440 672 670 175 351 705 707 16 |
| (0, 5)    | 0.054 135 267 454 169 862 724 041 107 128 968 098 589 9564 |
| (0, 6)    | 0.046 270 625 118 124 826 307 891 513 718 976 681 29 |
| (1, 0)    | 0.185 017 905 660 208 889 033 280 022 921 240 812 501 169 798 120 706 755 495 468 197 422 4 |
| (1, 1)    | 0.117 968 431 924 077 608 469 524 665 145 254 831 699 685 327 441 035 531 300 195 |
| (1, 2)    | 0.086 375 946 124 332 667 318 931 365 553 847 611 350 824 249 148 788 743 |
| (1, 3)    | 0.068 067 125 029 383 214 620 224 044 370 102 299 284 619 470 137 459 |
| (1, 4)    | 0.056 138 382 148 082 731 945 748 777 574 599 708 434 870 3163 |
| (1, 5)    | 0.047 756 313 537 008 115 832 269 130 540 577 117 248 03 |
| (1, 6)    | 0.036 762 960 762 327 517 031 166 177 241 246 |
| (1, 7)    | 0.029 877 749 676 422 718 102 966 09 |

Table 4. Some eigenvalues for the potential $V(r) = r^{1/2}$.

| $(l, \nu)$ | $\epsilon_l\nu$ |
|-----------|-----------------|
| (0, 0)    | 1.833 393 609 778 132 819 989 706 566 163 148 984 |
| (0, 1)    | 2.550 647 491 414 789 963 001 597 3569 |
| (0, 2)    | 3.051 181 948 950 148 127 778 090 |
| (0, 3)    | 3.452 131 943 857 522 6071 |
| (0, 4)    | 3.793 360 444 647 6296 |
| (1, 0)    | 2.300 496 239 515 583 918 636 898 196 682 148 |
| (1, 1)    | 2.854 335 925 747 438 604 342 984 490 |
| (1, 2)    | 3.285 833 295 818 405 737 010 872 |
| (1, 3)    | 3.647 385 421 454 765 449 82 |
| (1, 4)    | 3.962 676 500 693 6562 |
| (2, 0)    | 2.657 563 368 283 691 944 712 218 969 6955 |
| (2, 1)    | 3.120 328 492 061 008 079 338 057 75 |
| (2, 2)    | 3.502 451 547 428 846 232 747 96 |
| (2, 3)    | 3.832 543 915 845 346 8999 |
| (2, 4)    | 4.125 809 074 413 673 |
| (3, 0)    | 2.954 450 931 022 392 036 030 215 450 7054 |
| (3, 1)    | 3.702 704 997 614 159 955 936 68 |
| (3, 2)    | 4.007 367 339 627 547 5504 |
| (3, 3)    | 4.281 959 441 7211 |

Table 5. Some eigenvalues for the potential $V(r) = r^{1/3}$.

| $(l, \nu)$ | $\epsilon_l\nu$ |
|-----------|-----------------|
| (0, 0)    | 1.615 675 088 788 293 385 022 05 |
| (0, 1)    | 2.041 832 932 331 519 69 |
| (0, 2)    | 2.319 639 064 734 |
| (1, 0)    | 1.904 886 674 021 626 369 387 99 |
| (1, 1)    | 2.216 658 693 998 539 24 |
| (1, 2)    | 2.448 777 374 655 |

expressions of the bound-state eigenfunctions [8]. Present results suggest that the RPM quantization condition is more suitable for the accurate computation of the eigenvalues than the one given in terms of the solutions of the biconfluent Heun equation [8].

Table 2 shows results for $\alpha = -1/3$ obtained from Hankel determinants of dimension $D \leq 45$. The rate of convergence of the RPM for this example is slightly smaller than for the preceding one.

Table 3 shows results for $\alpha = -2/3$ where the Hankel determinants of dimension $D \leq 40$ were constructed from the coefficients $g_{2r+1}$ as indicated in section 2. The rate of convergence of the RPM for this case is noticeably greater than the one for the previous examples, which is the reason for the greater accuracy of the results shown in that table.

Tables 4–7 show results for $\alpha = 1/2$ ($D \leq 45$), $\alpha = 1/3$ ($D \leq 45$), $\alpha = 2/3$ ($D \leq 40$) and $\alpha = 3/2$ ($D \leq 45$), respectively. In the case $\alpha = 2/3$ the Hankel determinants were constructed from the coefficients $g_{2r+1}$. In all these cases the results are also quite accurate due to the exponential rate of convergence.

In two recent papers it was shown that the RPM proves to be preferable to other approaches for the calculation of the resonances of the Stark effect in hydrogen [10, 11] (see also [12] for the performance on other models). However, it has been stated that ‘...RPM is not able to get the wave function, but its logarithmic derivative. So the RPM method is not useful when we are focused on obtaining physical parameters derived from the wave functions’ [13]. Such a criticism is not entirely true because the RPM has been useful to obtain accurate expectation values from the Hellmann-Feynman theorem, even in the case of models with self-interaction [14].

4. Further comments and conclusions

Throughout this paper we have shown that the RPM is a remarkably suitable approach for the calculation of accurate eigenvalues of the Schrödinger equation (1). The interest in such power-law potentials stems from the fact that may be suitable models for the study of the bound states of a heavy quark and antiquark. We are not aware of results obtained by means of other
basis set and the calculation of the necessary matrix elements. On the other hand, the variational method requires a suitable calculations with different grids to mesh size equal to zero. The rest of the space. In addition to this, one has to extrapolate the potential in a neighbourhood of the origin with respect to numerical integration or a variational method. It will probably convenient than the one expressed in terms of such solutions.

In principle, one may resort to other approaches like other approaches for all problems and under all possible conditions. However, our experience shows that when the RPM applies, then it is difficult to obtain the same accuracy with other methods. The reason is the exponential rate of convergence of the RPM clearly shown in figure 1.

ORCID iDs

Francisco M Fernández @ https://orcid.org/0000-0003-0393-790X

Table 6. Some eigenvalues for the potential \( V(r) = r^{2/3} \).

| \((l, \nu)\) | \(\epsilon_{\nu}\) |
|------------|----------------|
| (0, 0)     | \(2.022 \, 306 \, 599 \, 257 \, 795 \, 366 \, 694 \, 630 \, 473 \, 241 \, 638 \, 339 \, 543 \, 808 \, 208 \, 636\) |
| (0, 1)     | \(3.063 \, 292 \, 934 \, 363 \, 098 \, 996 \, 761 \, 746 \, 839 \, 551 \, 207 \, 071 \, 417 \, 01\) |
| (0, 2)     | \(3.834 \, 514 \, 262 \, 915 \, 892 \, 348 \, 506 \, 786 \, 987 \, 792 \, 448 \, 41\) |
| (0, 3)     | \(4.475 \, 455 \, 263 \, 926 \, 046 \, 368 \, 753 \, 487 \, 903 \, 053\) |
| (0, 4)     | \(5.035 \, 727 \, 730 \, 937 \, 186 \, 483 \, 377 \, 806 \, 66\) |
| (0, 5)     | \(5.539 \, 745 \, 015 \, 667 \, 931 \, 120 \, 170\) |
| (0, 6)     | \(6.001 \, 649 \, 825 \, 519 \, 164 \, 41\) |
| (1, 0)     | \(2.674 \, 632 \, 066 \, 892 \, 448 \, 274 \, 035 \, 790 \, 138 \, 569 \, 168 \, 725 \, 041 \, 769 \, 190\) |
| (1, 1)     | \(3.516 \, 229 \, 138 \, 873 \, 600 \, 817 \, 283 \, 804 \, 160 \, 330 \, 404 \, 237 \, 6825\) |
| (1, 2)     | \(4.198 \, 921 \, 393 \, 458 \, 422 \, 829 \, 516 \, 632 \, 321 \, 619 \, 9609\) |
| (1, 3)     | \(4.787 \, 683 \, 913 \, 114 \, 832 \, 164 \, 935 \, 873 \, 702 \, 25\) |
| (1, 4)     | \(5.312 \, 760 \, 784 \, 478 \, 424 \, 504 \, 241 \, 1545\) |
| (1, 5)     | \(5.791 \, 063 \, 559 \, 826 \, 215 \, 590 \, 620\) |
| (1, 6)     | \(6.233 \, 158 \, 930 \, 659 \, 972 \, 95\) |

Table 7. Some eigenvalues for the potential \( V(r) = r^{3/2} \).

| \((l, \nu)\) | \(\epsilon_{\nu}\) |
|------------|----------------|
| (0, 0)     | \(2.708 \, 092 \, 416 \, 017 \, 969 \, 144 \, 951 \, 929 \, 434 \, 292 \, 19\) |
| (0, 1)     | \(5.585 \, 662 \, 539 \, 733 \, 075 \, 503 \, 934 \, 301 \, 85\) |
| (0, 2)     | \(8.266 \, 868 \, 775 \, 124 \, 008 \, 939 \, 4177\) |
| (0, 3)     | \(10.731 \, 720 \, 881 \, 160 \, 291 \, 6761\) |
| (0, 4)     | \(13.141 \, 917 \, 795 \, 591 \, 099\) |
| (1, 0)     | \(4.250 \, 826 \, 006 \, 586 \, 811 \, 136 \, 445 \, 756 \, 097 \, 70\) |
| (1, 1)     | \(6.966 \, 044 \, 020 \, 353 \, 490 \, 984 \, 091 \, 3607\) |
| (1, 2)     | \(9.520 \, 904 \, 383 \, 150 \, 697 \, 791 \, 0024\) |
| (1, 3)     | \(11.968 \, 551 \, 211 \, 219 \, 516 \, 0942\) |
| (1, 4)     | \(14.336 \, 606 \, 204 \, 183 \, 540\) |

It is not our purpose to state that the RPM is preferable to other approaches for all problems and under all possible conditions. However, our experience shows that when the RPM applies, then it is difficult to obtain the same accuracy with other methods. The reason is the exponential rate of convergence of the RPM clearly shown in figure 1.

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