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Large-order shifted $1/N$ expansions through the asymptotic iteration method

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Abstract

The perturbation technique within the framework of the asymptotic iteration method is used to obtain large-order shifted $1/N$ expansions, where N is the number of spatial dimensions. This method is contrary to the usual Rayleigh–Schrödinger perturbation theory, no matrix elements need to be calculated. The method is applied to the Schrödinger equation, and the non-polynomial oscillator potential $V(r) = r^2 + \frac{br^2}{(1+cr^2)}$ is discussed as an illustrative example.

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1. Introduction

The shifted $1/N$ expansion technique (SLNT) proposed by Sukhatme and Imbo [1], is an extremely powerful method of solving the Schrödinger equation, and has been used extensively to determine the eigenenergies for some important potentials [2–6]. The SLNT is an expansion in powers of $\Lambda^{-1/2}$, $\Lambda = N + 2\ell - a$, where N, ℓ and a stand for the number of dimensions, the angular momentum quantum number and a properly chosen shift parameter, respectively. The shifted parameter a is usually chosen so as to improve the convergence of the energy perturbation series, and to obtain the correct eigenenergies for the harmonic oscillator and the hydrogen atom to all orders.

After expanding the potential-energy function and the centrifugal term in Taylor series about an appropriate point r_0 one is left with the Hamiltonian operator for a harmonic oscillator plus a polynomial perturbation. Then one applies the perturbation theory and obtains the perturbation corrections for the eigenenergies and eigenfunctions.

In the literature, the Rayleigh–Schrödinger and the logarithmic perturbation schemes (referred to as RSPT and LPT, respectively) have been used for the calculation of these corrections.

As well known, the applications of the above two schemes were restricted by serious difficulties. They require considerable computational time and effort, and they involve, in

general, quite elaborate algebraic manipulations. Therefore, it was extremely laborious to advance beyond the first four perturbation expansion terms in the eigenenergy series [2].

In the last few years, considerable progress was made to obtain large-order shifted $1/N$ expansions [7–10]. For example, Maluendes *et al* [7] have reported an approach in which the coefficients of the SLNT of arbitrarily high orders could be generated by means of the hypervirial (HV) and Hellmann–Feynman theorems (HF), and thereby providing an excellent check for the convergence of the method.

However, the previous authors in their work did not give explicit expressions of their algorithm, each order getting progressively much more complicated than the previous one, and the derivations were tediously long. Thus, the need arises here to have a relatively simple, fast and effective method that will provide large-order shifted $1/N$ expansions.

The so-called perturbation technique within the framework of the asymptotic iteration method (AIM) [11] has emerged in recent years to be a very useful and powerful technique of attack. This method reproduced excellent results for many important potentials in relativistic and non-relativistic quantum mechanics. Through AIM one can actually obtain all the perturbation corrections to both eigenenergies and eigenfunctions for all states [12, 13]. These quantities can be calculated to any given accuracy, since the generation of successive corrections in the present perturbative framework only requires the solution of simple algebraic equation.

The method is also applicable in the same form to both the ground state and excited bound states without involving tedious calculations which appeared in the available perturbation theories.

Encouraged by its satisfactory performance, we feel tempted to extend AIM, and to see this time how the AIM can be used to obtain large-order shifted $1/N$ expansions for the three-dimensional Schrödinger equation with any arbitrary spherically symmetric potential $V(r)$ directly without either, using the base eigenfunctions of the unperturbed problem, or needing to calculate matrix elements.

As an illustration, the present technique is applied to the non-polynomial oscillator potential $V(r) = r^2 + \frac{br^2}{(1+cr^2)}, b \in (-\infty, \infty), c > 0$. This potential appears in several areas of physics. In the field theory, it provides a simple zero-dimensional model possessing a non-polynomial Lagrangian [14]. In laser physics, it arises out of the Fokker–Planck equation for a single-mode laser [15].

For this potential only a class of exact analytical solutions for certain parameter dependence $b = b(c)$ were obtained [16, 17]. Hence, it has been a subject of several investigations and many authors have studied the one-, two- and three-dimensional cases [18–20]. Roy, Roychoudhury and Roy have shown the supersymetric (SUSY) character of this potential and gave new solutions using the standard $1/N$ expansion method [21] and recently, Saad, Hall and Ciftci have developed a variational method and obtain the eigenenergies of this potential [22].

Keeping this in mind, this paper is organized as follows. In section 2, the formulation of SLNT through AIM is outlined to find the eigenenergies and eigenfunctions for any arbitrary spherically symmetric potential. The analytical expressions for AIM are cast in such a way that allows the reader to use them without proceeding into their derivation. In section 3, we explained how to obtain numerically the eigenenergies and the eigenfunctions for the non-polynomial oscillator potential $V(r) = r^2 + \frac{br^2}{(1+cr^2)}$, and therein we will compare the accuracy of our results with those obtained by [21, 22]. Finally, the paper ends with a brief summary and concluding remarks on the method and our findings.

2. Formalism of the asymptotic iteration method for SLNT

The radial part of the time-independent Schrödinger equation for central-field model in terms of the expansion parameter Λ in N-dimensional space with ($\hbar = 2m = 1$) is

$$\left\{-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\Lambda^2}{4r^2}\left(1 + \frac{2A}{\Lambda} + \frac{4B}{\Lambda^2}\right) + V(r)\right\}\chi_{n\ell}(r) = E_{n\ell}\chi_{n\ell}(r), \tag{1}$$

where $\Lambda = N + 2\ell - a$ is a constant which rescales the potential $V(r)$ at large-ℓ limit and will be determined below, $A = 1 - N + a$ and $B = (N - a)(N - a - 2)/4$.

SLNT begins with shifting the origin of the coordinate through the definition

$$x = \Lambda^{1/2}\left(\frac{r}{r_0} - 1\right), \tag{2}$$

where r_0 is chosen to minimize the effective potential $V_{\mathrm{eff}}(r) = \Lambda^2\left(\frac{1}{4r^2} + \frac{V(r)}{\Lambda^2}\right)$, so that

$$\Lambda^2 = 2r_0^3 V'(r_0). \tag{3}$$

Expansions about $r = r_0$ yield

$$\left\{-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \sum_{i=0}^{\infty}(\alpha_i g^i x^{i+2} + \beta_i g^i x^i + \xi_i g^{i+2} x^i)\right\}\chi_{n\ell}(x) = \epsilon_{n\ell}\chi_{n\ell}(x) \tag{4}$$

where

$$\alpha_i = (-1)^i\frac{i+3}{4} + \frac{r_0^{i+1}}{2(i+2)!}\frac{\mathrm{d}^{i+2}V(r_0)}{V'(r_0)\,\mathrm{d}r_0^{i+2}}, \qquad \beta_i = (-1)^i\frac{i+1}{2}A, \qquad \xi_i = (-1)^i(i+1)B, \tag{5}$$

and

$$\epsilon_{n\ell} = r_0^2 g^2(E_{n\ell} - V_{\mathrm{eff}}(r_0)), \qquad g = 1/\Lambda^{1/2}. \tag{6}$$

The construction of the AIM method starts with expanding the eigenenergy term $\epsilon_{n\ell}$ in powers of g. This power series is only convergent for small values of g as we shall see later, and equation (4) thus becomes

$$\begin{aligned}\Big[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} &+ \alpha_0 x^2 + \beta_0 + g(\alpha_1 x^3 + \beta_1 x) + g^2(\alpha_2 x^4 + \beta_2 x^2 + \xi_0) \\ &+ g^3(\alpha_3 x^5 + \beta_3 x^3 + \xi_1 x) + g^4(\alpha_4 x^6 + \beta_4 x^4 + \xi_2 x^2) + \cdots\Big]\chi_{n\ell}(r) \\ &= \left[\epsilon_{n\ell}^{(0)} + g\epsilon_{n\ell}^{(1)} + g^2\epsilon_{n\ell}^{(2)} + g^3\epsilon_{n\ell}^{(3)} + g^4\epsilon_{n\ell}^{(4)} + \cdots\right]\chi_{n\ell}(x).\end{aligned} \tag{7}$$

If we further insert the ansatz

$$\chi_{n\ell}(x) = \mathrm{e}^{-\gamma x^2/2} f_{n\ell}(x) \tag{8}$$

into equation (7) and then carry out the mathematics, in this case, the function $f_{n\ell}(x)$ will satisfy a new second-order homogeneous linear differential equation of the form

$$f''_{n\ell}(x) = \lambda_0(x, g) f'_{n\ell}(x) + s_0(x, g) f_{n\ell}(x), \tag{9}$$

where $\lambda_0(x, g) = 2\gamma x$, and

$$\begin{aligned}s_0(x, g) = (\alpha_0 - \gamma^2)x^2 &+ \beta_0 + \gamma - \epsilon_{n\ell} + g(\alpha_1 x^3 + \beta_1 x) + g^2(\alpha_2 x^4 + \beta_2 x^2 + \xi_0) \\ &+ g^3(\alpha_3 x^5 + \beta_3 x^3 + \xi_1 x) + g^4(\alpha_4 x^6 + \beta_4 x^4 + \xi_2 x^2) + \cdots,\end{aligned} \tag{10}$$

$$\epsilon_{n\ell} = \epsilon_{n\ell}^{(0)} + g\epsilon_{n\ell}^{(1)} + g^2\epsilon_{n\ell}^{(2)} + g^3\epsilon_{n\ell}^{(3)} + g^4\epsilon_{n\ell}^{(4)} + \cdots. \tag{11}$$

Here, it should be pointed out that, when we switch off g, equation (9) will be reduced to an exactly solvable eigenvalue problem within the framework of AIM [23–27].

To apply the perturbation expansion technique within the framework of AIM we rely on the symmetric structure of the right-hand side of equation (9). By differentiating this equation $(k+2)$ times with respect to x, $k = 1, 2, \ldots$, taking the ratio of the $(k+2)$th and $(k+1)$th derivatives, and then introducing, for sufficiently large k, the 'asymptotic' aspect and the termination condition of the method, respectively (details can be found in [23–27]), one can obtain

$$\varrho(x, g) \equiv \frac{s_k(x, g)}{\lambda_k(x, g)} = \frac{s_{k-1}(x, g)}{\lambda_{k-1}(x, g)}, \tag{12}$$

$$\delta_k(x, g) \equiv s_k(x, g)\lambda_{k+1}(x, g) - s_{k+1}(x, g)\lambda_k(x, g) = 0, \tag{13}$$

which, in turn, yields to a general solution of equation (9),

$$f_{n\ell}(x) \sim \exp\left(-\int^x \varrho(z, g)\,\mathrm{d}z\right). \tag{14}$$

Now we proceed to obtain the eigenenergies of equation (9) systematically in terms of the expansion parameter g. By expanding $\delta_k(x, g)$ about $g = 0$, equation (13) reads

$$\delta_k(x, g) = \delta_k^{(0)}(x) + g\delta_k^{(1)}(x) + g^2\delta_k^{(2)}(x) + g^3\delta_k^{(3)}(x) + g^4\delta_k^{(4)}(x) + \cdots. \tag{15}$$

According to the procedure of AIM [23–27] $\delta_k(x, g)$ must be zero; if this to be true for every g value, then every term of the above series must be zero. That is to say

$$\delta_k^{(j)}(x) = \frac{1}{j!}\left(\frac{\partial^j \delta_k(x, g)}{\partial g^j}\right)\bigg|_{g=0} = 0, \qquad j = 0, 1, 2, \ldots. \tag{16}$$

A quantitative estimate for $\epsilon_{n\ell}$ expansion terms can be obtained by comparing the terms with the same order of g in equations (9) and (15). Therefore, it is clear that the roots of $\delta_k^{(0)}(x) = 0$ give us the zeroth contribution energy terms $\epsilon_{n\ell}^{(0)}$. Likewise, the roots of $\delta_k^{(1)}(x) = 0$ give us the first correction terms $\epsilon_{n\ell}^{(1)}$, and so on. Therefore, the general solution for the eigenenergies $E_{n\ell}$ in conjunction with equations (6) and (11) is

$$E_{n\ell} = \frac{\Lambda^2}{r_0^2}\left(\frac{1}{4} + \frac{r_0^2 V(r_0)}{\Lambda^2}\right) + \frac{1}{r_0^2 g^2}\sum_{i=0}^{\infty} g^i \epsilon_{n\ell}^{(i)}. \tag{17}$$

Similarly we expand $\varrho(x, g) \equiv \frac{s_k(x,g)}{\lambda_k(x,g)}$ about $g = 0$, which in turn implies

$$\varrho(x, g) = \varrho^{(0)}(x) + g\varrho^{(1)}(x) + g^2\varrho^{(2)}(x) + g^3\varrho^{(3)}(x) + g^4\varrho^{(4)}(x) + \cdots, \tag{18}$$

with

$$\varrho^{(j)}(x) = \frac{1}{j!}\left(\frac{\partial^j \varrho(x, g)}{\partial g^j}\right)\bigg|_{g=0}, \qquad j = 0, 1, 2, \ldots. \tag{19}$$

By substituting equation (18) into the eigenfunction generator given in equation (14), in this case, the function $f_{n\ell}(x)$ is expressed as series in powers of g,

$$f_{n\ell}(x) = f_{n\ell}^{(0)}(x) f_{n\ell}^{(1)}(x) f_{n\ell}^{(2)}(x) f_{n\ell}^{(3)}(x) \ldots = \prod_{j=0}^{\infty} f_{n\ell}^{(j)}(x), \tag{20}$$

with

$$f_{n\ell}^{(j)}(x) = \exp\left(-g^j \int^x \varrho^{(j)}(z)\,\mathrm{d}z\right), \qquad j = 0, 1, 2, \ldots. \tag{21}$$

As a result, the eigenfunction $\chi_{n\ell}(x)$ general solution is

$$\chi_{n\ell}(x) = \mathrm{e}^{-\gamma x^2/2} \prod_{j=0}^{\infty} f_{n\ell}^{(j)}(x). \tag{22}$$

3. Numerical results for the eigenenergies and eigenfunctions of the potential $V(r) = r^2 + \frac{br^2}{(1+cr^2)}$

Within the framework of the asymptotic iteration method mentioned in the above section, the eigenenergies $E_{n\ell}$ of the non-polynomial oscillator potential $V(r) = r^2 + \frac{br^2}{(1+cr^2)}$ are calculated by means of equation (17).

To obtain the zeroth contribution energy terms $\epsilon_{n\ell}^{(0)}$, one should simply switch off g in equation (9), that will lead to an exactly solvable eigenvalue problem within the framework of AIM,

$$f''_{n\ell}(x) = 2\gamma x f'_{n\ell}(x) + \left((\alpha_0 - \gamma^2)x^2 + \beta_0 + \gamma - \epsilon_{n\ell}^{(0)}\right) f_{n\ell}(x). \tag{23}$$

For each iteration, the expression $\delta_k^{(0)}(x, 0) = 0$ in equation (13) depends on two variables namely γ and x. Since the problem is exactly solvable, the calculated eigenenergies $\epsilon_{n\ell}^{(0)}$ by means of this condition are independent of the choice of x once we set $\gamma = \sqrt{\alpha_0}$; therefore, the roots of $\delta_k^{(0)}(x, 0) = 0$ are

$$\epsilon_{n\ell}^{(0)} = \beta_0 + (2n + 1)(\alpha_0)^{1/2}, \qquad n = 0, 1, 2, \ldots. \tag{24}$$

As we noted before, the leading contribution term of the total energy is of order Λ^2 given in equation (17), and the next contribution is of order Λ and is given by $\beta_0 + (2n+1)(\alpha_0)^{1/2}$. In this case, it is customary to choose the shift parameter a so as to make this contribution vanish. This choice is physically motivated by requiring agreement between the $1/\Lambda$ expansions and the exact analytic results for the harmonic-oscillator and Coulomb potentials to all orders [2]. However, there are some difficult cases in which this simple choice is insufficient and it is really necessary to select an order-dependent value of a according to minimal sensitivity or other appropriate criterion [7]. Nevertheless, at this point, it is enough for us to compare the AIM results with the SLNT results. Therefore, we choose

$$a = 2 - 2(2n + 1)(\alpha_0)^{1/2}, \tag{25}$$

$\Lambda = N + 2\ell - a$, and $\Lambda^2 = 2r_0^3 V'(r_0)$.

Collecting all these terms and carrying out the mathematics, we obtain

$$N + 2\ell - 2 + 2(2n + 1)(\alpha_0)^{1/2} = \left(2r_0^3 V'(r_0)\right)^{1/2}, \tag{26}$$

which is an implicit equation for r_0. Once r_0 is determined, the leading term $\Lambda^2 V_{\mathrm{eff}}(r_0)$ can be calculated numerically. On the other hand, to obtain the higher order perturbative expansion terms, first one should go to equation (9), switch on g, and then replace $\epsilon_{n\ell}$ with $\epsilon_{n\ell}^{(0)} + g\epsilon_{n\ell}^{(1)}$, and terminate the iterations by imposing the condition $\delta_k^{(1)}(x) = 0$ as an approximation to equation (9). The first root of the resulting equation gives $\epsilon_{n\ell}^{(1)}$. Similarly, one can easily obtain the other perturbative expansion terms.

Moreover, throughout the present calculations, it is observed that the perturbation corrections of odd orders $\epsilon_{n\ell}^{(2i+1)}$ vanish for all i.

In table 1 an explicit list of calculations for $\epsilon_{0\ell}^{(i)}$ up to 6th order with different values of ℓ, b and c, including $\ell = -1$ which represents the lowest even state in the one-dimensional case are given, so that the reader may, if so inclined, reproduce our results.

Table 1. The calculated values of the coefficients in the energy expansion $\epsilon_{n\ell}$ for the non-polynomial oscillator potential with different values of ℓ, b and c.

ℓ	c	b	$\epsilon_{0\ell}^{(0)}$	$\epsilon_{0\ell}^{(1)}$	$\epsilon_{0\ell}^{(2)}$	$\epsilon_{0\ell}^{(3)}$	$\epsilon_{0\ell}^{(4)}$	$\epsilon_{0\ell}^{(5)}$	$\epsilon_{0\ell}^{(6)}$
0	0.1	−0.46	0	0	−0.021 504 914	0	0.014 728 06	0	−0.010 867
1	0.1	−0.5	0	0	−0.030 894 587	0	0.020 425 23	0	−0.003 4827
2	0.1	−0.54	0	0	−0.034 627 947	0	0.017 939 87	0	0.018 511
0	0.01	−0.0406	0	0	−0.000 018 842	0	$1.707\,706 \times 10^{-6}$	0	-1.7717×10^{-6}
1	0.01	−0.041	0	0	−0.000 049 912	0	$7.312\,060 \times 10^{-6}$	0	-7.6296×10^{-6}
−1	0.1	−0.42	0	0	−0.005 539 564	0	0.002 341 067	0	−0.001 8839

Table 2. Comparison between selected eigenenergies calculated from the standard shifted (1/N) expansion method $E_{n\ell}(1/N)$ [21], the exact super-symmetric values $E_{n\ell}$(SUSY) [21] and the eigenenergies $E_{n\ell}$(AIM) computed by means of equation (17) up to fourth and sixth orders.

ℓ	c	b	$E_{0\ell}(1/N)$	$E_{0\ell}$(SUSY)	$E_{0\ell}^{4\text{th}}$(AIM)	$E_{0\ell}^{6\text{th}}$(AIM)
0	0.1	−0.46	2.400 520	2.4	2.400 515 918 141 38	2.399 902 413 381 5471
1	0.1	−0.5	4.000 116	4.0	4.000 121 951 116 41	4.000 077 708 289 9992
2	0.1	−0.54	5.599 965	5.6	5.599 985 370 495 38	5.600 073 578 772 1094
0	0.01	−0.0406	2.939 999	2.94	2.940 000 014 311 55	2.939 999 885 762 7638
1	0.01	−0.041	4.899 974	4.9	4.900 000 021 365 54	4.899 999 901 768 3162
−1	0.1	−0.041	0.801 177	0.8	0.801 176 583 181 43	0.798 484 833 837 5296

Table 3. Comparison between selected eigenenergies for $n = 1, \ell = 1$ state calculated from the standard shifted $(1/N)$ expansion method $E_{n\ell}(1/N)$ [21], and the eigenenergies $E_{n\ell}$(AIM) computed by means of equation (17) up to fourth and sixth orders.

c	b	$E_{11}(1/N)$	$E_{11}^{4\text{th}}$(AIM)	$E_{11}^{6\text{th}}$(AIM)
0.1	0.1	9.276 635	9.276 665	9.276 835
0.5	0.1	9.117 522	9.117 546	9.117 881
1	0.1	9.070 745	9.070 749	9.070 945
1	0.5	9.353 303	9.353 316	9.354 385
0.1	1	11.622 346	11.622 378	11.623 002
1	1	9.705 584	9.705 589	9.707 955
100	100	9.994 694	9.994 691	9.994 664

In tables 2–4 the calculated AIM, together with the standard shifted expansion method $E_{n\ell}(1/N)$, the exact SUSY and the variational results are displayed for comparison purposes [21, 22].

In the tables the one-dimensional and the three-dimensional cases are discussed, and we have only considered the eigenenergies for the ground state $n = 0$ and the first excited state $n = 1$ with different values of ℓ. This was in order to make a clear comparison between the results of this method and the results of [21, 22]. Examination of the tables shows that the accuracy of the AIM is better than the accuracy of the standard shifted $1/N$ expansion method, and the predicted eigenenergies for the ground state $E_{0\ell}$(AIM) are all in excellent agreement with the results obtained by the super-symmetric and the variational methods [21, 22].

Proceeding in the same way, one can also obtain all the correction terms of the eigenfunction given in equation (22). As an illustration, in figure 1 we present our numerical results for the eigenfunction $(n = 0, \ell = 1)$, compared with the eigenfunction results

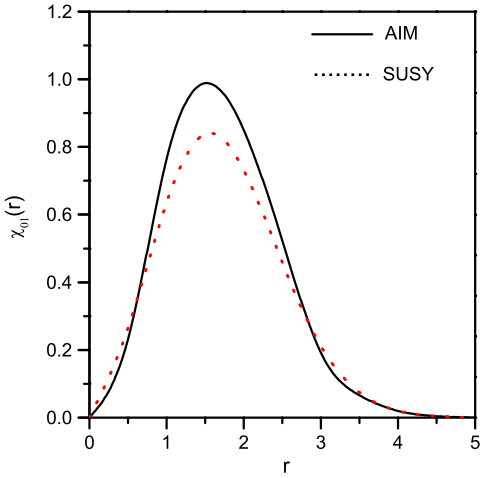

Figure 1. A comparison between the eigenfunction obtained by the super-symmetric method $\chi_{01}(r) \sim r^2(1 + cr^2)\exp(-r^2/2)$ [21], and the eigenfunction $\chi_{01}(r)$ computed by means of equation (22) up to fourth orders.

Table 4. Comparison between selected eigenenergies calculated from the variational method $E_{n\ell}$(var) [22], and the eigenenergies $E_{n\ell}$(AIM) computed by means of equation (17) up to fourth and sixth orders.

ℓ	c	b	$E_{0\ell}$(var)	$E_{0\ell}^{4\text{th}}$(AIM)	$E_{0\ell}^{6\text{th}}$(AIM)
1	0.1	0.1	5.186 373 003	5.186 344 633	5.186 361 169
2			7.243 961 840	7.243 947 208	7.243 943 566
3			9.294 359 111	9.294 353 460	9.294 343 830
1	0.5	0.1	5.100 857 624	5.100 988 230	5.100 893 484
2			7.118 980 872	7.119 024 139	7.119 046 917
3			9.131 812 402	9.131 822 737	9.132 452 529
1	1	0.1	5.065 569 522	5.065 616 321	5.065 790 121
2			7.073 726 362	7.073 717 362	7.073 777 736
3			9.078 911 720	9.078 902 850	9.078 922 349
1	0.1	0.5	5.893 595 1523	5.893 507 438	5.893 556 186
2			8.177 871 6934	8.177 807 825	8.177 785 414
3			10.429 204 118	10.429 166 01	10.429 121 63
1	0.1	1	6.704 238 8925	6.704 150 575	6.704 212 326
2			9.261 914 7808	9.261 831 304	9.261 776 909
3			11.760 620 963	11.760 554 75	11.760 462 43
1	1	1	5.651 393 3173	5.652 135 054	5.654 047 914
2			7.734 828 0429	7.734 784 398	7.735 439 296
3			9.787 669 7785	9.787 586 966	9.787 795 394
1	100	100	5.993 438 8734	5.993 565 505	5.993 156 839
2			7.996 024 6730	7.996 047 679	7.995 970 245
3			9.997 153 6386	9.997 159 961	9.997 137 678

obtained by the super-symmetric method $\chi_{01}(r) \sim r^{\ell+1}(1 + cr^2)\exp(-r^2/2)$ for the three-dimensional non-polynomial oscillator potential. The comparison is clearly excellent up to some normalization constant.

Finally, it is worthwhile to emphasize that the results of this work show the effectiveness of this approach in comparison with other techniques developed in the literature, and these results can, of course, be further improved by simply increasing the order of perturbation. We have also shown that, it is very easy task to implement the perturbation technique within the framework of the AIM without having to worry about the ranges of the couplings in the potential and the ranges of n and ℓ.

Moreover, this method is applicable in the same form to both the ground state, and excited bound states without involving tedious calculations which appeared in the available perturbation theories.

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