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On the radius of convergence of Rayleigh–Schrödinger perturbative solutions for quantum oscillators in circular and spherical boxes†

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Abstract. The energy eigenvalues of harmonic oscillators in circular and spherical boxes are obtained through the Rayleigh–Schrödinger perturbative expansion, taking the free particle in a box as the non-perturbed system. The perturbative series is shown to be convergent for small boxes, and an upper bound for the radius of convergence is established. Padé-approximant solutions are also constructed for boxes of any size. Numerical comparison with the exact eigenvalues—which are obtained by constructing and diagonalising the Hamiltonian in the basis of the eigenfunctions of the free particle in a box—corroborates the accuracy and range of validity of the approximate solutions, particularly the convergence and the radius of convergence of the perturbative series.

1. Introduction

The one-dimensional quantum mechanical problem of the harmonic and inverted oscillators in a box has been studied by several authors (Singh and Baijal 1955, Vawter 1973, Consortini and Frieden 1976, Rotbart 1978, Fernandez and Castro 1981). Recently, Aguilera-Navarro *et al* (1980) investigated the problem with the objective of finding approximate analytical expressions for the energy eigenvalues as functions of size of the box. Specifically, they obtained (i) exact solutions by constructing and diagonalising the Hamiltonian matrix in the basis of eigenstates of the free particle in a box, (ii) Rayleigh-Schrödinger perturbative solutions (valid for small boxes) taking the quadratic potential as the perturbation, (iii) asymptotic solutions valid for very large boxes, and (iv) Padé-approximant solutions (valid for boxes of any size) constructed as interpolations between (ii) and (iii). The accuracy and range of validity of these solutions were illustrated through their numerical comparison. However, no attempt was made to establish the convergence and the radius of convergence of the Rayleigh–Schrödinger perturbation series.

The present paper is an extension of Aguilera-Navarro *et al* (1980) in the sense that the same methods are used to study two- and three-dimensional harmonic oscillators in circular and spherical boxes, respectively. But, additionally, we show the

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convergence of the Rayleigh–Schrödinger perturbative series and estimate an upper bound for the radius of convergence. In § 2, we formulate the exact solution of the problems in two alternative ways: the first one, in terms of confluent hypergeometric functions, is not the most convenient for the numerical evaluation of the energy eigenvalues, but it is useful to establish the asymptotic form of the solution. The second one uses the eigenstates of the free particle in circular and spherical boxes—Bessel functions and spherical Bessel functions, respectively—to construct the matrix of the corresponding Hamiltonians; the diagonalisation of these matrices provides highly accurate energy eigenvalues. In § 3, the appropriate matrix elements are used to construct the Rayleigh–Schrödinger perturbative expansions. We also use Rellich's theorem to show the convergence of the Rayleigh–Schrödinger perturbative series for small boxes, and Kato's method to establish upper bounds for the radii of convergence. In § 4, we construct Padé-approximant solutions which interpolate between the perturbative and asymptotic solutions previously obtained. In § 5, we present the numerical results of our exact and approximate solutions. Comparison of these results confirms the convergence of the Rayleigh–Schrödinger perturbative series for boxes of sizes consistent with the estimates of § 3, and shows that the Padé-approximant solutions are in fair agreement with the exact solutions for boxes of any size.

2. Formulation of the exact solution

The problem to be solved is the eigenvalue problem

$$-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dr^2}+\frac{(D-1)}{r}\frac{d}{dr}-\frac{L^2}{r^2}\right)\psi+\tfrac{1}{2}\mu\omega^2r^2\psi=E\psi, \tag{1}$$

with the additional boundary condition

$$\psi(r=R)=0, \tag{2}$$

where R is the radius of the box. The bidimensional system is obtained by putting $D=2$ and $L^2=M^2$, while for the tridimensional system, $D=3$ and $L^2=l(l+1)$. Here, $M=0,1,2,\ldots$ and $l=0,1,2,\ldots$ are the magnetic and orbital quantum numbers, respectively.

Introducing the dimensionless variables $\xi=r/b$ and $\varepsilon=E/\hbar\omega$ where $b^2=\hbar/\mu\omega$, we obtain from (1)

$$\left(\frac{d^2}{d\xi^2}+\frac{(D-1)}{\xi}\frac{d}{d\xi}-\frac{L^2}{\xi^2}-\xi^2+2\varepsilon\right)\psi(\xi)=0. \tag{3}$$

The wavefunction can be written in the form

$$\psi(\xi)=\xi^\alpha\exp(-\xi^2/2)f(\xi), \tag{4}$$

where $\alpha=|M|$ or l, depending on the dimension of the problem we consider.

Introducing (4) in (3) and changing to the variable $z=\xi^2$, we find

$$zf''+(\alpha+D/2-z)f'+\tfrac{1}{2}(\varepsilon-\alpha-D/2)f=0. \tag{5}$$

Equation (5) is Kummer's equation and its solution is given by the confluent hypergeometric function (Abramowitz and Stegun 1965), namely,

$$f(z)={}_1F_1(\{\alpha+D/2-\varepsilon\}/2;\alpha+D/2;z). \tag{6}$$

Defining now

$$\eta = (\varepsilon - \alpha - D/2)/2 \qquad \text{or} \qquad \varepsilon = 2\eta + \alpha + D/2, \tag{7}$$

the boundary condition (2) reads

$${}_1F_1(-\eta; \alpha + D/2; z_0) = 0, \qquad z_0 = (R/b)^2. \tag{8}$$

Equation (8) is satisfied by discrete values of η which define the solutions of the problem. The eigenstates are characterised by the quantum numbers η and α with energy defined by (7).

It should be noted that obtaining the energy eigenvalues through the zeros of the confluent hypergeometric function requires hard computational effort (see however Killingbeck 1983). We shall use (8) to obtain the asymptotic behaviour of the eigenvalues in the region of very large boxes as follows.

The exact wavefunction, in the limit of very large boxes, can be written as

$$\begin{aligned} {}_1F_1(-\eta; \alpha + D/2; z_0) \xrightarrow[z_0 \to \infty]{} & (-z_0)^{\eta}\Gamma(\alpha + D/2)/\Gamma(\alpha + D/2 + \eta) \\ & + e^{z_0}(z_0)^{-\eta-\alpha-D/2}\Gamma(\alpha + D/2)/\Gamma(-\eta). \end{aligned} \tag{9}$$

For the jth level, η is expected to tend to j (positive integer). In such conditions, we obtain from (9)

$$\eta \sim j + e^{-z_0} z_0^{2j+\alpha+D/2}/\Gamma(j + \alpha + D/2) j!, \tag{10}$$

and the asymptotic energy eigenvalues are

$$\varepsilon_{\alpha j} \sim 2j + \alpha + D/2 + 2\, e^{-z_0} z_0^{2j+\alpha+D/2}/\Gamma(j + \alpha + D/2) j!, \tag{11}$$

with $j = 0, 1, 2, \ldots$ and $\alpha = 0, 1, 2, \ldots$.

Another way to obtain the exact numerical energy eigenvalues is by constructing and diagonalising the Hamiltonian matrix whose elements are constructed within the eigenspace of the free particle in a box. The matrix element for the bidimensional case is given by

$$\langle n|H|m\rangle = \left[\frac{1}{2}\frac{\beta_{\alpha n}^2}{\xi_0^2} + \frac{\xi_0^2}{6}\left(1 - \frac{2(1-m^2)}{\beta_{\alpha n}^2}\right)\right]\delta_{nm} + (1-\delta_{nm})4\xi_0^2\beta_{\alpha n}\beta_{\alpha m}(\beta_{\alpha n}^2 - \beta_{\alpha m}^2)^{-2} \tag{12a}$$

where $\beta_{\alpha n}$ is the nth zero of the Bessel function of order α.

For the tridimensional system the matrix element is given by

$$\langle n|H|m\rangle = \left[\frac{1}{2}\frac{\beta_{\alpha n}^2}{\xi_0^2} + \frac{\xi_0^2}{6}\left(1 - \frac{3-4l(l+1)}{2\beta_{\alpha n}^2}\right)\right]\delta_{nm} + (1-\delta_{nm})4\xi_0^2\beta_{\alpha n}\beta_{\alpha m}(\beta_{\alpha n}^2 - \beta_{\alpha m}^2)^{-2} \tag{12b}$$

and $\beta_{\alpha n}$ is the nth zero of the spherical Bessel function of order α.

The computation was done for several values of ξ_0, and the eigenvalues are listed in table 1. The matrix dimension was varied in such a way as to assure the convergence of the eigenvalues within six decimal places. In the present case, we have diagonalised matrices of order 20×20 for values of $0 \leqslant \xi_0 \leqslant 1$ and of order 50×50 to assure the convergence for $1 \leqslant \xi_0 \leqslant 5$.

Table 1(a). Energy eigenvalues for the bidimensional case. $M = 0$, $n = 1$; $M = 1$, $n = 1$.

Radius of convergence < 1.79.

	Perturbative	$P[1/5]$	$P[4/3]$	$P[2/3]$	$P[2/4]$	Exact
$M = 0$, $n = 1$.						
0.10	289.160 389	289.160 389	289.160 389	289.160 389	289.160 389	289.160 389
0.30	32.138 623	32.138 623	32.138 623	32.138 623	32.138 623	32.138 623
0.50	11.593 619	11.593 619	11.593 619	11.593 619	11.593 622	11.593 619
0.70	5.954 560	5.954 558	5.954 560	5.954 561	5.954 601	5.954 561
0.90	3.657 848	3.657 824	3.657 847	3.657 851	3.658 140	3.657 850
1.10	2.520 553	2.520 400	2.520 544	2.520 580	2.521 948	2.520 572
1.30	1.892 186	1.891 505	1.892 104	1.892 325	1.897 166	1.892 288
1.40	1.684 171	1.682 878	1.683 938	1.684 460	1.692 798	1.684 386
1.50	1.523 104	1.520 777	1.522 453	1.523 673	1.537 297	1.523 532
1.60	1.397 687	1.393 678	1.395 838	1.398 760	1.419 907	1.398 506
1.70	1.299 694	1.292 992	1.293 915	1.301 637	1.332 817	1.301 195
1.80	1.222 927	1.211 858	1.197 376	1.226 320	1.269 930	1.225 586
1.90	1.162 541	1.143 952	1.313 540	1.168 281	1.226 022	1.167 107
2.00	1.114 586	1.081 050	1.166 304	1.124 019	1.196 274	1.122 209
3.00	0.589 554	1.017 098	1.107 801	1.028 271	1.077 267	1.001 937
4.00	−5.211 561	1.001 569	1.214 547	1.053 443	1.022 744	1.000 003
5.00	−49.565 119	1.000 212	1.255 623	1.050 891	1.007 389	1.000 000
$M = 1$, $n = 1$.						
0.10	734.099 745	734.099 745	734.099 745	734.099 745	734.099 745	734.100 199
0.30	81.577 417	81.577 417	81.577 417	81.577 417	81.577 417	81.518 503
0.50	29.394 249	29.394 249	29.394 249	29.394 249	29.394 251	29.405 600
0.70	15.040 963	15.040 963	15.040 963	15.040 964	15.041 001	15.063 213
0.90	9.160 909	9.160 901	9.160 909	9.160 914	9.161 188	9.197 690
1.10	6.212 796	6.212 739	6.212 794	6.212 829	6.214 190	6.267 747
1.30	4.546 352	4.546 072	4.546 330	4.546 512	4.551 662	4.623 134
1.40	3.979 376	3.978 812	3.979 318	3.979 696	3.988 965	4.068 466
1.50	3.529 870	3.528 795	3.529 725	3.530 476	3.546 444	3.632 219
1.60	3.169 646	3.167 688	3.169 297	3.170 744	3.197 163	3.286 239
1.70	2.878 443	2.875 010	2.877 624	2.880 358	2.922 416	3.010 316
1.80	2.641 328	2.635 502	2.639 431	2.644 554	2.709 013	2.789 598
1.90	2.447 027	2.437 392	2.442 602	2.452 297	2.547 327	2.612 934
2.00	2.286 808	2.271 181	2.276 107	2.295 187	2.429 707	2.471 775
3.00	1.398 583	2.604 335	1.814 189	1.710 487	2.200 469	2.014 967
4.00	−2.380 372	2.030 065	1.886 697	1.724 971	2.075 468	2.000 050
5.00	−30.372 028	2.004 086	2.014 144	1.812 473	2.026 617	2.000 000

3. Rayleigh–Schrödinger perturbative solution

Considering our unperturbed system as the free particle in a box and the quadratic potential as the perturbation, we construct the Rayleigh–Schrödinger perturbative series for the energy eigenvalues.

The wavefunctions for the free particle in circular and spherical boxes satisfy the equation

$$\left(\frac{d^2}{dr^2}+\frac{D-1}{r}\frac{d}{dr}-\frac{L^2}{r^2}+\kappa^2\right)\psi^{(0)}=0, \tag{13}$$

with D and L^2 defined as in § 2, and $\kappa^2 = 2\mu E/\hbar^2$.

Table 1(b). Energy eigenvalues for the tridimensional case. $l=0$, $n=1$; $l=1$, $n=1$.

Radius of convergence < 1.72.
$l=0$, $n=1$.

	Perturbative	$P[1/5]$	$P[4/3]$	$P[2/3]$	$P[2/4]$	Exact
0.10	493.481 632	493.481 632	493.481 632	493.481 632	493.481 632	493.481 632
0.30	54.843 855	54.843 855	54.843 855	54.843 855	54.843 855	54.843 855
0.50	19.774 534	19.774 534	19.774 534	19.774 534	19.774 537	19.774 534
0.70	10.140 214	10.140 212	10.140 214	10.140 214	10.140 261	10.140 214
0.90	6.206 533	6.206 512	6.206 532	6.206 536	6.206 874	6.206 535
1.10	4.248 366	4.248 230	4.248 357	4.248 387	4.250 021	4.248 381
1.30	3.156 107	3.155 486	3.156 015	3.156 215	3.162 149	3.156 185
1.40	2.790 448	2.789 253	2.790 175	2.790 674	2.801 062	2.790 614
1.50	2.504 645	2.502 471	2.503 818	2.505 092	2.522 384	2.504 976
1.60	2.279 636	2.275 862	2.276 892	2.280 483	2.307 906	2.280 270
1.70	2.101 654	2.095 351	2.088 423	2.103 196	2.144 637	2.102 820
1.80	1.960 471	1.950 238	2.021 865	1.963 182	2.022 774	1.962 543
1.90	1.848 260	1.831 894	1.873 944	1.852 876	1.934 239	1.851 831
2.00	1.758 832	1.732 515	1.784 738	1.766 469	1.871 698	1.764 816
3.00	1.153 178	1.544 195	1.610 758	1.540 390	1.641 254	1.506 082
4.00	−4.341 728	1.504 181	1.773 849	1.593 339	1.542 653	1.500 015
5.00	−48.076 319	1.500 581	1.870 927	1.603 334	1.514 072	1.500 000
Radius of convergence < 1.840 $l=1$, $n=1$.						
0.10	1009.528 302	1009.538 302	1009.538 302	1009.538 302	1009.538 302	1009.538 302
0.30	112.187 571	112.187 571	112.187 571	112.187 571	112.187 571	112.187 571
0.50	40.428 277	40.428 276	40.428 277	40.428 277	40.428 280	40.428 277
0.70	20.694 514	20.694 513	20.694 514	20.694 515	20.694 559	20.694 515
0.90	12.614 909	12.614 895	12.614 908	12.614 911	12.615 240	12.614 910
1.10	8.569 177	8.569 083	8.569 169	8.569 189	8.570 818	8.569 186
1.30	6.288 103	6.287 660	6.288 006	6.288 168	6.294 284	6.288 150
1.40	5.514 623	5.513 754	5.514 293	5.514 758	5.525 703	5.514 722
1.50	4.903 392	4.901 782	4.902 059	4.903 661	4.922 374	4.903 590
1.60	4.415 743	4.412 902	4.399 541	4.416 255	4.446 914	4.416 123
1.70	4.023 929	4.019 125	4.032 462	4.024 865	4.073 067	4.024 628
1.80	3.707 558	3.699 723	3.714 804	3.709 212	3.781 909	3.708 801
1.90	3.451 299	3.438 898	3.459 915	3.454 130	3.559 127	3.453 442
2.00	3.243 353	3.224 167	3.254 730	3.248 064	3.392 893	3.246 947
3.00	2.310 416	2.688 286	2.615 770	2.567 552	2.846 334	2.531 292
4.00	−1.565 579	2.517 144	2.838 243	2.663 861	2.611 653	2.500 144
5.00	−34.035 847	2.502 500	3.078 434	2.742 382	2.537 958	2.500 000

The solutions of (13) must satisfy the boundary condition of (2). They are Bessel and spherical Bessel functions for the bidimensional and tridimensional cases, respectively, i.e.

$$\psi_b^{(0)} = AJ_M(\kappa r), \qquad \psi_t^{(0)} = Bj_l(\kappa r). \tag{14a,b}$$

The corresponding eigenvalues are given in terms of the zeros of the above solutions as

$$E_{\alpha n}^{(0)} = \hbar^2 \beta_{\alpha n}^2 / 2\mu R^2. \tag{15}$$

The Rayleigh–Schrödinger perturbative series was computed up to the third order and it is expressed by

$$\varepsilon_{\alpha n}=\frac{\beta_{\alpha n}^{2}}{2\xi_0^2}+\frac{\xi_0^2}{6}\left(1-\frac{3+4L_D^2}{2\beta_{\alpha n}^2}\right)+32\xi_0^6\sum_{k\neq n}\frac{\beta_{\alpha n}^2\beta_{\alpha k}^2}{(\beta_{\alpha n}^2-\beta_{\alpha k}^2)^5}$$
$$+256\xi_0^{10}\sum_{\substack{j\neq n\\ k\neq n}}\frac{\beta_{\alpha n}^2\beta_{\alpha k}^2\beta_{\alpha j}^2}{(\beta_{\alpha k}^2-\beta_{\alpha n}^2)^3(\beta_{\alpha j}^2-\beta_{\alpha n}^2)^2(\beta_{\alpha k}^2-\beta_{\alpha j}^2)^2}$$
$$-32\xi_0^{10}\left(1-\frac{3+4L_D^2}{2\beta_{\alpha n}^2}\right)\sum_{k\neq n}\frac{\beta_{\alpha n}^2\beta_{\alpha k}^2}{(\beta_{\alpha n}^2-\beta_{\alpha k}^2)^6}+\mathrm{O}(\xi_0^{14}),\qquad(16)$$

where $L_2^2=\frac{1}{4}-M^2$ for the bidimensional system and $L_3^2=-l(l+1)$ for the tridimensional one.

The coefficients in the expansion (16) were computed with the help of Olver's (1960) table of Bessel functions and the result can be written as

$$\varepsilon_{\alpha n}=a_{\alpha n}^{(0)}\xi_0^{-2}+a_{\alpha n}^{(1)}\xi_0^{2}+a_{\alpha n}^{(2)}\xi_0^{6}+a_{\alpha n}^{(3)}\xi_0^{10}.$$

In table 2 we present the coefficients $a_{\alpha n}^{(i)}$.

One of the objects of this paper is to prove the convergence of the perturbative series in the region of small boxes. An intuitive argument was given by previous authors as follows. As the perturbation matrix elements are proportional to ξ_0^2 and the unperturbed eigenvalues decrease with ξ_0^{-2}, we can say that the perturbation is small when compared with the unperturbed Hamiltonian for values of ξ_0 less than 1.

We present a more rigorous argument based on Rellich's theorem (Rellich 1969). This theorem states that if Hamiltonian can be written as a convergent power series in a certain parameter λ, or particularly,

$$H=H_0+\lambda V,$$

with V being a bounded operator, then the perturbed eigenvalues are analytic functions of λ, and its power series are convergent in the neighbourhood of $\lambda=0$.

Table 2(a). Coefficients for the perturbative series. Bidimensional case. E stands for powers of 10, in FORTRAN notation: $E\pm n=10^{\pm n}$.

n	α	$a_{\alpha n}^{(0)}$	$a_{\alpha n}^{(1)}$	$a_{\alpha n}^{(2)}$	$a_{\alpha n}^{(3)}$
1	0	2.891 593E+0	1.090 283E−1	−6.242 599E−4	−4.367 609E−6
2	0	1.523 563E+1	1.557 274E−1	1.834 281E−4	−1.781 526E−5
3	0	3.744 350E+1	1.622 155E−1	8.794 544E−6	−5.530 723E−7
4	0	6.952 014E+1	1.642 593E−1	6.123 589E−7	1.023 207E−7
5	0	1.114 662E+2	1.651 714E−1	8.544 759E−8	7.537 347E−9
1	1	7.340 985E+0	1.212 595E−1	−4.801 477E−4	−2.682 352E−6
2	1	2.460 923E+1	1.531 216E−1	1.166 585E−4	−8.692 686E−6
3	1	5.174 973E+1	1.602 254E−1	8.797 921E−6	3.077 487E−7
4	1	8.876 038E+1	1.629 112E−1	7.284 405E−7	2.880 339E−8
5	1	1.356 408E+2	1.642 092E−1	1.145 709E−7	4.353 350E−9
1	2	1.318 731E+1	1.034 746E−1	−3.511 470E−4	−1.234 053E−6
2	2	3.544 250E+1	1.431 428E−1	5.532 250E−5	−4.615 381E−6
3	2	6.751 035E+1	1.543 229E−1	7.527 763E−6	1.563 355E−7
4	2	1.094 601E+2	1.590 535E−1	6.981 589E−7	1.696 901E−8
5	2	1.612 776E+2	1.614 996E−1	1.194 422E−7	2.713 871E−9

Table 2(b). Coefficients for the perturbative series. Tridimensional case. $E\pm n = 10^{\pm n}$.

n	α	$a_{\alpha n}^{(0)}$	$a_{\alpha n}^{(1)}$	$a_{\alpha n}^{(2)}$	$a_{\alpha n}^{(3)}$
1	0	4.934 802E+0	1.413 364E−1	−5.577 473E−4	−4.412 653E−6
2	0	1.973 921E+1	1.603 341E−1	1.558 979E−4	−1.254 672E−5
3	0	4.441 322E+1	1.638 522E−1	9.142 044E−6	−5.170 651E−7
4	0	7.895 684E+1	1.650 835E−1	7.013 171E−7	8.479 062E−8
5	0	1.233 701E+2	1.656 535E−1	1.045 044E−7	5.663 096E−9
1	1	1.009 536E+1	1.873 032E−1	−4.104 872E−4	−3.349 338E−6
2	1	2.983 976E+1	1.736 484E−1	8.231 949E−5	−7.045 474E−6
3	1	5.944 993E+1	1.701 710E−1	8.197 784E−6	2.149 309E−7
4	1	9.892 891E+1	1.687 726E−1	7.221 382E−7	2.182 452E−8
5	1	1.482 772E+2	1.680 717E−1	1.188 506E−7	3.405 446E−9
1	2	1.660 873E+1	2.193 498E−1	−3.026 825E−4	−2.351 412E−6
2	2	4.135 962E+1	1.878 226E−1	3.484 773E−5	−4.441 162E−6
3	2	7.592 744E+1	1.781 908E−1	6.868 104E−6	1.114 024E−7
4	2	1.203 515E+2	1.739 370E−1	6.653 644E−7	1.327 369E−8
5	2	1.746 400E+2	1.716 770E−1	1.177 130E−7	2.181 202E−9

As our system is confined in the region $0 \leqslant r \leqslant R$, the harmonic potential is bounded, and as a consequence of Rellich's theorem, the perturbative series obtained in § 2 is convergent in the region of small boxes.

As the convergence is assured, it is natural to look for the region in which the above statement is assured (Kato 1949, 1950). This region is estimated as follows.

Consider the projector formally defined by

$$P_n(\lambda) = -\frac{1}{2\pi \mathrm{i}} \oint_{C_n} (H_0 + \lambda V - l)^{-1}\, \mathrm{d}l, \tag{17}$$

where the circuit C_n involves only the unperturbed eigenvalue $E_n^{(0)}$. Let it be, for instance, a circle of radius $d/2$ (where d is the distance between $E_n^{(0)}$ and its closest neighbour).

The perturbed wavefunction is obtained as a power series of λ, by applying $P_n(\lambda)$ over an unperturbed state.

$P_n(\lambda)$ can also be written as

$$P_n(\lambda) = -\frac{1}{2\pi \mathrm{i}} \oint_{C_n} R(0) \sum_{k=0}^{\infty} (-\lambda)^k [VR(0)]^k\, \mathrm{d}l, \tag{18}$$

where $R(0)$ is the unperturbed resolvent, namely

$$R(0) = (H_0 - l)^{-1}.$$

In order to obtain a convergent power series for the perturbed wavefunction, as well as for its eigenvalues, the series (18) must be convergent. A sufficient condition which satisfies our requirements is

$$|\lambda| \cdot \|V\|/(d/2) < 1 \tag{19}$$

and if V is a multiplicative operator, or

$$\hat{V}\psi = V(x)\psi$$

its norm is given by

$$\|V\| = \sup|V(x)|, \qquad 0 \leq x \leq R.$$

The upper limit for the convergence radius is obtained from expression (19), and for practical purposes it gives the result

$$(R/b) < (2/d)^{1/4}. \tag{20}$$

4. Padé-approximant solutions

The solutions in the two regions of small and very large boxes can be matched through the use of Padé approximants. First, we construct the two-point Padé approximants which reproduce the perturbative series (16) when $\xi_0 \to 0$, and the asymptotic eigenvalues (11) when $\xi_0 \to \infty$. Secondly, we present which we call one-point modified Padé approximants which reproduce the perturbative series in the limit $\xi_0 \to 0$; and in the region of $\xi_0 \to \infty$ their behaviour is quite different from the previous ones.

The two-point Padé approximants are constructed for the function $F(\xi_0)$ defined by

$$F(\xi_0) = \xi_0^2 \varepsilon(\xi_0) \tag{21}$$

which is an analytic function of the variable ξ_0.

$F(\xi_0)$ presents the following behaviour:

$$F(\xi_0) \xrightarrow{\xi_0 \to 0} a_0 + a_1\xi_0^4 + a_2\xi_0^8 + a_3\xi_0^{12} + O(\xi_0^{16}), \qquad F(\xi_0) \xrightarrow{\xi_0 \to \infty} (\alpha + 2n + D/2)\xi_0^2,$$

where the coefficients a_i are the ones obtained for the perturbative series (see table 2).

From this behaviour, we can construct two-point Padé approximants for $F(\xi_0)$,

$$P[N/\!/M] = \left(\sum_{n=0}^{N} c_n \xi_0^{2n}\right)\left(1 + \sum_{m=1}^{M} b_m \xi_0^{2m}\right)^{-1},$$

in the following way. The asymptotic form of $F(\xi_0)$ when $\xi_0 \to \infty$ requires $M = N - 1$ and the additional relation

$$c_N / b_{N-1} = \alpha + 2n + D/2.$$

We have performed the computation for $N = 4$ and the resulting Padé approximant, for the ground state of the tridimensional system, is

$$P[4/\!/3] = \frac{4.934\,802 - 1.397\,182\xi_0^2 + 0.102\,294\xi_0^4 - 0.045\,529\xi_0^6 - 0.001\,676\xi_0^8}{1 - 0.283\,128\xi_0^2 - 0.007\,912\xi_0^4 - 0.001\,1173\xi_0^6}$$

and the energy eigenvalues are found by using (21).

The one-point modified Padé approximants are constructed for the function

$$G(\xi_0) = [\varepsilon(\xi_0) - \alpha - 2n - D/2]\xi_0^2,$$

which presents the behaviour

$$G(\xi_0) \xrightarrow{\xi_0 \to 0} a_0 - (\alpha + 2n + D/2)\xi_0^2 + a_1\xi_0^4 + a_2\xi_0^8 + a_3\xi_0^{12}, \qquad G(\xi_0) \xrightarrow{\xi_0 \to \infty} 0.$$

The additional condition is that the degree of the numerator must be less than the degree of the denominator.

The one-point Padé approximants, constructed for the ground state of the tridimensional system, are

$$P[1/5]=\frac{4.934\,802-0.987\,214\xi_0^2}{1+0.103\,912\xi_0^2+0.002\,945\xi_0^4-0.002\,081\xi_0^6-0.000\,604\xi_0^8+0.000\,112\xi_0^{10}}$$

$$P[2/3]=\frac{4.934\,802-1.201\,894\xi_0^2+0.082\,682\xi_0^4}{1+0.060\,409\xi_0^2+0.006\,476\xi_0^4+0.000\,238\xi_0^6}$$

$$P[2/4]=\frac{4.934\,802-1.895\,733\xi_0^2+0.259\,874\xi_0^4}{1-0.080\,192\xi_0^2-0.000\,355\xi_0^4+0.002\,189\xi_0^6+0.000\,789\xi_0^8}$$

and the energy eigenvalues are found by using (22).

5. Numerical results and discussion

We present in table 1 our numerical results for some of the lowest eigenvalues of the two systems. In the first column we list the size of the boxes. In the last column we list the exact eigenvalues obtained by diagonalising the Hamiltonian matrix. The order of the matrices we have diagonalised was such that the convergence of the eigenvalues was assured up to six decimal places. For $0\leqslant\xi_0\leqslant 1$ we have diagonalised matrices of order 20×20 while for $1\leqslant\xi_0\leqslant 5$ the convergence was assured with matrices of order 50×50. The second column exhibits the perturbative eigenvalues which were computed with the help of (16). As can be seen, the perturbative series is convergent in the region estimated by (20).

We also present the eigenvalues computed by Padé-approximant technique. From these results we can conclude that the Padé approximants allow us to obtain explicit expressions for the energy eigenvalues valid for all sizes of boxes.

The reader should be warned that some Padé approximants present inherent singularities. For instance $P[4/\!/3]$, whose expression was given above, presents a singularity for $\xi_0\sim 1.75$.

Nevertheless the energies for the neighbouring values $\xi_0\sim 1.70$ and 1.80 are quite reasonable.

We should also point out that for $\xi_0\geqslant 5$, the energy eigenvalues have already converged to their asymptotic values. Other states of both systems show a similar trend.

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