Revista Brasileira de Fisica, Vol. 13, nº 4, 1983

On the Quantum Quartic Oscillator in a Box

V.C. AGUILERA-NAVARRO, J.F. GOMES*, A.H. ZIMERMAN
Instituto de Fisica Teórica, Caixa Postal 5956, São Paulo, 01405, SP, Brasil

and

E. LEY KOO**
Instituto de Física, Universidad Nacional Autonoma do México, México

Recebido em 10 de outubro de 1983

Abstract The energy eigenvalues of the quartic potential in a box are obtained exactly and perturbatively using the basis of eigenstates of the free particle in a box. The exact eigenvalues are obtained from the diagonalization of the Hamiltonian in that basis. The perturbative solution is constructed from the Rayleigh-Schrödinger expansion using the quartic potential as the perturbation. The perturbative series is shown to be convergent for small boxes, and an upper bound for the radius of convergence is estimated. Padé-approximant solutions, valid for boxes of any size, are also constructed. The numerical comparison of the perturbative and Padé-apprpximant solutions with the exact ones confirms the validity of the former, especially the convergence and the radius of convergence of the perturbative series.

1. INTRODUCTION

Recently Barakat and Rosner[1] obtained the eigenvalues of the pure quartic oscillator bounded by infinitely high potentials,

$$\left[\frac{d^2}{dx^2} + (E-x^4)\right]\psi(x) = 0 \quad , \quad -\frac{L}{2} \leqslant x \leqslant \frac{L}{2} \tag{1}$$

subject to the boundary conditions

$$\psi(-L/2) = \psi(L/2) = 0 \tag{2}$$

Their method of solution involves power series for the even and odd wavefunctions, compact recurrence relations for the corresponding coefficients, and numerical computation of the eigenvaiues via an iteration scheme.

In this paper we present some alternative solutions of the quartic oscillator in a box defined by eqs. (1) and (2). In section 2,

Work partially supported by FINEP, Rio de Janeiro under contract 43/82/01 50/00.

*With fellowship of FAPESP, São Paulo.

**Work partially supported by ININ, México.

we formulate the exact solution of the problem through the construction and diagonalization of the Hamiltonian in the basis of eigenfunctions of the free particle in a box. In section 3, we construct the Rayleigh-Schrödinger perturbative solution using the quartic potential as the perturbation. The perturbative series is shown to be convergent for small boxes through the use of Rellich's theorem, and an upper bound for the radius of convergence is estimated following Kato's method. In section 4, we construct Padé-approximant solutions (which are expected to give the energy levels for boxes of any size) as an interpolation between the perturbative series solutions (valid for very small boxes) and the asymptotic solutions (valid for very large boxes and corresponding to the limit of the unbounded oscillator[2-6]). Finally, in section 5, we present and compare the numerical results of our exact and approximate solutions. The convergence of the perturbative solutions is explicitly illustrated for boxes of sizes consistent with the radius of convergente estimated according to the discussion of section 3. The Padé-approximant solutions show a fair agreement with the exact solutions for boxes of any size.

2. EXACT SOLIJTION

Our procedure to obtain the exact eigenvalues of the problem consists in diagonalizing the Harniltonian matrix constructed through free-particle wavefunctions, namely

$$|2n+1> = (2/L)^{1/2} \cos[(2n+1)\pi x/L] \tag{3a}$$

for the even levels and

$$|2n> = (2/L)^{1/2} \sin(2n\pi x/L) \tag{3b}$$

for the odd ones.

The wavefunctions (3a) and (3b) obviously satisfy the bondary conditions (2). In order to obtain the exact eigenvalues, we have diagonalized finite rnatrices corresponding to a finite nurnber of wavefunctions.

I'he convergence and accuracy can be assured by changing the dimension of the basis sub-space.

I'he Hamiltonian matrix elements are given by

$$\langle N|H|N'\rangle = \left[N^2\pi^2/L^2 + (L/2)^4(1/5 - 4/N^2\pi^2 + 24/N^4\pi^4)\right]\delta_{N'N}$$

$$+ (-1)^{(N-N')/2}(L/2)^4\left[1/(N-N')^2\pi^2 - 3/2(N-N')^4\pi^4\right.$$

$$\left. - 1/(N+N')^2\pi^2 + 3/2(N+N')^4\pi^4\right](1-\delta_{N'N}) \qquad (4)$$

where N and N' are both even ($=2n$) or odd ($=2n+1$) depending on the parity of the level to be computed.

The diagonalization of the Hamiltonian matrix was made for several values of Land the first ten eigenvalues are listed in Table 1 In the present case, for small values of L, the quartic term can be thought of as a perturbation over the free particle in a box, and we expect the lower dimension of the matrix to assure convergence up to six decimal places. For values of $L/2$ less then 2, we havediagonalized matrices of order 5, 10, 15 and 20. With order 15, we have assured the convergence of the first ten eigenvalues. For values of $L/2$ between 2 and 3, the convergence was assured with a 40x40 matrix.

3. PERTURBATIVE RAYLEIGH-SCHRÖDINGER SOLUTION

Considerlng our unperturbed system as the free particle in a box and the quartic potential as the perturbation, we have computedthe perturbative Rayleigh-Schrödinger series up to the third order for the ten lowest energy levels. As an illustration, we have for the ground and first excited states, respectively,

$$E^{(+)}(L) = 2.467401(L/2)^{-2} + 0.041099(L/2)^4 - 0.000306(L/2)^{10} + 0.000003(L/2)^{16} \qquad (5a)$$

$$E^{(-)}(L) = 9.869604(L/2)^{-2} + 0.114078(L/2)^4 - 0.000515(L/2)^{10} + 0.000002(L/2)^{16} \qquad (5b)$$

One of the purposes of this paper is to prove the convergente of the above series for small boxes. An intuitive argument was given by previous authors[7,8,9], as follows. As the matrix elements are proportional to $(L/2)^4$, and the difference between unperturbed energy levels deci-eases with $(L/2)^{-2}$, we can say that the perturbation is small compared with the unperturbed system for values of $(L/2)$ less than 1.

We now give a more rigorous argument based on Rellich's theorem[10], which states that if the Hamiltonian can be written as a convergent power series in some perturbative parameter, or particularly

$$H = H_0 + \lambda V$$

with V being a bounded operator, then the perturbed eigenvalues are analytic functions of λ and they are convergent power series in a neighbourhood of $\lambda=0$. The proof of this theorem can be found in Rellich's book[10].

As the convergence of the perturbative series in assured, it is natural to estimate the convergence region. This is obtained as follows[11].

Consider the projector formally defined by

$$P_n(\lambda) = -\frac{1}{2\pi i}\oint_{C_n} (H_0+\lambda V-\ell)^{-1} d\ell \tag{6}$$

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 the nearest eigenvalue. The perturbed wave function can be obtained by applying $P_n(\lambda)$ over any trial function.

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

$$P_n(\lambda) = \frac{i}{2\pi}\oint_{C_n} R(0) \sum_{k=0}^{\infty} (-1)^k \lambda^k [VR(0)]^k \,, \quad \text{where } R(0) = (H_0-\ell)^{-1} \tag{7}$$

In order to obtain a convergent series for the perturbed wavefunction, the series (7) must be convergent. The sufficient condition which satisfies our requirements is[11]

$$|\lambda| . ||V|| \, (d/2)^{-1} < 1 \tag{8}$$

and if V is a multiplicative operator, its norm is given by

$$||V|| = \sup V(x) \,, \quad -L/2 \leqslant x \leqslant L/2$$

From eq. (1), by making the change of variable $x = yL/2$, we see that the perturbative parameter is $(L/2)^6$, where now the boundary conditions are $\psi(+1) = \psi(-1) = 0$.

The upper bound for the convergence radius is obtained from eq. (8), and the result for pratical purposes is

$$L/2 < (d/2)^{1/6} \tag{9}$$

where d is expressed in terms of the unperturbed energy levels in the box multiplied by $(L/2)^2$.

4. PADÉ-APPROXIMANT SOLUTIONS

Modified one-point Padé-approximant was constructed with help of expressions like (5a) and (5b), valid in the region of small boxes, and the asymptotic eigenvalues obtained by diagonalization of the Hamiltonian matrix for large boxes. These asymptotic eigenvalues are numerically obtained for boxes with size $L/2$ greater then 3, which are named D_N.

The Padé-approximants are constructed for the function $G(L)$ defined by

$$G(L) = [E_N(L) - D_N](L/2)^2 \tag{10}$$

and they have the form

$$P_{N/M} = \sum_{n=0}^{N} c_n (L/2)^{2n} / \sum_{m=0}^{M} b_m (L/2)^{2m}, \quad b_0 = 1 \tag{11}$$

We should point out that M must be greater then N in order to reproduce the asymptotic behaviour (see eq. (10)). We have performed the computation for $M=7$ and $N=2$, and the resulting approximant can be written as $[x \equiv L/2]$

$$P_{2/7} = \frac{c_0 + c_1x^2 + c_2x^4}{1 + b_1x^2 + b_2x^4 + b_3x^6 + b_4x^8 + b_5x^{10} + b_6x^{12} + b_7x^{14}} \tag{12}$$

The coefficients for the ground and first excited states are given in the list below.

ground state	first excited state
$c0 = 2.467401$	$c0 = 9.869604$
$c1 = -1.905316$	$c1 = -5.889344$
$c2 = 0.315769$	$c2 = 0.839951$
$b1 = -0.342447$	$b1 = -0.211728$
$b2 = -0,019190$	$b2 = 0.003592$
$b3 = -0.024904$	$b3 = -0.010176$
$b4 = -0.004998$	$b4 = -0.001470$
$b5 = -0.001828$	$b5 = -0.000608$
$b6 = -0.000247$	$b6 = -0.000064$
$b7 = -0.000065$	$b7 = -0.000019$

The eigenvalues are obtained by using eq. (10).

5. NUMERICAL RESULTS AND DISCUSSION

We present in Table 1 our numerical results for the first ten eigenvalues of a pure quartic bounded potential. We discuss first the exact eigenvalues, which are obtained by diagonalizing the Hamiltonian matrix for several values of L. We observe that the eigenvalues rapidly decrease to its unbounded behavior. For values of $L/2$ greater than 3, the eigenvalues do not change substantially, and we can take it almost as the unbounded ones.

In second place we observe that the perturbative eigenvalues are shown to agree very well with the exact ones, for values of $L/2$ less than 1.7. This agreement also verifies the good estimate for the radius of convergence. In Table 1 the radius of convergence is estimated using eq. (9).

As a third point, we have that the eigenvalues obtained by the modified one-point Padé-approximant are shown to match very well in the region of small boxes (perturbative solution) and the region of very large boxes (obtained by diagonalizing the Hamiltonian matrix for $L/2 = 3$). This result is due to the fact that this Padé-approximant has information either from small and large boxes behavior.

Table 1. Energy levels for several box sizes.

N=0. Radius of convergence d < 1.24

$L/2$	Perturbative	Padé	Exact
0.1	246.740114	246.740114	246.740106
0.5	9.872173	9.872173	9.872172
0.8	3.872116	3.872116	3.872115
1.0	2.508197	2.508199	2.508197
1.1	2.098567	2.098582	2.098566
1.2	1.796851	1.796946	1.796850
1.3	1.573341	1.574093	1.573335
1.4	1.408481	1.403023	1.408452
1.5	1.288742	1.285631	1.288611
2.0	1.128540	1.063745	1.072620
2.5	5.017693	1.053940	1.060451
3.0	95.218101	1.058365	1.060363

N=1. Radius of convergence d < 1.24

$L/2$	Perturbative	Padé	Exact
0.1	986.960451	986.960451	986.960418
0.5	39.485547	39.485547	39.485546
0.8	15.467928	15.467928	15.467927
1.0	9.983169	9.983171	9.983169
1.1	8.322392	8.322403	8.322392
1.2	7.087292	7.087345	7.087291
1.3	6.158855	6.159091	6.158854
1.4	5.459300	5.460300	5.459295
1.5	4.935656	4.940029	4.935630
2.0	3.900481	3.830613	3.882506
2.5	5.933144	3.755976	3.800480
3.0	68.869411	3.784057	3.799674

N=2. Radius of convergence d < 1.35

$L/2$	Perturbative	Padé	Exact
0.1	2220.661006	2220.661006	2220.660930
0.5	88.836315	88.836315	88.836312
0.8	34.762523	34.762523	34.762521
1.0	22.364373	22.364373	22.364373
1.1	18.583270	18.583271	18.583269
1.2	15.747359	15.747365	15.747360
1.3	13.587812	13.587836	13.587818
1.4	11.929474	11.929571	11.929506
1.5	10.654338	10.654693	10.654483
2.0	7.723157	7.800756	7.783707
2.5	3.633719	7.586946	7.460468
3.0	-68.614220	7.616175	7.455702

N=3. Radius of convergence d < 1.43

$L/2$	Perturbative	Padé	Exact
0.1	3947.841778	3947.841778	3947.841643
0.5	157.924647	157.924647	157.924642
0.8	61.756966	61.756966	61.756963
1.0	39.654041	39.654040	39.654039
1.1	32.883907	32.883906	32.883906
1.2	27.779680	27.779678	27.779680
1.3	23.861416	23.861405	23.861417
1.4	20.816167	20.816134	20.816175
1.5	18.433540	18.433454	18.433580
2.0	12.559499	12.577592	12.583568
2.5	9.107625	11.673249	11.666097
3.0	-55.746637	11.693011	11.644771

N=4. Radius of convergence d < 1.49

$L/2$	Perturbative	Padé	Exact
0.1	6168.502768	6168.502769	6168.502559
0.5	246.751621	246.751621	246.751613
0.8	96.458304	96.458304	96.458301
1.0	61.869281	61.869281	61.869279
1.1	51.249205	51.249205	51.249203
1.2	43.219173	43.219175	43.219171
1.3	37.026989	37.026997	37.026988
1.4	32.181393	32.181423	32.181390
1.5	28.351563	28.351668	28.351556
2.0	18.386790	18.405985	18.385989
2.5	15.809674	16.926889	16.337912
3.0	-9.791335	18.868224	16.267339

N=5. Radius of convergence d < 1.54

$L/2$	Perturbative	Padé	Exact
0.1	8882.643979	8882.643979	8882.643677
0.5	355.317567	355.317567	355.317555
0.8	138.868708	138.868708	138.868703
1.0	89.015459	89.015459	89.015456
1.1	73.687121	73.687121	73.687118
1.2	62.077331	62.077329	62.077329
1.3	53.100812	53.100806	53.100810
1.4	46.047861	46.047838	46.047858
1.5	40.439690	40.439610	40.439681
2.0	25.296398	25.285068	25.292437
2.5	21.627944	21.429051	21.460899
3.0	15.606391	21.431404	21.238971

N=6. Radius of convergence d < 1.59

$L/2$	Perturbative	Padé	Exact
0.1	12090.265409	12090.265409	12090.264998
0.5	483.622605	483.622605	483.622589
0.8	188.988980	188.988980	188.988973
1.0	121.094568	121.094568	121.094564
1.1	100.200624	100.200624	100.200621
1.2	84.358471	84.358470	84.358468
1.3	72.089060	72.089057	72.089057
1.4	62.424345	62.424333	62.424342
1.5	54.710370	54.710329	54.710365
2.0	33.371432	33.364294	33.368925
2.5	27.320832	27.043798	27.075426
3.0	28.143698	26.908310	26.530807

N=7. Radius of convergence d < 1.62

$L/2$	Perturbative	Padé	Exact
0.1	15791.367059	15791.367060	15791.366522
0.5	631.666790	631.666790	631.666768
0.8	246.819469	246.819469	246.819460
1.0	158.107472	158.107472	158.107467
1.1	130.790994	130.790994	130.790990
1.2	110.064442	110.064442	110.064438
1.3	93.994365	93.994363	93.994361
1.4	81.314554	81.314548	81.314551
1.5	71.168837	71.168817	71.168833
2.0	42.650697	42.646845	42.649471
2.5	33.426740	33.228790	33.255403
3.0	35.519688	32.702383	32.106660

N=8. Radius of convergence d < 1.66

$L/2$	Perturbative	Padé	Exact
0.1	19985.948930	19985.948930	19985.948250
0.5	799.450146	799.450146	799.450119
0.8	312.360345	312.360345	312.360334
1.0	200.054586	200.054587	200.054581
1.1	165.458842	165.458844	165.458842
1.2	139.196109	139.196119	139.196128
1.3	118.817891	118.817929	118.817972
1.4	102.719949	102.720085	102.720226
1.5	89.816656	89.817100	89.817501
2.0	53.065825	53.123754	53.149897
2.5	37.171063	39.623057	40.080430
3.0	-14.382779	36.452001	37.947739

Finally, we would like to add that Rellich's theorem is also applicable to other systems, provided that the potential is bounded.

In the confined hydrogen atom or harmonic oscillator, the perturbative parameter is L or L^4, respectively. The upper bound for the radius of convergence is obtained in the same way as we did, replacing $(L/2)^6$ for the appropriate perturbative parameter.

We wish to point out that our exact numerical results differ slightly from those of Ref.1. The reason is due to the fact that those authors take only 100 terms in their eqs. (3) and (4) (let us remark that the symbol L in their Tables 1 and 2 should be substituted by $L/2$). We believe that by taking more terms in their eqs. (3) and (4) the corresponding results will become closer to ours.

One of us (JFG) gratefully acknowledges Drs. J.F. Perez and B.M. Pimentel for useful discussions about Rellich's theorem. He is also grateful to FAPESP for a post-graduate grant. We also thank Dr. R. Barakat for an helpful correspondence.

REFERENCES

1. R.Barakat and R.Rosner, Phys.Lett. *83*A, 149 (1981). See also F.M. Fernández and E.A.Castro, Phys.Lett. *88*A, 4 (1982). An approximate solution in the whole straight line was discussed by F.T. Hioe and E. W. Montroll, J. of Math. Phys. 16,1949 (1975).
2. J.E. Kilpatrick and M.F.Kilpatrick, J.Chem.Phys. *16*, 781 (1948).
3. S.Chan and D.Stellman, J.Molec. Spectrosc. *10*, 278 (1963).
4. F.C. Auluck and D.S.Kothari, Proc. Cambridge Phylos. Soc. 41 , 175 (1945).
5. K.K. Singh and J.S. Baljal, Prog.Theor.Phys. 4, 214 (1955).
6. R.P. Bell, Proc. R. Soc. (London) A 183, 328 (1945).
7. V.C.Aguilera-Navarro, W.M.Kloet and A.H.Zimerman, Rev. Bras. Fís. *1*, 55 (1971).
8. V.C.Aguilera-Navarro, E.Ley Koo and A.H.Zimerman, J.Phys. A*13*,3585 (1980).
9. V.C.Aguilera-Navarro, E.Ley Koo and A.H.Zimerman, Rev. Bras. Fís. *10*, 251 (1980).
10. F. Rellich, *Perturbation Theory of Eigenvalue Problem*, N.Y., Gordon and Breach, 1969.

11. T.Kato, Prog. Theor. Phys. 4, 514 (1949); 5, 95 (1950).

12. G. Baker Jr., *Essentials of Padé Approximants*, N.Y., Ac. Press, 1975.

Resumo

As autoenergias do potencial quártico numa caixa são obtidas exatamente e perturbativamente usando como base os autoestados de partícula livre numa caixa. Os autovalores exatos são obtidos a partir da diagonalização do hamiltoniano com respeito àquela base. A solução perturbativa é construída da expansão de Rayleigh-Schrodinger usando o potencial quártico como perturbação. Mostra-se que a série perturbativa é convergente, para caixas pequenas, e estima-se um limite superior para o raio de convergência. Constroem-se, também, soluções aproximantes (de Padé), válidas para caixas de qualquer tamanho. A comparação numérica das soluções perturbativas e as de Padé com as exatas confirma a validade daquelas, e, em especial, a convergência e o raio de convergência da série perturbativa.