

# A NON-PERTURBATIVE METHOD FOR THE $KX^2 + \beta X^4$ INTERACTION

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## ABSTRACT

A numerical procedure is presented, yielding rapidly convergent and stable eigenvalues for the anharmonic interaction  $\kappa X^2 + \beta X^4$ , with both positive and negative values of  $\kappa$  and  $\beta$ . This non-perturbative method consists basically of the diagonalization of a finite pre-established Hamiltonian matrix, whose eigenvalue equation resembles the Schrödinger equation. This method can also be used successfully for other kind of potentials. It is similar in some aspects to the Calogero's method to compute eigenvalues of differential operators.

## RESUMEN

Se presenta una técnica numérica que produce eigenvalores estables y rápidamente convergentes para la interacción anarmónica  $\kappa X^2 + \beta X^4$ , con valores tanto positivos como negativos de  $\kappa$  y  $\beta$ . Este método no perturbativo consiste básicamente en la diagonalización de una matriz hamiltoniana finita preestablecida, cuya ecuación de eigenvalores asemeja a la ecuación de Schrödinger. Este método puede ser usado exitosamente para otros potenciales. En algunos aspectos es similar al método de Calogero para calcular eigenvalores de operadores diferenciales.

## 1. INTRODUCTION

In the past few years, a great deal of analytical and numerical research on the calculation of the eigenvalues and eigenfunctions of the Schrödinger equation for the quartic anharmonic interaction

$$V(x) = \kappa x^2 + \beta x^4, \quad -\infty < x < \infty, \quad (1)$$

have been carried out. Interest in this kind of potential has stemmed from the fact that it is a simple, non-trivial nonlinear interaction having applications in molecular physics and field theory. Several methods have been applied to this problem by many authors.

Since the work of Bender and Wu<sup>(1)</sup>, who proved that the perturbation series in terms of the parameter  $\beta$  for the ground state of the anharmonic oscillator is divergent, perturbative-type methods have explored new approaches. Some of these recent techniques can be found in Refs. 2-8. Parallel to this, other non-perturbative methods have also been applied to obtain approximate solutions of the Schrödinger equation for the potential given in Eq. (1) (see for example Pefs. 9-19).

It is well known that this interaction represents different physical systems according to the location of the parameters  $\kappa$  and  $\beta$  on the real line. We have the following three cases:

a)  $\kappa > 0, \beta > 0$ . These ranges give rise to the anharmonic oscillator which has been widely studied in the past. In this case, most of the work deals with analytical expressions, or numerical quantities, for the approximants to the energy eigenvalues.

b)  $\kappa < 0, \beta > 0$ . For these ranges we have the double well, another confinement problem. It has been studied, among others, in Refs. 5, 16-19, where approximants to both eigenvalues and eigenfunctions are calculated. It is found also that the energy spectrum has its lower eigenvalues bunched in pairs when the two minima of the potential are sufficiently separated.

c)  $\kappa > 0, \beta < 0$ . None on the papers mentioned previously, report any explicit calculation for this non-confinement potential, but

Chaudhuri and Mukherjee<sup>(19)</sup>, suggest a study through the stabilization method<sup>(20)</sup> and the renormalization series approach<sup>(17,21)</sup>. On the other hand, Flessas, Whitehead and Rigas<sup>(22)</sup> have obtained a class of exact solutions of the Schrödinger equation for the potential  $V(x) = \kappa x^2 + \beta x^4$ ,  $x > 0$ ,  $\kappa \geq 0$ ,  $\beta < 0$ , and have shown that the corresponding eigenvalues are continuous, however, they have cut off this potential for both positive and negative values of  $x$ .

In spite of the great number of papers on anharmonic oscillators the preceding remarks attempt to show that it may be desirable to have a method that besides yielding accurate and rapidly convergent results for cases (a) and (b) above, was able to deal with the anharmonic interaction (1) with  $\kappa > 0$ ,  $\beta > 0$ .

In this paper, a stable numerical procedure with these features is presented. It will be seen in Sec. 2, that this method consists basically in the diagonalization of a finite, pre-established Hamiltonian matrix (whose eigenvalue equation resembles the one-dimensional Schrödinger equation) which is fitted *via* an extremal property where the potential is involved. In Sec. 3, the results of diagonalization in cases (a) and (b) are given. The eigenvalues yielded by this procedure are compared with those calculated by other methods, and their stable nature is shown. It is suggested that the proper values obtained in case (c) are the approximants to the resonance energies of this non-confinement potential. This suggestion stems from the acceptable agreement of the lowest eigenenergy obtained by this method for the model potential

$$V(x) = \begin{cases} \frac{1}{2} x^2, & x \leq 0, \\ \frac{1}{2} x^2 \exp(-\lambda x^2), & x \geq 0, \end{cases} \quad (2)$$

and those given by Hazi and Taylor<sup>(20)</sup> for the resonance energies of this problem. We conclude in Sec. 4 with a discussion of the main results presented in this paper.

## 2. THE METHOD

The method that we will describe in this section is based on the suggestion made in a previous work related with the harmonic oscillator<sup>(23)</sup>. In that paper, a discrete equation in a N-dimensional space for the eigenvectors and exact eigenvalues of the linear oscillator is obtained by replacing the usual position and momentum operators by finite matrices, obtained by truncating the infinite matrices for these operators in the energy representation. Such eigenvalue equation has the form

$$-\frac{\hbar^2}{2m} \sum_{j,k}^N \frac{\phi_n(x_j)}{(x_i - x_k)(x_k - x_j)} + V(x_i) \phi_n(x_i) = E_n \phi_n(x_i) \quad , \quad (3)$$

where  $i = 1, 2, \dots, N$ ;  $n = 0, 1, \dots, N-1$ ;  $\Sigma'$  means the sum over the values which make a non-null denominator;  $\hbar$  is the modified Planck's constant;  $m$  is the mass of the particle subject to the potential  $V(x) = \frac{1}{2}m\omega^2 x^2$ ; the points  $x_1, x_2, \dots, x_N$  are the eigenvalues of the finite matrix representing the position operator (it turns out that, except for a constant, they are also the N zeros of the N-th Hermite function);  $E_n$  is given by

$$E_n = \begin{cases} (n + \frac{1}{2}) \hbar\omega, & 0 \leq n \leq N-2 \quad , \\ \frac{N-1}{2} \hbar\omega, & n = N-1 \quad ; \end{cases} \quad (4)$$

and finally,  $\phi_n(x_i)$ ,  $i=1, 2, \dots, N$ , are the components of the eigenvector corresponding to  $E_n$ . It should be said that Eq. (3) is the representation of the Hamiltonian in the x-basis, where the elements  $p_{jk}$  of the finite matrix associate to the momentum operator are given by

$$p_{jk} = \begin{cases} 0, & j = k \quad , \\ (-i\hbar) \frac{1}{(x_j - x_k)}, & j \neq k \quad , \end{cases} \quad (5)$$

where  $i$  stands for the imaginary unity. It is also shown in Ref. 23 that the points  $x_1, x_2, \dots, x_N$  satisfy the equation

$$\sum_{j=1}^N \frac{1}{(x_i - x_j)^3} = \frac{m}{2\hbar^2} \frac{dV(x_i)}{dx_i} \quad (6)$$

for all  $x_i$ . This equation is the necessary condition for an extremal property of these zeros: the function

$$\text{Tr } H(z_1, z_2, \dots, z_N) = \text{Tr } H(z) = \frac{\hbar^2}{2m} \sum_{i,j}^N \frac{1}{(z_i - z_j)^2} + \sum_{i,j}^N V(z_i) \quad , \quad (7)$$

where  $-\infty < z_i < \infty$  takes a stationary value in  $z_i = x_i$ . It can be shown that Eq. (7) (and therefore the extremal property) holds for certain polynomial solutions of the Schrödinger equation, and that  $\text{Tr } H(x)$  is an absolute minimum if  $V'(x_i) > 0$  for all  $x_i$ . This fact makes plausible the conjecture made in Ref. 23 about Eqs. (3) and (6). In that paper it is guessed that these equations are expected to hold for  $V(x)$  different from the harmonic one. The guess comes from the resemblance of Eq. (3) with the Schrödinger equation and from the physical meaning of the extremal property of  $\text{Tr } H(z)$ . One of the purposes of this work is to test numerically this conjecture for the potentials (1) and (2).

A glance at Eq. (3) shows that in order to handle it as an eigenvalue equation, it is necessary to have determined the points  $x_i$  previously. This can be carried out by using Eq. (6). This is the major difficulty of the method from a numerical point of view. The nonlinear nature of Eq. (6) makes difficult to get some information about the dependence of its solution on the number  $N$  and on the parameters involved in  $V(x)$ . But, in principle, we can solve numerically this equation and obtain the set of  $N(N \geq 2)$  points  $x_i$  which hereafter will be denoted by  $x_i^N$  and ordered as usual:  $x_1^N < x_2^N < \dots < x_N^N$ . After the replacing of these values in Eq. (3), we can diagonalize it and obtain the  $N$  eigenvalues and  $N$  eigenvectors which from now on will be denoted by  $E_n^N$  and  $\phi_n^N(x) = (\phi_n^N(x_1^N), \phi_n^N(x_2^N), \dots, \phi_n^N(x_N^N))$ , respectively.

In order to be able to compare the numerical results yielded by

this method for the potential (1) with those reported in the literature, Eqs. (3) and (6) must be rewritten by putting  $\hbar=m=1$  and  $2V(x)$  equal to the right-hand side of Eq. (1). Hereafter we will bear in mind these changes whenever we refer to those equations with potential (1).

### 3. NUMERICAL RESULTS

It is not difficult to prove the following general properties of Eqs. (3) and (6): If  $V(x)$  is a symmetric function, the points  $x_i^N$  are symmetrically located around the origin and Eq. (3) has solutions of definite symmetry, *i.e.*,  $\phi_n^N(-x)$  differs from  $\phi_n^N(x)$  at the most by a change of sign, if the points  $x_i^N$  has been properly ordered. More properties of the solutions of Eqs. (1) and (6) in the specific case of potential (1) will be described numerically in this section. Before continuing, let us make a remark on the computer technique used to obtain such solutions. Newton's method was used to solve Eq. (6) and the iterations were stopped when the maximum difference of two consecutive iterative values of points  $x_i^N$  was less than  $10^{-15}$ . Such approximation gave as a result that Eq. (6) was satisfied at least within eleven significant figures among all the values of  $\kappa$  and  $\beta$  considered. This is not a good approximation but eigenvalues in good agreement with those reported in the literature can be obtained by diagonalizing the Hamiltonian involved in Eq. (1) as shown in the following

A.  $\kappa > 0, \beta > 0$

First of all, it should be noticed that there will be no lack of generality in our results if  $\kappa$  is constrained to be 1 for the present (a simple scaling is enough to recover  $\kappa > 0$ ,  $\kappa$  arbitrary). For this value of  $\kappa$ , it is possible to find a solution of Eq. (6) for  $\beta$  lying in  $[0,1000]$  and for  $N=2,3,\dots,35$ . Numerical work gives evidence of the existence of solutions for larger values of  $\beta$  and  $N$ .

As expected, the points  $x_i^N(1,\beta)$  were found to be symmetrically located around zero. It turns out that  $|x_i^N(1,\beta)|$ , with fixed  $N$  and  $i=1,2,\dots,N$ , is a very rapidly decreasing function for small  $\beta$  whereas for large  $\beta$ , it decreases very slowly as illustrated in Fig. 1 where the fifteen positive points  $x_i^N$ , corresponding to  $N=30$ , are plotted against the anharmonic parameter  $\beta$ .

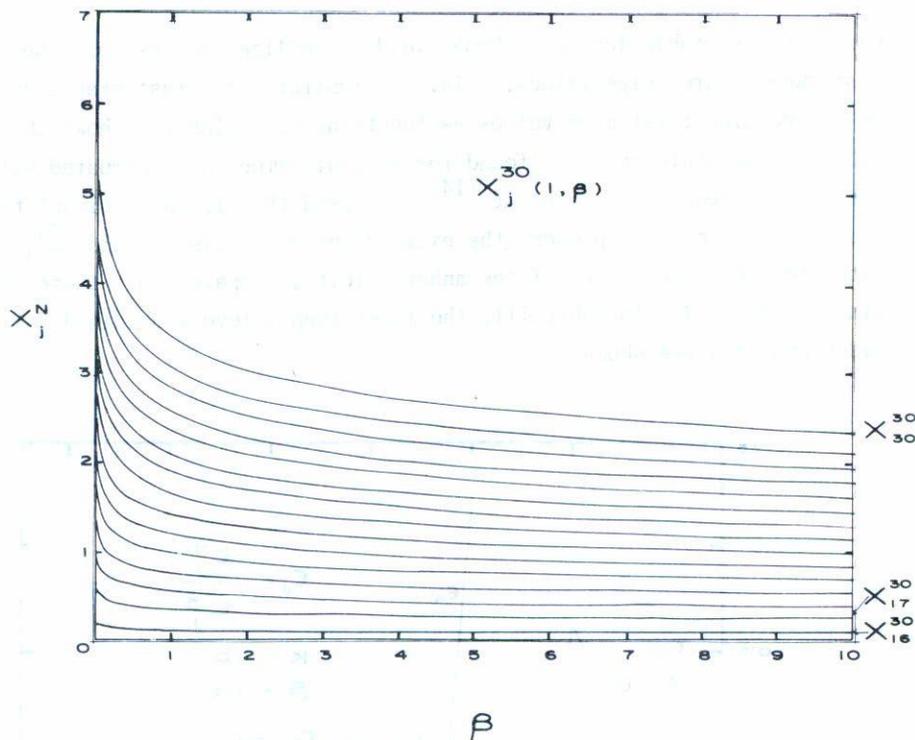


Fig. 1. Plots of the fifteen positive points  $x_i^N$ ,  $i=16,17,\dots,30$ , used to fit the Hamiltonian matrix whose diagonalization yields approximations for the eigenvalues of the anharmonic oscillator  $V(x)=x^2+\beta x^4$  ( $0 \leq \beta \leq 10$ ), against  $\beta$ .

Once the points  $x_i^N$  have been calculated, we replace them in Eq.(1) in order to solve for the proper values  $E_n^N$  and eigenvectors  $\phi_n^N(x)$ . When the resultant eigenvalues are arranged in increasing order for different consecutive values of  $N$ , we obtain a family of sequences that rapidly converge to stable values of  $E_n^N$  for  $n$  fixed. However, a spurious eigenenergy, *i.e.*, a non-stable eigenvalue that does not correspond to any energy sequence, always appears among the  $N$  eigenvalues in every diagonalization. Its numerical value depends on  $N$  and it can be identified very easily. It plays the same role as the eigenvalue  $E_{N-1} = [(N-1)/2]\hbar\omega$  of the harmonic oscillator [see Eq. (4)].

The number  $N$  for which the stable value (up to 15 figures) of  $E_n^N$  is attained depends on  $n$  and  $\beta$ . For instance, if  $\beta=1$ ,  $E_0^N$  is stable for  $N \geq 13$

whereas  $E_6^N$  is stable for  $N \geq 20$ ;  $N=35$  yields stabilized values for the first twenty-three eigenvalues. Fig. 2 illustrates the fast stabilization of the nine first eigenvalues as functions of  $N$ . Table I shows the stable ground state energies found for several values of  $\beta$  compared with those calculated by Biswas *et.al.* <sup>(14)</sup>, who used the Hill determinant technique. In Table II we present the excited energy levels  $E_3^{35}$  and  $E_7^{35}$ , calculated for some values of the anharmonicity, compared with those obtained in Ref. 14. In Table III, the first twenty levels obtained for  $\beta=1000$  and  $N=35$  are shown.

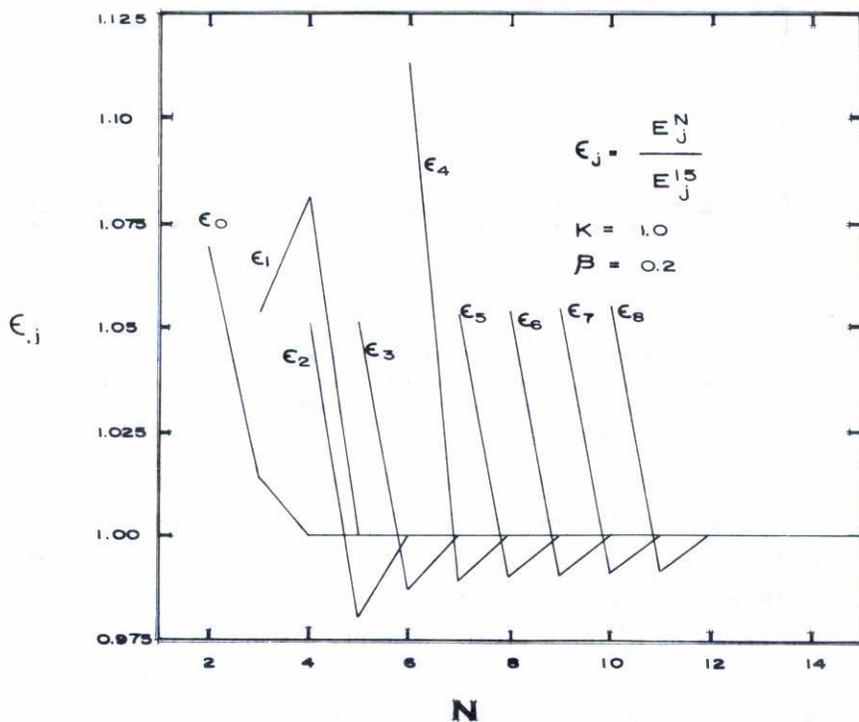


Fig. 2. Fast stabilization of the nine lowest approximants to eigenenergies for the anharmonic oscillator  $V(x) = x^2 + 0.2x^4$ , calculated by the present method. The plots are those of the ratios  $\epsilon_j = E_j^N / E_j^{15}$  against parameter  $N$ , for  $j=0,1,\dots,8$ .

TABLE I

$\beta$	$E_0^{(35)}$	$E_0^{(Bis)}$
0.2	1.118 292 654 367 03	1.118 292 654 367 03
0.4	1.204 810 327 372 50	1.204 810 327 372 49
0.8	1.337 545 208 148 17	1.337 545 208 148 17
2	1.607 541 302 468 54	1.607 541 302 468 54
10	2.449 174 072 118 38	2.449 174 072 118 38
50	4.003 992 768 277 62	4.003 992 768 277 62
60	4.243 081 446 423 64	4.243 081 446 423 64
100	4.999 417 545 137 59	4.999 417 545 137 58
500	8.461 642 629 081 18	. . .
1000	10.639 788 711 328 0	. . .

Table I. Ground state energies (in a.u.) of the anharmonic oscillator for several values of the anharmonicity.  $E^{(35)}$  are the stable values yielded by the present method and  $E^{(bis)}$  are those obtained by Biswas *et.al.*, (see Ref. 14).

On the other hand, it is found that, as expected, the eigenvectors  $\phi_n^N(x)$  have a definite parity: their components satisfy

$$\phi_n^N(x_j^N) = (-1)^{N-1-n} \phi_n^N(-x_j^N), \quad n=0,1,\dots,N-1,$$

where  $-x_j^N$  is also an element of the set of points satisfying Eq.(6). Besides, the linear interpolation of the components  $\phi_n^N(x_j^N)$ ,  $j=1,2,\dots,N$ , denoted from now on by  $\mathcal{L}(\phi_n^N)$ , has exactly  $N-1-n$  nodes. Fig. 3 shows  $\mathcal{L}(\phi_0^{35})$ ,  $\mathcal{L}(\phi_1^{35})$  and  $\mathcal{L}(\phi_2^{35})$ , obtained for  $\beta=0.1$ .

Two interesting features of this interpolating process can be pointed out. The first is the way in which it depends on  $N$ . The plots of  $\mathcal{L}(\phi_0^{15})$  and  $\mathcal{L}(\phi_0^{35})$  shown in Fig. 4 illustrate this dependence. The

TABLE II

$\beta$	$E_3^{(35)}$	$E_3^{(\text{Bis})}$	$E_7^{(35)}$	$E_7^{(\text{Bis})}$
3	17.859 316 502 141 4	17.859 316	48.073 337 128 514 4	48.073 337
6	22.009 467 099 122 2	22.009 467	59.743 658 359 573 8	59.743 658
9	24.965 808 107 073 2	24.965 808	68.006 918 953 755 0	68.006 918
10	25.806 276 215 055 6	25.806 276	70.351 051 939 234 6	70.351 051
50	43.321 550 474 406 9	43.321 550	118. 953 883 032 244	118.953 88
100	54.385 291 571 603 1	54.385 291	149. 545 657 443 288	149.545 65
500	92.620 596 454 251 5	. . .	255. 092 750 615 571	. . .
1000	116. 603 198 937 293	. . .	321. 244 760 274 354	. . .

Table II. Third and seventh excited energy levels (in a.u.) of the anharmonic oscillator for some values of parameter  $\beta$ .  $E^{(35)}$  are the eigenvalues calculated by the present method and  $E^{(\text{Bis})}$  are those obtained by Biswas *et. al.*, (see Ref. 14).

TABLE III

J	$E_j^{35}$	j	$E_j^{35}$
0	10.639 788 711 328 04	10	502.886 399 284 715 7
1	38.086 833 459 382 28	11	567.686 243 636 189 9
2	74.681 404 200 164 81	12	634.394 242 871 855 2
3	116.603 198 937 293 1	13	702.906 871 196 509 9
4	162.802 374 196 975 3	14	773.133 614 216 448 3
5	212.594 183 409 734 3	15	844.994 531 747 478 9
6	265.519 951 678 280 2	16	918.418 407 996 414 7
7	321.244 760 274 354 6	17	993.341 319 846 245 1
8	379.511 311 178 728 8	18	1069.705 509 825 030
9	440.114 532 233 655 5	19	1147.458 485 682 109

Table III. The first twenty energy levels of the anharmonic oscillator calculated by the present method for  $\beta=1000$  with  $N=35$ .

envelopes of these curves become smoother as  $N$  is increased and in the case of  $\beta = 0$  (harmonic oscillator) the unnormalized ground state wave function can be fitted pretty well with the envelope of  $\mathcal{L}(\phi_0^{35})$ . The second is the resemblance of the interpolation  $\mathcal{L}[(\phi_n^N)^2]$  to the square of the  $n$ -th eigenfunction of the harmonic oscillator. In Fig. 5 we plot  $\mathcal{L}[(\phi_0^{35})^2]$ ,  $\mathcal{L}[(\phi_1^{35})^2]$  and  $\mathcal{L}[(\phi_2^{35})^2]$  obtained for two different values of  $\beta$ . The dependence of these interpolations on  $\beta$  is also illustrated in this figure. If  $\mathcal{L}[(\phi_n^N)^2]$  approximates the square of the wave function (as suggested by the  $\beta = 0$  case) then, from Fig. 5 it is clear that the confinement of the particle is greater for large  $\beta$ . This confinement increases rapidly if  $\beta$  is small and slowly if  $\beta$  is large.

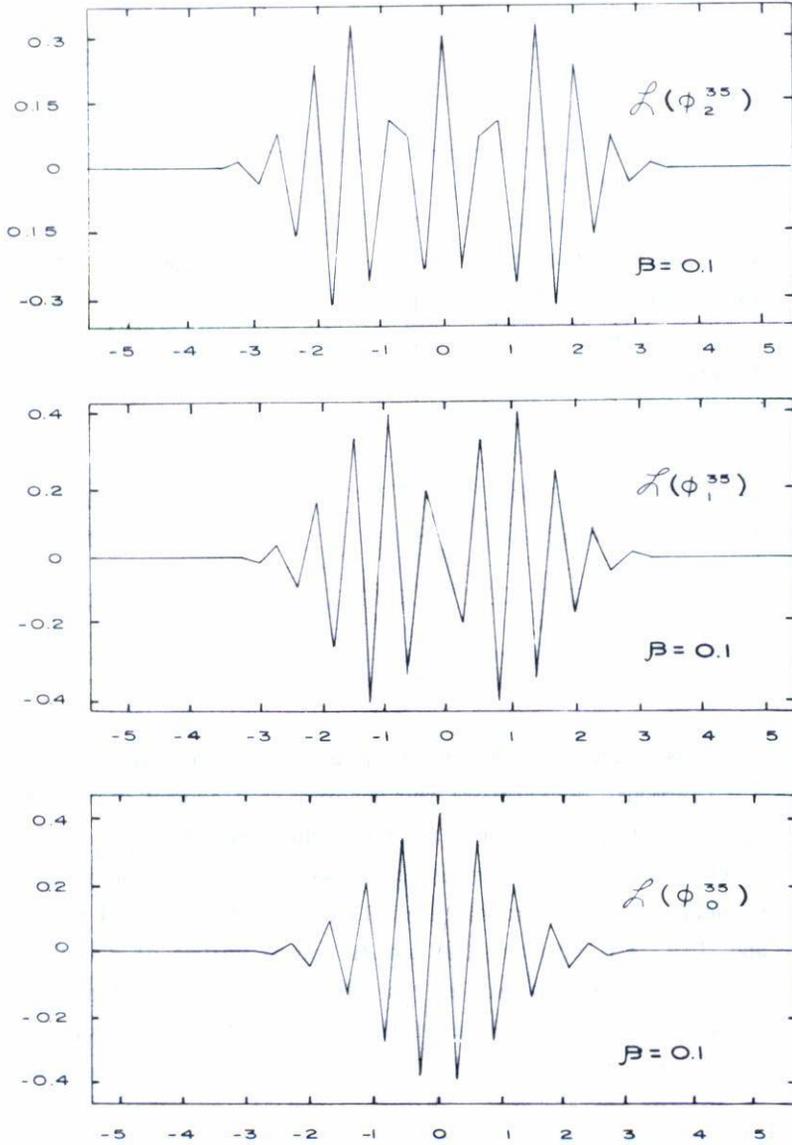


Fig. 3. Linear interpolation  $\mathcal{L}(\phi_j^{35})$  of the first three eigenvectors  $\phi_j^{35}$ , yielded by the present method for the anharmonic oscillator  $V(x) = x^2 + 0.1 x^4$ .

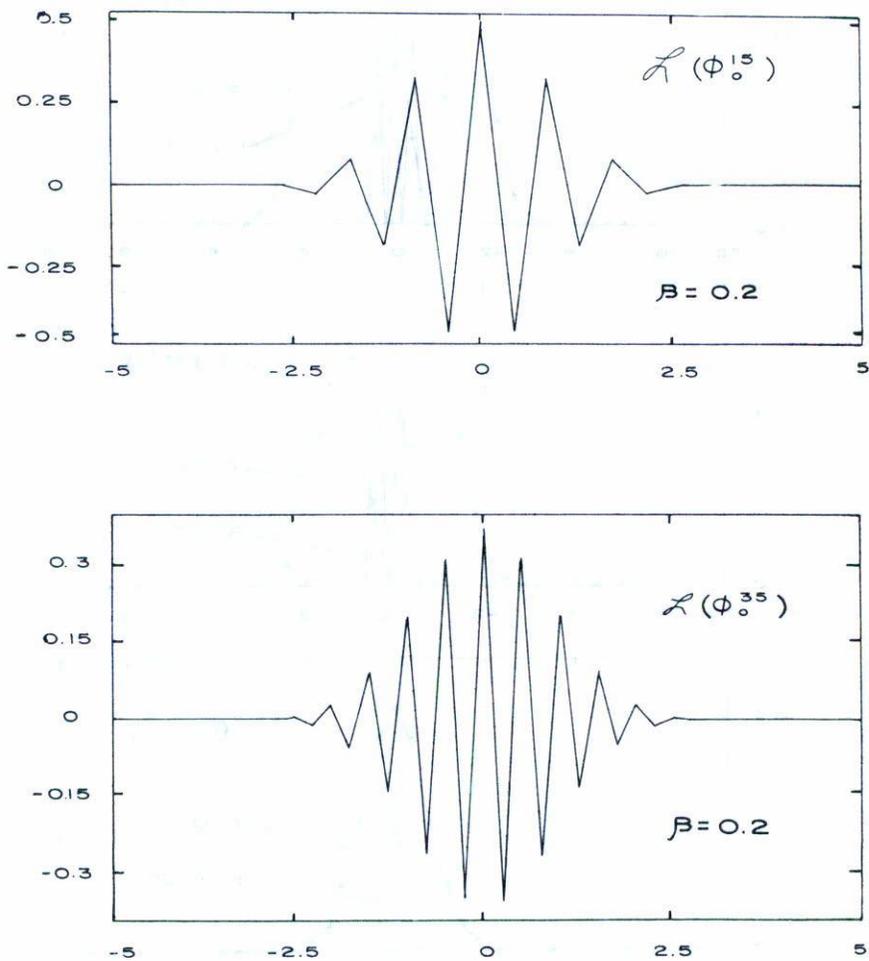


Fig. 4. Dependence on the parameter  $N$  of the linear interpolation  $\mathcal{L}(\Phi_0^N)$  of the first eigenvector  $\Phi_0^N$  obtained by the present method for the anharmonic potential  $V(x) = x^2 + 0.2x^4$ , with  $N=15$  and  $N=35$ .

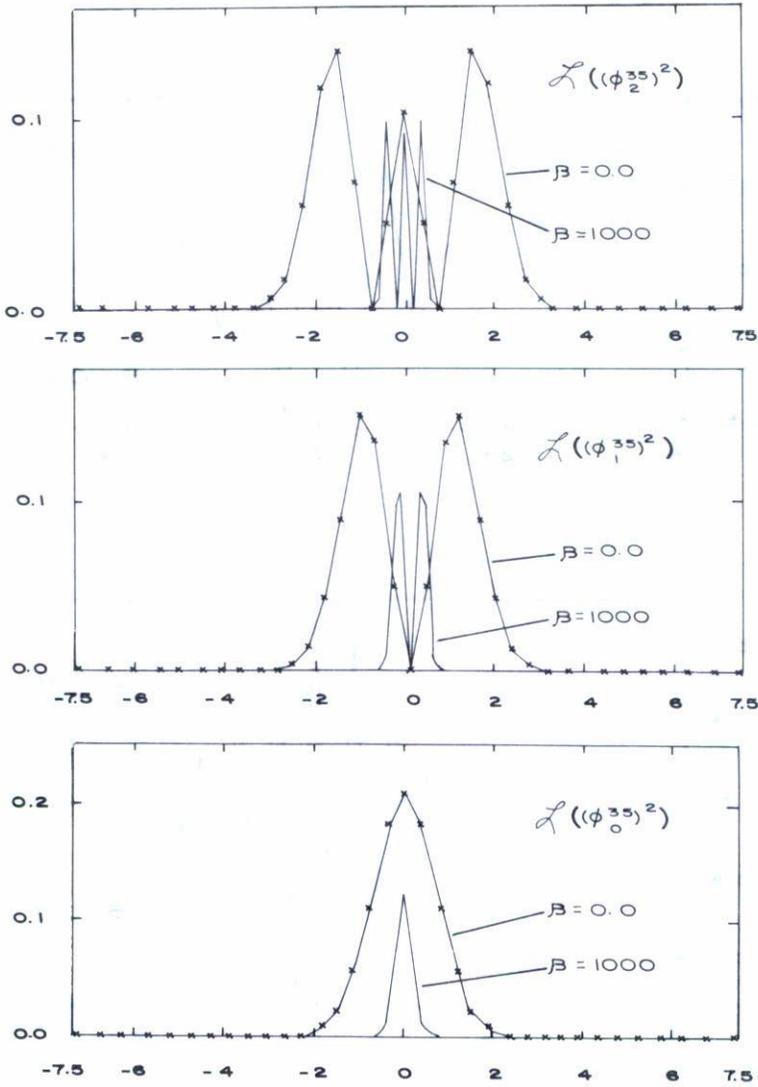


Fig. 5. Linear interpolations  $\mathcal{L}[(\phi_i^{35})^2]$  of the vectors formed by the squared components  $(\phi_i^{35})^2$  of the first three corresponding eigenvectors  $\phi_j^{35}$  obtained for the anharmonic potential  $V(x) = x^2 + \beta x^4$  by the present procedure for  $\beta=0.0$  and  $\beta=1000$ .

B.  $\kappa < 0$   $\beta > 0$

In this case, parameter  $\beta$  will be constrained to be 1 and  $\kappa$  will be allowed to lie in  $[-100, 100]$ . It is possible to find solutions of Eq.(6) for several values of  $N$  in the whole range of  $\kappa$ . The plots of the fifteen positive functions  $x_j^{30}(\kappa, 1)$  shown in Fig. 6 suggest the existence of solutions for larger values of  $\kappa$ .

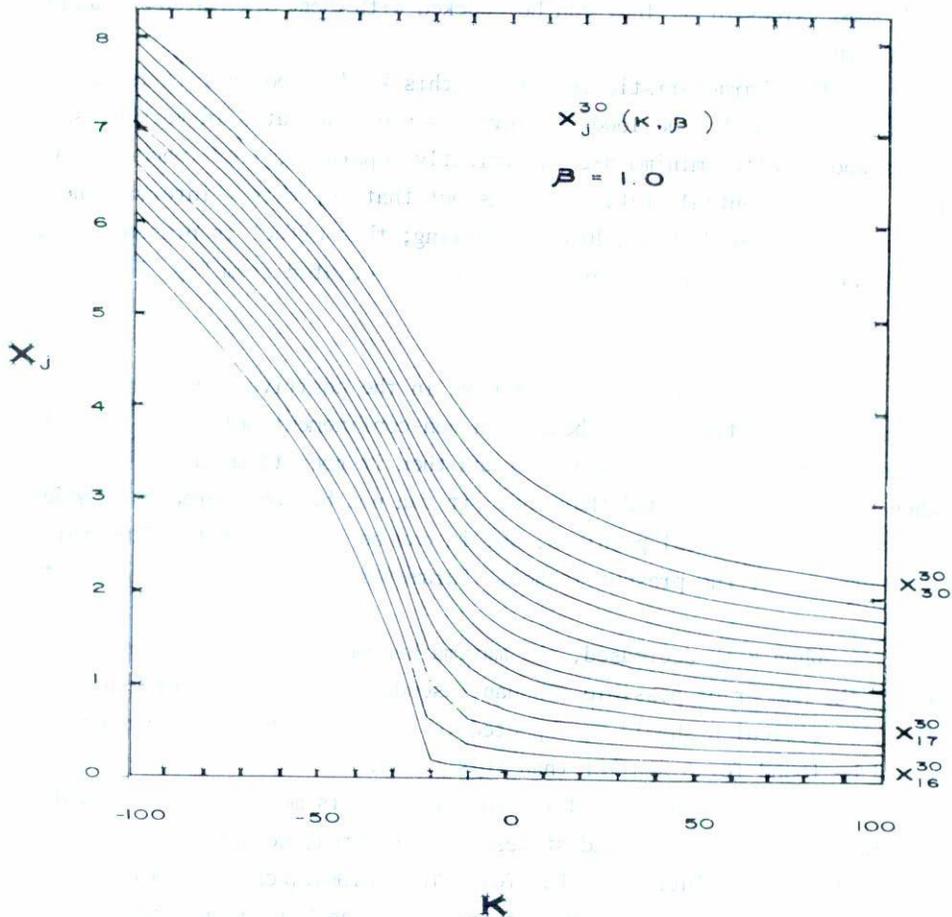


Fig. 6. Plots of the fifteen positive points  $x_i^N$ ,  $i=16, 17, \dots, 30$ , used to fit the Hamiltonian matrix whose diagonalization yields approximants for the potential  $V(x) = \kappa x^2 + x^4$  ( $-100 \leq \kappa \leq 100$ ), against  $\kappa$ .

Table IV shows the stable eigenvalues  $E_n^{35}$ ,  $n=0,1,2,3$ , calculated for various values of  $\kappa$  and compared with those obtained by Chan and Stelman<sup>(24)</sup>, Chaudhuri and Mukherjee<sup>(19)</sup> and Killingbeck<sup>(17)</sup>. Table V exhibits the eigenvalues  $E_0^{35}$  and  $E_1^{35}$  yielded by this method for the potential

$$V(x) = -x^2 + \lambda x^4 + \frac{1}{4\lambda} \quad (8)$$

with some values of  $\lambda$ . They can be checked with those calculated by Banerjee and Bhatnagar<sup>(16)</sup>.

The characteristic feature of this kind of potentials is shown in Tables IV and V: the lower eigenvalues are associated in very close pairs when the two minima are sufficiently separated, i.e., when  $\kappa \ll 0$  [ $\lambda \ll 1$  in potential (8)]. It turns out that for this  $\kappa$  interval the lower eigenstates do not exhibit tunneling; this effect is present in certain range of  $\kappa$  close to zero, as can be appreciated from Fig. 7.

### C. $\kappa > 0$ , $\beta < 0$

If  $\kappa$  and  $\beta$  are allowed to move in the positive and negative semiaxes, respectively, (1) becomes a non-confinement potential: it has two symmetrical maxima around zero and then it goes to minus infinity when  $|x|$  is increased and therefore, it can not be considered as a model potential for physical problems, but it can be worked out to illustrate some aspects of the present method. Parameter  $\kappa$  will be constrained to be 1.

When  $\beta$  is decreased, the maxima become smaller and, along with this, the number of possible resonant pseudostates should diminish. Therefore, a critical  $\beta$  should be expected to exist such that no pseudostate could be found for  $\beta$  smaller than this value.

If we are interested in studying *via* this method the limit values of  $\beta$  for which only few pseudostates are permitted, we have to take  $N$  small and to look for solutions of Eq. (6). The minimal  $\beta$  can be found by this way and, as expected, it increases negatively as  $N$  is decreased. Approximate values to the minimal ones are -0.005 and -0.011 for  $N=30$  and  $N=16$  respectively. Table VI shows the first eigenvalues obtained for an extremal and common  $\beta$  with  $N=2,3,4$ .

TABLE IV

$\kappa$	$E^{35}$	$E^{CS}$	$E^{CM}$	$E^k$
0	1.060 362 090 484 197	1.060 362 63	. . .	. . .
	3.799 673 029 801 397	3.799 675 46		
	7.455 697 937 986 741	7.455 702 48		
	11.644 745 511 378 16	11.644 750 2		
-1	0.657 653 005 180 715	. . .	0.658	
	2.834 536 202 119 305		2.835	
	6.163 901 256 963 070		6.164	
	10.038 646 120 711 58		10.032	
-10	-20.633 576 702 947 80	. . .	. . .	-20.633 576 7
	-20.633 546 884 404 91			-20.633 546 8
	-12.379 543 786 013 30			-12.379 543 7
	-12.375 673 720 705 61			-12.375 673 8
-100	-2485.867 880 342 076	. . .	. . .	. . .
	-2485.867 880 342 075			
	-2457.643 822 698 833			
	-2457.643 822 698 833			

Table IV. The first four eigenvalues for the double well  $\kappa x^2 - x^4$  with some values of  $\kappa$ .  $E^{35}$  are the stable values calculated by the present method and  $E^{CS}$ ,  $E^{CM}$ , and  $E^k$  are those obtained by Chan and Stellman (see Ref. 25), Chaudhuri and Mukherjee (see Ref. 19), and Killingbeck (see Ref. 17), respectively. All of these values are given in a.u.

If we put  $N=2$ , Eq. (6) can be solved only if  $\beta \geq -1/8$ . When the equal sign holds, the nonstable approximant  $(9\sqrt{2} + 2)/8$  to the ground energy level can be obtained. The agreement of the results yielded by this procedure in cases A and B with those calculated by other methods and the continue nature of the eigenvalues obtained in the present case (they tend to those given by Eq. (4) as  $\beta$  goes to zero), suggest that  $\beta = -1/8$  as in approximate value to the real minimal bound of parameter

TABLE V

$\lambda$	$E_0^{35}$	$E_1^{35}$	$E_0^{BB}$	$E_1^{BB}$
0.01	1.404 048 605 297 706		1.404 048 605 297 7	
	1.404 048 605 297 707		1.404 048 605 297 7	
0.03	1.382 601 444 053 782		1.382 601 444 053 8	
	1.382 605 783 831 367		1.382 605 783 831 4	
0.07	1.323 274 074 208 529 <sup>a</sup>		1.323 374 074 208 5	
	1.343 365 616 287 377		1.343 365 616 287 4	
0.1	1.234 507 162 786 0 15		1.234 507 162 786 0	
	1.346 940 868 922 550		1.346 940 868 922 5	
0.2	0.941 750 342 076 866		0.941 750 342 076 9	
	1.535 530 204 085 822		1.535 530 204 085 8	

<sup>a</sup>This eigenvalue differs from that given in Ref. 16 by the fifth significant figure. However, that particular stable value was always obtained by this procedure for different values of N.

Table V. The first two eigenvalues for the potential  $-x^2 + \lambda x^4$  with some values of  $\lambda$ .  $E^{35}$  are the stable values calculated by the present method and  $E^{BB}$  are those obtained by Banerjee and Bhatnagar (see Ref. 16). All of these values are given in a.u.

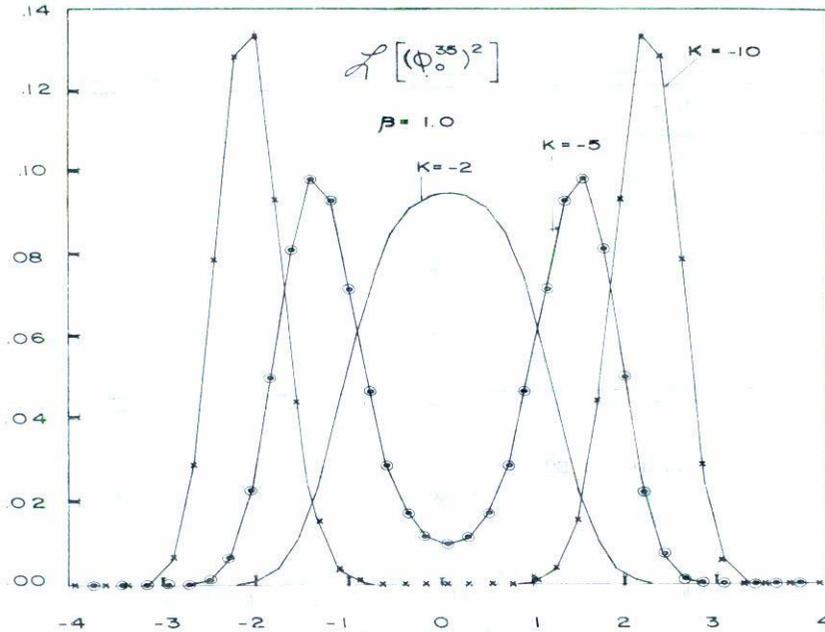


Fig. 7. Linear interpolations,  $\int (\phi_0^{35})^2$  of the vectors formed by the squared components  $(\phi_0^{35})^2$  of the first corresponding eigenvector  $\phi_0^{35}$  obtained by the present method for the double well  $V(x) = \kappa x^2 + x^4$  with  $\kappa = -2, -5, -10$ .

$\beta$  in the Schrödinger Equation. This suggestion is reinforced by testing the procedure for other non-confinement potential, used to model the elastic scattering phenomena: we choose that given in Eq. (2) and worked out by Hazi and Taylor<sup>(20)</sup>. This potential has a barrier whose size decreases when  $\lambda$  is increased, giving way to the occurrence of only few resonances for suitable  $\lambda$ .

We find numerically that a maximal value of  $\lambda$  exists in this case. It is obtained with  $N=2$  and its value is approximately 0.295. Table VII shows the first two nonstable eigenvalues calculated for some values of  $\lambda$  with  $N=2,3$  and compared with those reported in Ref. 20. These numbers are not much fortunate, but, before something about this approximation can be said, the following points should be considered. First, the selected values of  $\lambda$  make the potential a difficult one to deal with, however, to ob-

TABLE VI

	N = 2	N = 3	N = 4
$E_0^N$	0.981 840	0.930 280	0.937 817
$E_1^N$	...	2.821 050	2.273 847
$E_2^N$	...	...	4.366 091

Table VI. Approximants  $E_j^N$  (in a.u.) for the first two eigenvalues of the potential  $V(x) = x^2 + \beta x^4$  with  $\beta = -0.07$ , yielded by the present method.

tain those values of  $E_0^2$  (or  $E_0^3$ ) it is sufficient to diagonalize a simple  $2 \times 2$  (or  $3 \times 3$ ) matrix. Second, the proper instable nature of these eigenvalues makes themselves poor approximations to the real ones. Nevertheless, these results suggest that the above discussion about the eigenvalues of the Schrödinger Equation for interaction (1) with  $\beta < 0$  and the minimal bound for this parameter, makes sense.

#### 4. FINAL REMARKS

As shown in Sec. 3, the technique presented in this paper yields good approximants for the eigenenergies and eigenfunctions of nontrivial problems: by the very simple diagonalization of, e.g., certain  $3 \times 3$  matrix an acceptable approximation to the ground energy level of some complicated potentials can be obtained, and if a greater accuracy and/or more eigenvalues are desired, the diagonalization of a matrix of suitable order yields this at once. Besides, the linear interpolations of the corresponding eigenvectors yield the expected form of the eigensolutions of the Schrödinger Equation. Thus, the numerical results shown in Sec. III suggest that Eq. (3) can be considered in some sense as the projection of

TABLE VII

$\lambda$	$E_0^2$	$E_0^3$	$E_0^{\text{HT}}$
0.125	0.461 986	0.465 602	0.472 940
0.15	0.452 035	. . .	0.466 105
0.19	0.433 281	. . .	0.453 536
0.225	0.412 441	. . .	0.441 333

Table VII. Comparison of the first approximant  $E_0^{\text{N}}$  yielded by the present method for the potential studied by Hazi and Taylor and the resonant energies  $E_0^{\text{HT}}$  obtained by them for extremal values of  $\lambda$  (see Ref. 20). These values are in a.u.

the Schrödinger Equation on a finite dimensional space for some potentials, and Eq. (5) as the representative of the differential operator  $-\hbar^2 d/dx$ .

Recently, F. Calogero has introduced a method to compute the eigen values of differential operators<sup>(25,26)</sup>. The procedure presented in this paper is similar to Calogero's technique: both are based on the substitution of the differential operator  $d/dx$  by a finite matrix with non-diagonal elements given by Eq. (5). They have, however, two different features: the matrix to be diagonalized is Hermitian and the initial conditions are, apparently, absent in the method outlined in Sec. 2.

The aim of future work will be to search for the relation between the initial conditions and Ec. (6), and for the theoretical justification of this technique.

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