Rayleigh-Ritz Variational Eigenvalues and Transition Moments for the Potentials
$$V(x) = \beta x^2 + \gamma x^p, \quad (p = 4, 6, 8)$$

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The Schrodinger equation is nunierically solved for the one-dilllensional potential $V(x) = \beta x^2 + \gamma x^p$ ($p = 4, 6, 8$) using successive assuming a variationally scaled hasis set of harmonic oscillator eigenstates and using successive approximations in the framework of the Rayleigh-Ritz variational method. For each case studied ($\beta = 0$; 1 and $\gamma = 0.001$; 1.0; 10.0; 1000.0; 40000.0) the first 21 eigenvalues are obtained with 30 significant figures and the accuracy of the corresponding wave functions is verified by a cross comparison of the transition moments computed from two different expressions. The results are compared to the ones obtained by other numerical methods and from the calculation of the transition monients it is shown that the eigenfunctions are also determined with high precision.

I. Introduction

The Simple Harmonic Oscillator (SHO) is a very useful mode: in classical and quantum mechanics and has been applied to the study of different systems in physics. In quantum mechanics its usefulness and theoretical importance is mainly due to the fact that it presents an exact solution to the Schrödinger equation and it is limiting case that describes the behaviour of many physical systems in the so called small oscillation regime. However, in other regimes, most of the physical systems are modelled by anharmonic potentials[1], which do not exhihit exact solutions to the wave equation. Iii molecular physics, for instance, one can find many examples of molecular vibrations tliat are described by a iharmonic potentials[2]. Also anharmonic terms contribute to douhle symmetric and asymmetric potential wells, very commonly found in molecular physics[3] and solid state physics[4], as, for instance, in the description of some magnetic and ferroelectric transitions[5]. Therefore, it is not surprising that since the early days of quantum mechanics theoreticians have

given special attention to this class of prohlems and specially to the study of the quartic anliarmonic oscillator, whose Hamiltonian is given by

$$H = \alpha p^2 + \beta x^2 + \gamma x^4 \tag{1}$$

Milne[6] performed the first numerical calculation on the pure quartic potential ($\beta = 0.0$ and $\gamma = 1.0$) obtaining the energy of the ground state and the first excited state with a precision of 4 figures. The eigenvalues and eigenfunctions of this system have also been studied by McWeeny antl Coulson[7] by using a variational tecnhique, where the trial wave function expansion contains, at most, eight SHO states. Besides the energy levels, they have also computed the transition probabilities. Since then, many authors[8–28] have studied anharmonic systems using different methods.

The Hamiltonian drscrihed in Eq.(1) was one of the first models studied hy perturhation theory. For that model Render and Wu[24] have shown that the standard Rayleigh-Schrödinger perturbation series diverges for any $\gamma > 0$. Furthermore, Bender[25] has extended this result by proving tliat the series also diverge for

any finite anliarmonic even power. Some authors[26-28] have overcome this clifficulty by considering a. renormalized series expansion which converges for any strengtli of the anliarmonic perturbation. Cohen and Kais[28] have used low-order variational perturbation theory to study quartic, sextic and octic anharmonic potentials. They have computed the ground state energy for these potentials and the first, second and tliird excited states for the quartic potential. These results have been obtained for $0.15 \leq y \leq 100$ and with an accuracy of 6 significant figures. The ground state energy for these anharmonic potentials has also been recently obtained by Weniger et al.[29] by performing tlie summation of the ordinary and renormalized perturbation series, and by using a nonlinear sequence of transformations. They obtained the ground state energy of tlie quartic potential with 62 figures, and tlie ground state of the sextic and octic potentials with **33** and 21 digits respectively.

Another method that has been used to study anliarmonic potentials is tlie Hill's determinant approach[10,19,23]. Oiie of the most successful calculation using this method has been peiformed by Banerjee[30] and Banerjee et al.[31]. By scaling the basis set used in their calculation they mcre able to obtain tlie energies of a large number of excited states, for $0.00001 \leq \gamma \leq 40000$, with an accuracy of 15 figures. For tlie quartic anharrnonic potential the transition moinents between the lower states were also calculated.

Tasili aiid Demiralp[32] have applied algebraic methods to calculate the energies of the yuartic and sextic potentials. The ground and the first five even excited states of the quartic potential were computed with an accuracy of 30 figures, and also, the ground state and the first three even excited states of the sextic potential.

Despite all data available on these anharmonic potentials, there are very few results for properties other than energy. It is well known that acceptable values of energy do not always iinply correct wave functions. Clearly there is a lack of information mainly related to the wave functions. In view of these facts, calculations that can furnish other properties than energy are highly desirable.

In this contribution results are reported of the application of tlie Rayleigh-Ritz variational method, in successive approximations, for the systems described by the Hamiltonian

$$H = \alpha p^2 + \beta x^2 + \gamma x^p \text{ , for } p = 4, 6, 8 \text{ .} \quad (2)$$

Tlie eigensolutions have been obtained by considering their expansion in a finite number of variationally scaled eigenstates of the SHO. Up to 350 basis functions have been included in the expansion ior the study of the pure anliarmonic oscillators ($a = 1$; $\beta = 0$; $\gamma = 0.001$, 1.0, 10.0, 1000.0 and 40000.0 for $p = 4, 6, 8$) and the SHO perturbed by anharmonic terrns ($a = 1$; $\beta = 1$) for the values of γ aiid p as in the latter case. For each value of β and γ, 21 converged eigenvalues have been obtained with a precision of at Ieast 30 figures.

The transition moments have been computed by using two different expressions, which allow very reliable study of the convergence and accuracy of the wave functions. Moreover, from the transition moments and energy eigenvalues, the intensities of the transitions have been obtained These transitions are of particular interest in a spectroscopic test of the method, as they are very strongly dcpendent on the wave functions.

In section II a brief review of the computational method is given. In section III the results are shown and compared to the literature results, and finally in section IV the conclusions are presented.

II. Details of the calculation

The Rayleigh-Ritz variational method used to obtain solutions to tlie Schrodinger equation

$$H|\Psi> = E|\Psi> \quad (3)$$

consists in assuming a linearly independent basis set of real orthonorinal functions $\{|n>\}$, which satisfy the boundary conditions[33], and writing down an approximiate solution to the Eq. (**3**) as finite linear expansion,

$$|\Psi> = \sum_{n=1}^{M} C_n |n> , \quad (4)$$

where C_n's are expansion coefficients to be determined and the functions $\{|n>\}$ satisfy

$$<m|n> = <n|m> = \delta_{mn} \text{ .} \quad (5)$$

Since the Hamiltonian is Hermitian and tlie basis is real: the matrix $\mathcal{H}$ which represents H is symmetric, such that

$$H_{mn} = <m|H|n> = H_{nm} . \tag{6}$$

The trial wavefunction defined in Eq. (4) is normalized, and this iinplies that the coefficients C_n satisfy the condition

$$<\Psi|\Psi> = \sum_{m,n=1} C_m C_n <m|n> = \sum_{n=1} C_n^2 = 1 . \tag{7}$$

and the expectation value of the Hamiltonian is given by:

$$
\begin{aligned}
E &= <\Psi|H|\Psi> = \sum_{m,n=1} C_m <m|H|n> \\
C_n &= \sum_{m,n=1} C_m C_n H_{mn} .
\end{aligned}
\tag{8}
$$

The problem consists in finding the set of coefficients for which $<4|H|\Psi>$ is minimum. Introducing tlie Lagrange's undetermined multipliers ϵ, in order to satisfy the constrain given in Eq. (7), we build the functional,

$$J(C_1, C_2, C_3 ..., C_M; \epsilon) = <\Psi|H|\Psi J> - \epsilon <\Psi|\Psi> , \tag{9}$$

and minimize it by imposing the condition, $\partial J/\partial C_k = 0$. Taking into account the condition given in Eq. (6) the following result can be obtained,

$$\sum_{n=1}^{M} H_{kn} C_n - \epsilon C_k = 0 \tag{10}$$

In matrix notation the set of equations (10) can be written as

$$\mathcal{H}C = \epsilon C , \tag{11}$$

which is the standard eigenvalue problem for the matrix $\mathcal{H}$. Since $\mathcal{H}$ is symmetric Eq.(11) can be solved to yield M orthonormal eigenvectors C_k and the corresponding eigenvalues ϵ_k. To this extent, with the linear variational approach, the eigenvalue equation, Eq.(3), can be solved in a finite subspace spanned by $\{|n>)$, $\{n = 1, 2, ..., M\}$. The successive approximations are then obtained by increasing the number M of basis functions of the subspace until tlie requested accuracy of the eigenvalues ϵ_k is attained.

A very important point concerning the convergence of tlie eigenvalues in this method is based on the MacDonald's theorem[34]. MacDonald has shown that if tlie matrix $\mathcal{H}$ is symmetric and the basis set has the properties discussed above, the eigenvalues in the M-th approximation split up from those of the (M+1)-th approximation obeying the rule:

$$\epsilon_0^{M+1} \leq \epsilon_0^M \leq \epsilon_1^{M+1} \leq ...\epsilon_m^{M+1} \leq \epsilon_m^M \leq \epsilon_{m+1}^{M+1} . \tag{12}$$

Thus the eigenvalue, ϵ_k^M, of the M-th approximation is greater or equal to the k-th eigenvalue of any succeeding approximation. Therefore, assuming convergence of the process $\epsilon_k^M \geq \epsilon_k^0$, where ϵ_k^0 is the k-th correct eigenvalue, and when M one has exact eigenvalues and eigenvectors. The eigenvalues ϵ_k (k = 0, 1, 2, ..., M − 1) are associated to the ground state and the excited states of the system. To perform the calculations in this work, tlie basis set chosen was composed by the eigenvectors of tlie SHO whose Hamiltonian is given by:

$$H_0 = p^2/2 + (w^2 x^2)/2 . \tag{13}$$

Due to the $x \rightarrow -x$ symmetry of the Hamiltonian H, Eq.(2), even and odd states are obtained by a separate diagonalization in a sub-space of M even or odd basis functions.

With this basis set and using the operators $a^\dagger$ and a, defined as

$$x = (a^\dagger + a)/\sqrt{2w} \quad p = i(a^\dagger - a)\sqrt{w/2} , \tag{14}$$

such that

$$aa^\dagger - ata = 1 , \tag{15}$$

and

$$
\begin{aligned}
a^\dagger|n> &= \sqrt{n+1}|n+1>, \\
a|n> &= \sqrt{n}|n-1>, \\
a^\dagger a|n> &= n|n>, ,
\end{aligned}
\tag{16}
$$

tlie matrix elements of the Hamiltonian, Eq.(2), can be directly derived and are given by

a) for $p = 4$

$$
\begin{aligned}
H_{j,j} &= (\alpha w + \beta/w)(n + 1/2) + \gamma(6n^2 + 6n + 3)/(4w^2) , \\
H_{j,j+1} &= [(\beta/w - \alpha/w)/2 + \gamma(4n + 6)/(4w^2)]\sqrt{(n + 1)(n + 2)} , \\
H_{j,j+2} &= \gamma[\sqrt{(n + 1)(n + 2)(n + 3)(n + 4)}/(4w^2) , \\
H_{j,1} &= 0 , \text{for } j > 1 + 2 ,
\end{aligned}
\tag{17}
$$

b) for $p = 6$

$$
\begin{aligned}
H_{j,j} &= (\alpha w + \beta/w)(n + 1/2) + \gamma(20n^3 + 30n^2 + 40n + 15)/(8w^3) , \\
H_{j,j+1} &= [(\beta/w - \alpha/w)/2 + \gamma(15n^2 + 45n + 45)/(8w^3)]\sqrt{(n + 1)(n + 2)} , \\
H_{j,j+2} &= \gamma[(6n + 15)\sqrt{(n + 1)(n + 2)(n + 3)(n + 4)}]/(8w^2) , \\
H_{j,j+3} &= \gamma[\sqrt{(n + 1)(n + 2)(n + 3)(n + 4)(+5)(n + 6)}]/(8w^3) , \\
H_{j,1} &= 0 , \text{for } j > 1 + 3 .
\end{aligned}
\tag{18}
$$

c) for $p = 8$

$$
\begin{aligned}
H_{j,j} &= (\alpha w + \beta/w)(n + 1/2) + (70n^4 + 140n^3 + 350n^2 + 280n + 105) , \\
H_{j,j+1} &= [(\beta/w - \alpha/w)/2 + \gamma(56n^3 + 180n + 316n + 168)/(16w^4)]\sqrt{(n + 1)(n + 2)} , \\
H_{j,j+2} &= \gamma[(28n^2 + 140n + 210)\sqrt{(n + 1)(n + 2)(n + 3)(n + 4)}]/(16w^4) , \\
H_{j,j+3} &= \gamma[(8n + 28)\sqrt{(n + 1)(n + 2)(n + 3)(n + 4)(+5)(n + 6)}]/(16w^4) , \\
H_{j,j+4} &= \gamma[\sqrt{(n + 1)(n + 2)(n + 3)(n + 4)(+5)(n + 6)(n + 7)(n + 8)}]/(16w^4) , \\
H_{j,1} &= 0 , \text{for } j > 1 + 3 ,
\end{aligned}
\tag{19}
$$

where $j = n/2 + 1$ for matrix elements between even states, and $j = (n + 1)/2$ for the matrix elements between odd states.

Banerjee et al.[30,31] have shown that the introduction of the scaling parameter tu, defined in Eq.(13), is of paramount importance in order to improve the convergence of the numerical results. Balsa et al.[35] have used tliis scaling form in the calculation of the energy levels of a symmetric double well potential. They have deterinined two scaling parameters, associated to states of even and odd parity, by minimising tlic expectation value of the Hamiltonian of this anharmonic oscillator evaluated in the ground and first excited state of tlie renormalized SHO sliown in Eq.(13). One problein involved in this approach is that one gcts two non-orthogonal sets of basis functions to desciibe states of different parities. This makes the calculation of some properties like for instance tlie transition moments be-tween states of opposite parity, extremely difficult. In order to avoid these prohlems we have built a pseudo-state as a linear coinbination of the ground state and the first excited state of the renormalized SHO, nameiy, $2\phi >= (|0 > +|1 >)/\sqrt{2}$ and determined **w** by minimising the pseudo-energy $< \phi|H|\phi >$, where H is given by Eq.(2). Following this procedure the scaling factor w, for each form of the anharmonic potential, is determined from the following set of equations:

$$
\alpha w^3 - \beta w - 9\gamma/2 = 0 \quad \text{for} \quad p = 4 ,
\tag{20a}
$$

$$
\alpha w^4 - \beta w^2 - 45\gamma/2 = 0 \quad \text{for} \quad p = 6 ,
\tag{20b}
$$

$$
\boldsymbol{\alpha w^5} - \beta w^3 - 525\gamma/4 = 0 \quad \text{for} \quad p = 8 ,
\tag{20c}
$$

In this way, after determining w, one obtains a basis set that has embodied a. better approximate asymptotic behaviour characteristic of each type of potential and of the defining parameters β and γ. As it will be shown in

the next section, this effect is remarkable iii improving considerably the convergence of tlie eigenvalues. Incorporating this procedure into the Rayleigh-Ritz variational scheme described above, tlie yielded results are as good as the ones produced by other methods used for determining the energies. Moreover, it allows one to obtain highly accurate wave functions.

Eq.(11) was solved by using a standard diagonalization routine from the IMSL packages properly modified to run in extended precision on a SUN Sparc 2 workstation. Although in this precision tlie results are expressed with 35 figures, tlie final results have been considered up to 30 digits in order to avoid round off errors.

Due to the properties of the basis set used, it is quite simple to calculate transition moments, μ_{ij}, in terms of the matrix element of the momentum and position operators for two given states $|j>$ and $|j>$ siiice they are given by,

$$\mu_{ij}^{x} = <j\psi_i|x|\psi_j> \quad \text{and}$$
$$\mu_{ij}^{p} = i/(\epsilon_j - \epsilon_i)<j\psi_i|x|\psi_j> . \quad (21)$$

For exact wave functions oiie has

$$\mu_{ij}^{x} = \mu_{ij}^{p} \quad (22)$$

Thus if an approximate calculation is performed for two states of the system, and Eq.(22) is satisfied within some precision, it gives great credit to the approximate wave functiors.

These transition moments have been calculated and the above criterion has been used to verify tlie accuracy of the wave functions. From the transition moments the intensities of the transitions of tlie systems studied have been obtained by using the formula

$$I_{ij} = \Delta\epsilon_{ij}|\mu_{ij}|^2 \quad (23)$$

III. Results and discussion

As has been reviewecl in tlie former section, tlie Rayleigh-Ritz variational method is computationally very simple, specially in the cases where the matrix elements of H can be determined in closed form. Its great advantage resides in the fact. tliat the eigeiivalues and eigenvectors are obtained by solving an ordinary eigenvalue problem in a given Hilbert sub-space, and

tlie coiivergence of the results is determined by increasing tlie dimension of this sub-space.

It is also well known that for basis set dependent methocls, the numerical convergence is strongly dependent on the the basis set used and in particular on the scaling of this basis set[28,30,32]. Banerjee[30], Balsa et al.[35], and Haut and Magnus[23] have pointed out this difficulty and by scaling the basis set used in their calculations were able to improve considerably tlie convergente of their results, i.e., the nurnber of basis functions necessary to converge a given eigenvalue was reduced whenever an optimal scaling parameter was introduced into the basis set.

Ill order to study this effect on anharmonic oscillators clescribed by Eq.(2), in the context of the variational method, run test calculations were performed using arithmetics double precision. In table I the results are presented for the octic anharmonic oscillator with $3 = 1.0$ and $\gamma = 10.0$. Two groups of eigenenergies were computed by using various scaled basis functions of different dimensions (ϵ_n^{ω}, ω obtained from eq.(20c)) and non-scaled basis functions with the same dimensions (ϵ_n, $\omega = 1$). The variation in tlie number of basis functions (M=20; 50; 100; 200) has allowed one to study how the convergence of a given eigenenergy depends on tlie number of scaled or non-caled basis functions.

From the data of table I it is very clear the role of the parameter w in reducing the number of functions necessary to converge an eigenvalue. For instance, for $M = 20$ and $n = 10$, while the scaled result (ϵ_{10}) is correct to 3 figures, the corrcsponding non-scaled result (ϵ_{10}) is meaningless and it only approaches the scaled result when the nuinber of non-scaled basis functions increases five times. The other data shown also give support to this conclusion, namely, that to obtain a specific result in a given precision using a non-scaled basis set it is necessary five times more functions than when a scaled basis is used. These results demonstrate clearly tlie necessity of tlie scaling of the basis set if one wants to calculate energies of excited states with great accuracy. Tlierefore the calculations for the anharmonic oscillator were performed by adopting as a basis set tlie simple harmonic oscillator basis set properly scaled. The results obtained by using arithmetic extended precision are shown in Tables II to IV.

Table I - Convergence of the energies for $H = p^2 + x^2 + 10.0x^8$ as a function of the diinensionality of the basis set M, and the scaling parameter w

M	20	50	100	200	260 (extended precision)
ϵ_0	2.122 483 10	2.114 588 39	2.114 544 65	2.114 544 62	
ϵ_0^w	2.114 545 14	2.114 544 62	2.114 544 62	2.114 544 62	2.114 544 621 942 113...
ϵ_1	7.956 511 42	7.929 806 68	7.922 683 40	7.929 683 08	
ϵ_1^w	7.929 684 36	7.929 683 08	7.929 683 08	7.929 683 08	7.929 683 082 350 762.....
ϵ_{10}	4.275.828 11	197.091 103	158.018 109	158.599 179	
ϵ_{10}^w	158.701 205	158.599 179	158.599 179	158.599 178	158.599 178 256 695 2.....
ϵ_{11}	7.274.617 30	290.731 218	183.363 477	183.310 361	
ϵ_{11}^w	183.515 811	183.310 360	183.310 360	183.310 360	183.310 359 774 028 6.....
ϵ_{18}	258.373.179	6.624.826 83	573.018 109	391.183 178	
ϵ_{18}^w	902.105.460	391.179 490	391.177 574	391.177 574	391.177 573 500 914 9.....
ϵ_{19}	349.383.179	13978.985 0	1039.000 56	460.878 733	
ϵ_{19}^w	1.181.269 74	425.474 714	425.467 152	425.467 152	425.467 151 611 511 4.....

Table II - Energy eigenvalues for the potentials $V(x)^a = x^2 + \gamma x^4$, $V(x)^b = \gamma x^4$

n	Refs. [30,31,32][†]	This work
		$\gamma = 0.001$
0 a	1.000 748 692 673 185 699 538 485 009 30	1.000 748 692 673 185 699 538 485 009 30
b		0.106 036 209 048 418 289 964 704 601 67
1 a	3.003 739 748 168 73	3.003 739 748 168 729 116 488 725 074 63
b		0.379 967 302 980 139 416 878 309 418 85
2 a	5.009 711 872 788 107 487 036 992 247 36	5.009 711 872 788 107 487 036 992 247 36
b		0.745 569 793 798 673 839 215 659 134 72
3 a	7.018 652 592 057 52	7.018 652 592 057 516 298 848 295 384 08
b		1.164 474 551 137 816 202 085 037 328 14
4 a	9.030 549 566 074 710 815 378 279 511 65	9.030 549 566 074 710 815 387 279 511 65
b		2.123 837 291 823 594 002 414 971 111 36
5 a	11.045 390 587 179 3	11.045 390 587 179 328 907 106 222 159 6
b		2.123 837 291 823 594 002 414 971 111 36
10 a	21.163 338 105 703 820 534 172 441 060 7	21.163 338 105 703 820 534 172 441 060 7
b		5.025 625 451 668 291 903 974 458 810 54
15 a		31.353 127 858 007 434 950 274 410 908 6
b		8.445 746 627 494 195 892 888 833 727 66
20 a		41.613 369 936 637 374 222 307 671 602 2
b		12.260 463 900 099 945 502 076 297 141 8
306 a		718.581 443 342 190 (200)[‡]
94 b		94.053 727 785 0899 (200)

Table II - (Continued)

n	$\gamma = 1.0$	
0 a	1.392 351 641 530 291 855 657 507 876 61	1.392 351 641 530 291 855 657 507 876 61
b	1.060 362 090 484 18	1.060 362 090 484 182 899 647 046 016 69
1 a	4.648 812 704 212 08	4.648 812 704 212 077 536 377 032 917 26
b	3.799 673 029 801 40	3.799 673 029 801 394 168 783 094 188 51
2 a	8.655 049 957 759 309 688 116 539 457 38	8.655 049 957 759 309 688 116 539 457 38
b	7.455 697 937 986 74	7.455 697 937 986 738 392 156 591 347 19
3 a	13.156 803 898 049 9	13.156 803 898 049 875 079 209 772 040 4
b	11.644 745 511 378 2	11.644 745 511 378 162 020 850 373 281 4
4 a	18.057 557 436 303 252 894 771 239 646 5	18.057 557 436 303 252 894 771 239 646 5
b	16.261 826 018 850 2	16.261 826 018 850 225 937 894 954 430 4
5 a	23.297 441 451 223 2	23.297 441 451 223 189 084 864 481 992 1
b	21.238 372 918 236 0	21.238 372 918 235 940 024 149 711 113 6
10 a	53.449 102 139 665 264 600 831 506 459 8	53.449 102 139 665 264 600 831 506 459 8
b		50.256 254 516 682 919 039 744 588 105 3
15 a	88.610 348 800 799 2	88.610 348 800 799 158 873 039 105 371 3
b	84.457 466 274 942 0	84.475 466 274 941 958 928 888 337 276 6
20 a	127.617 777 795 355	127.617 777 795 354 918 333 962 283 058
b		122.604 639 000 999 455 020 762 971 418
103 a		1076.670 367 768 23 (200) 66
b		586.704 762 262 455 (200)

Table II - (Continued)

n	$\gamma = 10.0$	
0 a	2.449 174 072 118 386 918 268 793 906 19	2.449 174 072 118 386 918 268 793 906 19
b		2.284 480 871 733 850 825 161 485 250 36
1 a	8.599 003 454 807 77	8.599 003 454 807 772 602 764 990 244 51
b		8.186 147 386 182 675 125 248 492 828 76
2 a	16.635 921 492 413 757 783 361 917 932 2	16.635 921 492 413 757 783 361 917 932 2
b		16.062 814 275 997 813 350 593 092 257 4
3 a	25.806 276 215 055 7	25.806 276 215 055 640 449 726 578 901 7
b		25.087 843 686 306 179 792 003 111 490 7
4 a	35.885 171 222 253 873 712 281 269 098 2	35.885 171 222 253 873 712 281 269 098 2
b		35.035 042 098 274 008 211 021 736 621 4
5 a	46.729 080 900 817 1	46.729 080 900 817 113 005 813 013 742 9
b		45.756 687 374 881 201 165 532 725 820 7
10 a	109.772 570 864 332 974 973 673 879 837	109.772 570 864 332 974 973 673 879 837
b		108.273 818 121 813 220 945 361 388 122
15 a		183.902 508 794 209 186 902 225 748 664
b		181.958 095 174 932 852 408 157 446 461
20 a		266.487 427 864 640 818 603 917 650 703
b		264.143 687 422 589 262 764 132 914 854
96 a		2090.298 203 894 81 (200) 44
b		742.368 700 123 280 (100)

Table II - (Continued)

n		$\gamma = 1000.0$	
0	a	10.639 788 711 328 046 063 622 042 669 4	10.639 788 711 328 046 063 622 042 669 4
	b		10.603 620 904 841 828 996 470 460 166 9
1	a	38.086 833 459 382 3	38.086 833 459 382 264 084 978 363 212 3
	b		37.996 730 298 013 941 687 830 941 885 1
2	a	74.681 404 200 164 813 260 852 269 799 1	74.681 404 200 164 813 260 852 269 799 1
	b		74.556 979 379 867 383 921 565 913 471 9
3	a	116.603 198 937 293	116.603 198 937 293 111 438 331 251 471
	b		116.447 455 113 781 620 208 503 732 814
4	a	162.802 374 196 975 230 178 579 711 889	162.802 374 196 975 230 178 579 711 889
	b		162.618 260 188 502 259 378 949 544 304
5	a	212.594 183 409 734	212.594 183 409 734 263 575 398 187 004
	b		212.383 729 182 359 400 241 497 111 136
10	a	502.886 399 284 715 911 615 348 140 903	502.886 399 284 715 911 615 348 140 903
	b		502.562 545 166 829 190 397 445 881 053
15	a		844.994 531 747 478 869 245 278 098 816
	b		844.574 662 749 419 589 288 883 372 766
20	a		1262.552 291 546 149 517 549 578 829 58
	b		1262.046 390 009 994 550 207 629 714 18
94	a		9406.774 101 872 33 (200)
44	b		3445.770 268 915 85 (100)

Table II - (Continued)

n		$\gamma = 40000.0$	
0	a	36.274 458 133 736 835 470 376 382 678 5	36.274 458 133 736 835 470 376 382 678 5
	b		36.263 873 389 915 441 722 315 919 221 5
1	a	129.973 351 403 294	129.973 351 403 293 737 863 018 371 678
	b		129.946 989 723 931 049 713 531 282 308
2	a	255.017 677 289 573 984 846 933 213 430	255.017 677 289 573 984 846 933 213 430
	b		254.981 282 792 887 413 314 885 879 077
3	a	398.290 246 956 059	398.290 246 956 059 019 025 436 878 813
	b		398.244 694 592 561 811 893 552 384 294
4	a	556.200 474 630 523 658 811 864 176 747	556.200 474 630 523 658 811 864 176 747
	b		556.146 626 825 503 152 776 113 242 718
5	a	726.403 686 448 353	726.403 686 448 352 769 272 621 134 827
	b		726.342 136 734 664 504 130 470 536 577
10	a	1718.834 435 887 075 492 178 358 411 30	1718.834 435 887 075 492 178 358 411 30
	b		1718.739 727 871 798 067 892 631 491 93
15	a		2888.527 499 879 298 584 801 687 017 59
	b		2888.404 716 948 181 709 423 278 634 28
20	a		4193.167 611 849 741 596 417 741 132 95
	b		4193.019 672 853 774 562 746 293 934 82
134	a		50479.108 313 054 6 (300) 44
	b		11784.368 555 239 6 (100)

† The results with 15 figures are from Refs. [30,31], and the results with 30 figures shown in the first column are from Ref. [32].

‡ The numbers in parenthesis are the dimensionality of the basis set used to obtain the corresponding eigenvalue.

Table III - Energy eigenvalues for the potentials $V(x)^a = x^2 + \gamma x^6$, $V(x)^b = \gamma x^6$

n	Refs. [23,31,32][†]	This work
		$\gamma = 0.001$
0 a	1.001 848 815 572 31	1.001 848 815 572 311 415 227 866 707 19
b		0.203 577 863 214 933 416 683 992 431 87
1 a	3.012 780 960 690 10	3.012 780 960 690 096 756 104 056 922 08
b		0.771 524 075 710 671 309 547 885 037 50
2 a	5.044 799 925 784 58	5.044 799 925 784 583 191 032 763 598 75
b		1.613 447 946 022 862 632 069 678 330 64
3 a	7.110 092 855 860 92	7.110 092 855 860 927 832 960 605 109 31
b		2.655 890 464 720 029 768 365 358 300 09
4 a	9.281 581 748 732 25	9.281 581 748 732 248 587 607 305 178 73
b		3.861 385 327 647 156 434 752 124 206 34
5 a	11.377 808 617 207 5	11.377 808 617 207 452 232 004 763 337 7
b		5.210 295 709 191 235 974 251 218 412 68
10 a	23.070 422 451 241 3	23.070 422 451 241 295 399 193 295 722 1
b		13.715 396 327 616 204 838 796 455 228 5
15 a		36.344 703 557 617 830 345 134 290 674 0
b		24.588 869 155 071 952 410 510 878 863 9
20 a		51.143 548 882 008 326 450 384 115 334 3
b		37.394 276 908 320 909 163 249 688 372 9
122 a		581.115 864 939 999 (200)[‡]
54 b		153.227 907 463 499 (200)

Table III - (Continued)

n	$\gamma = 1.0$	
0 a	1.435 624 619 003 39	1.435 624 619 003 392 315 761 272 220 54
b	1.144 802 454	1.144 802 453 797 052 763 765 457 534 15
1 a	5.003 395 937 720 27	5.003 395 937 720 266 476 828 385 453 49
b	4.338 598 712	4.338 598 711 513 981 191 647 336 888 06
2 a	9.966 621 999 718 11	9.966 621 999 718 110 281 520 795 353 93
b	9.073 084 561	9.073 084 560 921 433 856 016 249 096 66
3 a	15.989 440 787 825 7	15.989 440 787 825 731 057 565 828 410 2
b	14.935 169 63	14.935 169 634 910 736 015 711 954 951 3
4 a	22.910 180 430 728 6	22.910 180 430 728 544 504 095 956 817 7
b	21.714 165 42	21.714 165 422 196 722 281 689 785 148 6
5 a	30.622 590 570 533 3	30.622 590 570 533 258 205 697 934 283 1
b	29.299 645 94	29.299 645 937 401 893 129 784 070 647 0
10 a	78.958 068 575 484 3	78.958 068 575 484 337 095 976 822 943 7
b	77.127 341 46	77.127 341 463 825 437 987 342 432 632 2
15 a		140.499 179 846 639 410 629 935 429 165
b	138.273 372 7	138.273 372 655 952 608 204 833 544 621
20 a		212.844 175 309 416 744 848 810 533 095
b	210.283 472 3	210.283 472 311 600 498 055 995 090 161
54 a		915.544 136 875 464 (200)
52 b		861.663 845 391 680 (200)

Table III - (Continued)

n	$\gamma = 10.0$	
0 a	2.205 723 269 595 632 351 009 973 387 17	2.205 723 269 595 632 351 009 973 387 17
b		2.035 778 632 149 334 166 839 224 318 71
1 a	8.114 843 118 819 54	8.114 843 118 819 540 781 823 060 402 53
b		7.715 240 757 106 713 095 478 850 375 02
2 a	16.641 218 108 251 080 173 659 025 662 6	16.641 218 108 251 080 173 659 025 662 6
b		16.134 479 460 228 626 320 696 783 306 4
3 a	27.155 085 604 631 4	27.155 085 604 631 357 643 884 048 321 0
b		26.558 904 647 200 297 683 653 583 000 9
4 a	39.289 330 675 370 355 991 128 134 360 7	39.289 330 675 370 355 991 128 134 360 7
b		38.613 853 276 471 564 347 521 242 063 4
5 a	52.849 512 678 258 2	52.849 512 678 258 226 625 331 320 397 2
b		52.102 957 091 912 359 742 512 184 126 8
10 a	138.185 313 922 455	138.185 313 922 454 771 811 479 135 560
b		137.153 963 276 162 048 387 964 552 285
15 a		247.141 875 779 098 707 208 785 335 035
b		245.888 691 550 719 524 105 108 788 639
20 a		375.384 077 480 477 969 325 655 152 378
b		373.942 769 083 209 091 632 496 883 729
52 a		1534.586 031 014 87 (200)
52 b		1532.249 074 634 99 (200)

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Table III - (Continued)

n		$\gamma = 1000.0$	
0	a	6.492 350 132 329 671 550 549 557 845 32	6.492 350 132 329 671 550 549 557 845 33
	b		6.437 697 289 493 980 265 849 317 987 45
1	a	24.525 316 086 919 2	24.525 316 086 919 226 970 227 292 335 3
	b		24.397 733 489 019 132 142 754 481 576 1
2	a	51.182 480 106 305 690 884 693 028 921 5	51.182 480 106 305 690 884 693 028 921 5
	b		51.021 703 955 526 556 380 090 598 066 4
3	a	84.175 583 775 589 6	84.175 583 775 589 653 396 702 214 671 0
	b		83.986 630 844 383 653 533 485 368 249 0
4	a	122.321 705 320 204 002 373 196 508 244	122.321 705 320 204 002 373 196 508 244
	b		122.107 725 589 205 606 382 014 468 961
5	a	165.000 436 566 548	165.000 436 566 547 511 900 020 979 448
	b		164.764 017 240 466 083 001 932 848 271
10	a		434.045 298 101 345 512 660 230 370 047
	b		433.718 914 071 761 548 874 540 259 029
15	a		777.964 806 824 184 823 287 477 555 482
	b		777.568 316 178 873 681 632 809 146 861
20	a		1182.966 819455 762 460 681 135 502 69
	b		1182.510 864 853 335 025 242 385 073 64
52	a		4846.221 518 384 51 (200)
44	b		4845.491 886 861 69 (200)

Table III - (Continued)

n	$\gamma = 40000.0$	
0 a	16.211 718 264 749 243 619 248 517 555 9	16.211 718 264 749 243 619 248 517 555 9
b		16.189 951 563 977 905 415 143 966 337 4
1 a	61.407 828 604 359 5	61.407 828 604 359 446 042 405 219 523 1
b		61.357 051 395 175 074 518 438 375 795 4
2 a	128.376 742 015 189 214 870 771 197 740	128.376 742 015 189 214 870 771 197 740
b		128.312 792 386 130 299 027 029 656 399
3 a	211.290 344 511 508	211.290 344 511 508 045 686 885 950 736
b		211.215 194 540 335 893 766 202 123 976
4 a	307.169 772 116 720 722 853 603 759 312	307.169 772 116 720 722 853 603 759 312
b		307.084 672 356 835 080 905 957 063 738
5 a	414.453 587 749 840	414.453 587 749 839 357 036 687 753 697
b		414.359 566 574 035 131 395 024 189 244
10 a	1090.875 114 099 14	1090.875 114 099 135 679 139 092 152 53
b		1090.745 323 279 226 960 296 801 145 96
15 a		1955.638 455 340 907 078 089 756 764 36
b		1955.480 789 251 172 492 715 948 023 17
20 a		2974.038 694 954 773 922 155 350 255 94
b		2973.857 384 859 726 366 410 280 393 30
54 a		12888.953 283 037 7 (200)
52 b		12185.766 963 594 7 (200)

† The results with 15 figures are from Refs. [31], the results with 10 figures are from Ref. [23] and the results with 30 figures shown in tlie first column are from Ref. [32].

‡ The numbers in parenthesis are tlie dimensionality of the basis set used to obtain the corresponding eigenvalue.

Table IV - Energy eigenvalues for the potentials $V(x)^a = a^2 + \gamma x^8$, $V(x)^b = \gamma x^8$

	Refs. [23,31,32][†]	This work
n		$\gamma = 0.001$
0 a	1.005 857 514 124 73	1.005 857 514 124 725 434 954 425 738 89
b		0.307 912 091 132 698 572 693 982 275 28
1 a	3.047 977 747 263 14	3.047 977 747 263 143 844 185 441 467 62
b		1.194 621 641 039 160 869 434 733 726 72
2 a	5.190 981 966 774 52	5.190 981 966 774 522 472 642 475 392 04
b		2.573 414 330 365 634 252 387 539 385 91
3 a	7.507 661 558 294 38	7.507 661 558 294 379 808 945 757 150 38
b		4.356 386 735 379 096 125 378 735 796 83
4 a	10.045 355 306 963 2	10.045 355 306 963 195 024 446 420 377 6
b		6.482 929 386 932 291 613 938 475 154 03
5 a	12.821 359 688 194 8	12.821 359 688 194 779 360 517 763 324 5
b		8.916 669 035 580 931 391 309 358 456 92
10 a	30.155 816 187 584 6	30.155 816 187 584 623 974 984 517 481 9
b		25.005 415 682 225 611 603 016 788 810 3
15 a		52.643 047 612 031 064 797 047 492 228 1
b		46.596 822 905 118 091 078 576 406 381 3
20 a		79.640 344 977 125 747 461 160 270 531 1
b		72.865 294 931 865 592 595 263 270 880 2
54 a		358.243 303 621 796 (200)[‡]
66 b		478.734 846 190 657 (350)

Table IV - (Continued)

n		$\gamma = 1.0$	
0	a	1.491 019 895 662 21	1.491 019 895 662 204 964 171 080 060 65
	b	1.225 820 114	1.225 820 113 800 492 191 591 086 026 65
1	a	5.368 778 061 748 13	5.368 778 061 748 129 766 350 976 013 68
	b	4.755 874 414	4.755 874 413 960 759 869 312 240 999 04
2	a	10.993 737 335 502 0	10.993 737 335 502 952 897 752 212 439 5
	b	10.244 946 98	10.244 946 977 236 854 744 232 174 213 0
3	a	18.191 100 018 514 9	18.191 100 018 514 917 400 711 796 474 5
	b	17.343 087 97	17.343 087 970 585 589 169 568 180 239 1
4	a	26.743 448 558 041 2	26.743 448 558 041 230 743 799 176 639 1
	b	25.809 006 75	25.809 006 751 297 331 886 444 795 462 1
5	a	36.509 236 308 241 3	36.509 236 308 241 279 310 147 001 597 1
	b	35.497 898 81	35.497 898 805 171 056 993 806 138 456 9
10	a	100.856 494 453 769	100.856 494 453 768 697 604 008 803 072
	b	99.548 352 86	99.548 352 857 648 863 712 754 062 265 2
15	a		187.033 687 331 259 315 068 420 807 794
	b	185.505 293 2	185.505 293 235 389 551 277 054 853 629
20	a		291.791 143 251 422 457 929 488 615 934
	b	290.081 964 0	290.081 963 968 710 943 098 244 204 283
54	a		1388.713 875 262 89 (260)
66	b		1905.877 750 623 26 (350)

Table IV - (Continued)

n	$\gamma = 10.0$	
0 a	2.114 544 621 942 13	2.114 544 621 942 128 798 277 886 872 77
b		1.942 793 953 544 307 505 607 253 369 23
1 a	7.929 683 082 350 76	7.929 683 082 350 761 613 209 060 037 62
b		7.537 552 982 886 395 898 224 727 868 97
2 a	16.711 022 381 994 9	16.711 022 381 994 848 208 955 679 238 1
b		16.237 146 721 347 753 262 010 893 793 5
3 a	28.022 750 232 932 1	28.022 750 232 932 082 828 935 284 671 1
b		27.486 942 060 835 328 266 440 902 851 3
4 a	41.494 702 572 696 9	41.494 702 572 696 905 419 144 248 748 7
b		40.904 519 104 314 059 527 286 150 099 3
5 a	56.898 990 129 970 3	56.898 990 129 970 355 063 974 034 858 4
b		56.260 378 162 989 102 460 331 271 220 7
10 a	158.599 178 256 695	158.599 178 256 695 222 415 236 134 678
b		157.773 506 764 804 517 157 198 792 139
15 a		294.970 637 993 639 869 745 812 583 889
b		294.006 076 414 271 545 574 147 419 183
20 a		460.827 516 327 071 031 343 553 479 368
b		459.748 929 949 759 980 132 189 323 766
54 a		2198.552 388 988 43 (280)
66 b		3020.612 672 625 91 (350)

Table IV - (Continued)

n		$\gamma = 1000.0$
0	a	4.949 487 440 032 74 4.949 487 440 032 743 317 630 830 089 82
	b	4.880 077 771 126 799 539 288 753 002 64
1	a	19.090 814 267 022 6 19.090 814 267 022 583 053 324 746 853 5
	b	18.933 477 064 496 900 157 573 315 361 2
2	a	40.974 799 857 386 5 40.974 799 857 386 465 236 145 855 214 7
	b	40 785 868 535 783 686 481 149 504 231 8
3	a	69.257 537 833 103 0 69.257 537 833 103 032 422 947 840 871 8
	b	69.044 076 806 302 236 586 651 963 387 2
4	a	102.982 586 803 735 102.982 586 803 734 782 392 755 014 886
	b	102.747 506 525 550 889 078 172 529 563
5	a	141.574 023 285 519 141.574 023 285 518 995 295 260 530 984
	b	141.319 680 539 210 202 624 956 735 158
10	a	396.637 899 756 015 396.637 899 756 015 014 653 604 050 057
	b	396.309 130 894 197 416 118 158 484 213
15	a	738.893 919 049 729 662 821 498 118 466
	b	738.509 874 126 377 479 155 957 927 441
20	a	1155.266 528 759 685 736 050 787 380 37
	b	1154.837 099 041 850 516 595 899 265 97
56	a	5846.705 212 744 82 (300)
66	b	7587.435 987 214 91 (350)

Table IV - (Continued)

n		$\gamma = 40000.0$	
0	a	10.238 868 235 479 0	10.238 868 235 479 038 325 373 895 482 7
	b		10.205 604 674 423 289 110 055 321 192 1
1	a	39.670 505 945 098 2	39.670 505 945 098 277 199 062 176 889 3
	b		39.595 184 973 435 343 875 145 946 794 8
2	a	85.384 995 313 354 9	85.384 995 313 354 958 305 051 998 357 7
	b		85.294 634 655 606 684 310 396 774 361 1
3	a	144.492 517 309 256	144.492 517 309 256 412 745 636 736 231
	b		144.390 435 161 638 751 583 559 885 119
4	a	214.986 131 730 873	214.986 131 730 873 063 288 138 572 506
	b		214.873 713 506 491 916 667 606 357 953
5	a	295.660 523 015 270	295.660 523 015 270 561 323 123 938 080
	b		295.538 895 062 722 837 547 711 230 955
10	a	828.950 218 446 122	828.950 218 446 122 972 294 628 965 280
	b		828.793 004 632 089 851 500 875 488 468
15	a		1544.613 913 076 516 886 891 970 780 41
	b		1544.430 268 731 485 715 662 715 821 81
20	a		2415.292 040 752 289 470 866 089 585 70
	b		2415.086 695 115 848 931 705 402 346 13
56	a		12226.053 469 597 4 (300)
62	b		14368.197 681 248 7 (200)

† The results with 15 figures are from Refs. [31], the results with 10 figures are from Ref.[23] and the results with 30 figures shown in the first column are from Rei. [32].

‡ The numbers in parenthesis are the dimensionality of the basis set used to obtain the corresponding eigenvalue.

In Tables II, III and IV are presented selected energies eigenvalues for the quartic, sextic and octic potentials respectively, and for each potential were considered two values of 3, namely, $3 = 0$ and $3 = 1$. In the first column of these tables are displayed the quantum nuinbers together with the indices a and b associated to the eigenvalues for the cases $3 = 0$ and $= 1$, respectively. The numbers in parenthesis indicate the number of basis functions necessary to obtain the indicated eigenvalue converged to 15 figures. The other shown eigenvalues, were chosen among the first 21 eigenvalues converged within 30 figures and compared to those from references [23,30,31,32]. Thc data on Tables II,III and IV extend the list of known eigenenergies for those class of potentials,especially to the case of pure anharmonic potentals ($3= 0$), where the literature results are rather scarce. The agreement of tlie 30 figures values with those of ref.[32], obtained by a different method and basis set, is a very important result since it provides the necessary reliability test for the present calculation. For the case $p = 4$, tlie two approaches yield eigenvalues with given precision with practically the same number of basis functions. The maxiinun difference in the number of basis function between the two methods was two. For $p = 6$ and $p = 8$, as expected, the number of basis functions increases in order to yield results as precise as the results for $p = 4$. For a given potential M also increases as g increases, and this effect is more pronounced for $y \geq 10.0$. This was also an expected result, since it reflects the enhancement of the anharmonic effects.

One of the main advantages of the present method is that the wave function is automatically obtained from the diagonalization proccss. In this way one can easily calculate properties other than energy, as for instance, the moments of all orders. These moments can be readily expressed in terms of the expansion coeficients obtained froin Eq.(10), by using the operators a and $a^\dagger$ defined in Eq.(14), and Eqs.(16) and (4).

The transition moments μ_{ij}^x and μ_{ij}^p (Eq.(21)) were calculated in order to verify the accuracy of the wave functions. This has been achieved by cross comparing them, and verifying up to which precision Eq.(22) is satisfied. It is clear that this convergence criterion is a measure of the quality of the wave functions involved in a given transition. In Table V these results are shown for $y = 0$, $y = 40000.0$ and $p = 4,6,8$, since they have presented the worst numerical convergence. The transition moments from the ground state up tp 41th excited state are displayed ill Table V.

The deliberate choice in displaying the transition moments for the transitions of the kind $(0 \rightarrow j)$ only is because it allows one to estimate the error of the wave function of a given j state. As the ground state has an eigenvalue converged to 30 digits the difference between tlie values of μ_{0j}^x and μ_{0j}^p (see Eq.(21)) comes from the accuracy of the eigenvalue ϵ_j and from the corresponding wave function ψ_j. Then, if ϵ_j is known within a certain precision, one can have a measure of the quality of the wave function ψ_j comparing $\&$ and μ_{0i}^p. As an example Iet one consider the case $p = 8$ in table V. For the transitions $(0 \rightarrow 5, 11, 15)$ both eigenvalues are converged to 30 figures ($M = 310$) and transition moments are converged to 29 figures. It means that the wave function for the 5th, 11th and 15th excited states is as accurate as the corresponding eigenvalues. For the transition $(0 \rightarrow 25)$ the eigenvalue is computed with 29 figures and the transition moments are given with 26 converged figures. Finally, for the transition $(0 \rightarrow 41)$, to an energy converged to 22 figures the transition moments are calculated with 19 figures of accuracy. Thercfore, from this calculation it is possible to infer the quality of the wave function for a given state.

The link between experiment and theory can be spectroscopically done by calculating the relative intensities of the transitions obtained from Eq. (23). The intensities for the pure anharmonic potentials ($\beta = 0, \gamma = 40000.0$) are given in table VI. As for the results shown in Table V these parameters have been chosen since they correspond to the worst numerical conver-

Table V - Transition moments from tlie ground state to some excited states for the potentials $V(x) = 40000x^p$, p = 4, 6, 8 for $M = 310$.

Transition $0 \to j$	$|\mu_{0j}^x|/|\mu_{0j}^p|$
	$p = 4$
5	2.610 093 376 944 638 058 551 714 968 09 (-4)
	2.610 093 376 944 638 058 551 714 968 09 (-4)
11	2.401 265 632 274 585 742 429 398 28 (-8)
	2.401 265 632 274 585 742 429 398 29 (-8)
15	4.721 912 082 101 892 371 772 16 (-11)
	4.721 912 082 101 892 371 772 17 (-11)
25	7.748 120 771 284 540 715 (-18)
	7.748 120 771 284 540 717 (-18)
41	1.023 263 91 (-28)
	1.023 263 97 (-28)
	$p = 6$
5	1.494 623 795 102 176 573 704 041 179 83 (-3)
	1.494 623 795 102 176 573 704 041 179 83 (-3)
11	4.428 039 373 596 569 326 300 970 665 45 (-6)
	4.428 039 373 596 569 326 300 970 665 45 (-6)
15	1.014 332 862 589 766 734 153 703 223 98 (-7)
	1.014 332 862 589 766 734 153 703 223 90 (-7)
25	9.115 688 879 368 155 767 669 81 (-12)
	9.115 688 879 368 155 767 669 80 (-12)
41	3.568 873 175 892 101 91 (-18)
	3.568 873 175 892 101 99 (-18)
	$p = 8$
5	2.717 852 510 243 525 894 706 347 531 91 (-3)
	2.717 852 510 243 525 894 706 347 531 92 (-3)
11	3.236 000 991 052 978 977 464 563 123 87 (-5)
	3.236 000 991 052 978 977 464 563 123 88 (-5)
15	1.909 961 769 204 809 472 648 320 482 22 (-6)
	1.909 961 769 204 809 472 648 320 482 23 (-6)
25	1.950 779 662 723 707 927 947 676 06 (-9)
	1.950 779 662 723 707 927 947 676 05 (-9)
41	4.048 838 402 953 542 174 7 (-14)
	4.048 838 402 953 542 174 6 (-14)

Table VI - Intensities (I_{0j}) round to 19 figures

$0 \rightarrow j$	$40000 \ x^4$	$40000 \ x^6$	$40000 \ x^8$
1	0.988 799 697 849 891 320	0.978 584 638 220 218 880	0.972 495 023 940 028 105
3	0.011 153 138 534 448 786	0.020 497 856 925 721 910	0.025 209 245 365 863 184
5	0.000 047 012 185 069 746	0.000 889 471 217 996 448	0.002 107 677 769 752 330
7	0.000 000 151 005 542 241	0.000 027 184 640 990 318	0.000 173 813 479 096 417
9	0.000 000 000 423 947 334	0.000 000 824 082 435 745	0.000 013 165 774 402 916
11	0.000 000 000 001 097 872	0.000 000 024 193 087 830	0.000 000 992 964 853 346
13	0.000 000 000 000 002 694	0.000 000 000 699 015 274	0.000 000 074 656 604 754
15	0.000 000 000 000 000 006	0.000 000 000 019 952 804	0.000 000 005 596 780 938
17	$< 10^{-19}$	0.000 000 000 000 564 476	0.000 000 000 418 797 103
19		0.000 000 000 000 015 859	0.000 000 000 031 296 235
21		0.000 000 000 000 000 443	0.000 000 000 002 336 358
23		0.000 000 000 000 000 012	0.000 000 000 000 174 277
25		$< 10^{-18}$	0.000 000 000 000 012 991
27			0.000 000 000 000 000 968
29			0.000 000 000 000 000 072
31			0.000 000 000 000 000 005
$\sum I_{0j}$	0.999 999 999 999 999 999	0.999 999 999 999 999 999	0.999 999 999 999 999 999

gence case.

From these results one can see that those intensities satisfy the well known Thomas-Reiche-Kuhn sum rule[36] that reads,

$$\sum_j (\epsilon_j - \epsilon_i)|\mu_{ij}|^2 = 1 \qquad (1)$$

in oiie part in 10^{18}

IV. Conclueions

It can be concluded from the present calculations that the Rayleigh-Ritz variational method, in the framework of successive approximations and with a variationally scaled basis set of SHO functions, can be used to obtaiii highly accurate energies and wavefunctions for yuaitic, sextic and octic anharmonic potentials. Due to the properties of the basis set the matrix elements can be easily computed, and tlie wave functions can be used to calculate properties otlier than energies to test the accuracy of the eigenvalues aiid the quality of the wave functions.

As a variational calculation and supported by Mac-Donald's theorem[34], the results of this contribution can safely be said to be exact in the given precision. It is important to realize that the present method does not apply to the Hamiltonian shown in Eq.(1), when $\gamma < 0.0$. In tliis case there will be unbounded states and consequenily, tlie conditions of discreteness of the eigenvalues and quadratic integrability of the solutions concerned are not satisfied, [33,34].

Finally it should be noted that from the preseiit results the thermodynamic properties of these anharmonic potentials can be determined very accurately. In particular cne can easily obtain the specific heat which can be compared to some known approximate results[37]. This calculatioii is under way.

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