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Scaling-variational treatment of anharmonic oscillators

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The scaling-variational method is applied to anharmonic-oscillator models with the Hamiltonian $H=p^2+hx^2+gx^{2k}$ to enable the discussion of two important aspects not previously analyzed. First, it is shown that the introduction of a scaling factor which is variationally optimized assures us of the correct dependence of the approximate eigenvalue with g. Second, it is shown that quantities $\bar{E}_n=\langle\phi_n\mid H\phi_n\rangle$ are very good approximations to the exact eigenvalues whenever the trial function ϕ_n satisfies the quantum virial theorem.

I. INTRODUCTION

The application of the scaling-variational method (SVM) was first introduced by Fock[1] and then it was analyzed thoroughly by Lowdin.[2] This author applied the SVM to the bound states of atoms and molecules. The application of this method has been restricted in practice to the ground state because, in this case, the expectation values of the Hamiltonian operator give upper bounds for the eigenvalues regardless of what the trial function is. As a general rule, the variation method yields an upper bound for the lowest eigenvalue corresponding to a given symmetry class whenever the trial function possesses the appropriate symmetry.

Recently, some interesting applications of the SVM have been reported. For example, Kreuzer *et al.*[3] used it in order to increase the rate of convergence of a 2×2 algorithm. Dmitrieva and Plindov[4,5] combined the SVM with perturbation theory to study the quartic anharmonic oscillator, i.e.,

$$H=p^2+x^2+gx^4,\quad p=-i\frac{d}{dx}\ . \tag{1}$$

By way of a nonlinear transformation on g, these authors arrived at a perturbative polynomial which is valid for large and small values of this parameter. Killingbeck[6] obtained an excellent approximation to the lowest eigenvalue associated with the Hamiltonian (1) for the whole range of g values considered through a scaling transformation of the harmonic-oscillator ground-state function ϕ_0^0,

$$H^0\phi_n^0=E_n^0\phi_n^0\ , \tag{2}$$

$$H^0=p^2+x^2\ . \tag{3}$$

The purpose of this communication is to show two aspects related to the SVM, which are of extreme importance and have not been noted previously. For the aim of discussing these points, we will consider at present the applications of the SVM to an even anharmonic oscillator with the Hamiltonian

$$H=p^2+hx^2+gx^{2k}\ . \tag{4}$$

First, we will demonstrate that when one introduces a scaling factor that is variationally optimized, a proper g dependence of the approximate eigenvalue is assured. This fact explains in a simple manner the success of Killingbeck's results. Then, we will show that quantities

$$\bar{E}_n=\langle\phi_n\mid H\phi_n\rangle \tag{5}$$

are very good approximations of H eigenvalues E_n for the complete range of n and g values whenever the trial functions ϕ_n satisfy the quantum virial theorem (VT) (n denotes the number of zeros of ϕ_n). In a more precise manner: We will prove that $\bar{E}_n$ increases with n at the same rate as E_n (especially when n is large), i.e.,

$$\lim_{n\to\infty}\bar{E}_n/E_n=\text{const}\neq0\ . \tag{6}$$

This result is obtained for two quite different basis sets: the harmonic-oscillator basis set $\{\phi_n^0\}$ and the particle in a box basis set $\{\phi_n^B\}$. This property suggests that the aforementioned behavior does not depend on the chosen basis set. Furthermore, when g and n are large enough, the two main terms in $\bar{E}_n$ are identical (except for the numerical coefficients) to those obtained from the WKB method.[7–9] In Sec. II, we present briefly the SVM which is applied to the pure $2k$ oscillators [$h=0$ in Eq. (4)] and to the anharmonic oscillators ($h\neq0$) in Secs. III and IV, respectively.

II. SCALING-VARIATIONAL METHOD

From a normalized function $\phi(x)$ belonging to the Hilbert space associated with our problem, we can construct a variational function $\phi(a,x)$ by means of the introduction of an adjustable parameter a in the following way[10]:

$$\phi(a,x)=a^{1/2}\phi(ax)=e^{G}\phi(x) , \tag{7}$$

where

$$G\equiv G(a)=\frac{i}{2}(\ln a)(xp+px) . \tag{8}$$

The parameter a is adjusted in such a manner that the functional energy

$$E(a)=\langle\phi(a,x)\,|\,H\phi(a,x)\rangle \tag{9}$$

possesses an extremum

$$\frac{\partial E}{\partial a}(a_0)=0 . \tag{10}$$

The function $\phi(a_0,x)$ calculated by this method will fulfill the VT:

$$\langle[H,G]\rangle(a_0)=0 , \tag{11a}$$

$$2\langle T\rangle(a_0)=\langle xV'\rangle(a_0) . \tag{11b}$$

In what follows, we will use the following notation to denote the expectation value of any operator U:

$$\langle U\rangle(a)\equiv\langle\phi(a,x)\,|\,U\phi(a,x)\rangle , \tag{12}$$

$$\langle U\rangle\equiv\langle U\rangle(1) . \tag{13}$$

When $V(x)$ is a homogeneous function of s degree, the optimum a_0 is obtained at once from Eqs. (11),

$$a_0=[s\langle V\rangle/(2\langle T\rangle)]^{1/(s+2)} . \tag{14}$$

The substitution of (14) in Eq. (9) gives us the approximate energy $E(a_0)$ as a function of $\langle T\rangle$ and $\langle V\rangle$, i.e.,

$$E(a_0)=[(s/2)^{2/(s+2)}+(2/s)^{s/(s+2)}]\times\langle T\rangle^{s/(s+2)}\langle V\rangle^{2/(s+2)} . \tag{15}$$

$E(a_0)$ represents the minimum value of $E(a)$ when $s>-2$, because

$$\frac{\partial^2 E}{\partial a^2}(a_0)=2(s+2)\langle T\rangle>0 . \tag{16}$$

III. PURE $2k$ OSCILLATORS

In this section we discuss the pure $2k$ oscillators whose general Hamiltonian is

$$H=p^2+gx^{2k} . \tag{17}$$

Owing to the fact that the potential energy is a homogeneous function with degree $2k$, Eq. (15) gives us

$$E(a_0)=(k^{1/(k+1)}+k^{-k/(k+1)})\langle p^2\rangle^{k/(k+1)}\times\langle x^{2k}\rangle^{1/(k+1)}g^{1/(k+1)} . \tag{18}$$

The correct dependence of $E(a_0)$ with g is due to the fact that the approximate function $\phi(a_0,x)$ satisfies the VT (Ref. 11) (just the same as the exact function does). If we use the unscaled function $\phi(x)$, then $\langle H\rangle$ has a linear g dependence for any k value. The second following result is perhaps even more important than the preceding one. If $\phi(x)=\phi_n^0(x)$ is an eigenfunction corresponding to the harmonic-oscillator model then, for large enough n values, it is deduced that

$$\langle p^2\rangle=(n+0.5) , \tag{19}$$

$$\langle x^{2k}\rangle=(2k)!(k!)^{-2}2^{-k}(n+0.5)^k . \tag{20}$$

Under these conditions, Eq. (18) predicts, in addition, the correct dependence of the eigenvalue with the quantum number n:

$$E_n(a_0)=C_k(n+0.5)^{2k/(k+1)}g^{1/(k+1)} , \tag{21}$$

$$C_k=(k^{1/(k+1)}+k^{-k/(k+1)})\times[(2k)!(k!)^{-2}2^{-k}]^{1/(k+1)} . \tag{22}$$

So we see that the SVM predicts the proper behavior of the eigenvalues of H for large values of n (regardless the value of C_k) and

$$\lim_{n\to\infty}(n+0.5)^{-2k/(k+1)}E_n(a_0)=\text{const}\neq 0 . \tag{23}$$

Perhaps one might suspect that this last result is a consequence of the choice of the basis set $\{\phi_n\}$. However, this is not the case, as we will show in the following. Let us consider the set of eigenfunction corresponding to the particle in a box $\{\phi_n^B\}$:

$$p^2\phi_n^B(b,x)=E_n^B\phi_n^B(b,x),\quad x\in[-b,b] , \tag{24}$$

$$\phi_n^B(b,b)=\phi_n^B(b,-b)=0 . \tag{25}$$

The average value of the Hamiltonian (17) in this basis set

$$E_n(b)=\langle\phi_n^B\,|\,H\phi_n^B\rangle \tag{26}$$

satisfies the following equation:

$$b\frac{\partial}{\partial b}E_n(b)=-2\langle T\rangle(b)+2kg\langle x^{2k}\rangle(b) . \tag{27}$$

Obviously, in order to satisfy the VT [Eq. (11)], it is necessary to choose $b=b_0$ in such a way that

$$\frac{\partial}{\partial b}E_n(b_0)=0 . \tag{28}$$

This last condition gives us the result

$$E_n(b_0)=(k^{1/(k+1)}+k^{-k/(k+1)})\left[\frac{\pi}{2}\right]^{2k/(k+1)} \times\langle x^{2k}\rangle^{1/(k+1)}(n+1)^{2k/(k+1)}g^{1/(k+1)} , \tag{29}$$

where

$$\langle x^{2k}\rangle\equiv\langle x^{2k}\rangle(b=1) .$$

Again, the VT produces the correct dependence of $E_n(b_0)$ with g. When $n\gg 1$,

$$\langle x^{2k}\rangle\cong(2k+1)^{-1} \tag{30}$$

and $E_n(b_0)$ satisfies Eq. (23), because

$$E_n(b)\cong C_k^B(n+1)^{2k/(k+1)}g^{1/(k+1)} , \tag{31}$$

$$C_k^B=(k^{1/(k+1)}+k^{-k/(k+1)})\left[\frac{\pi}{2}\right]^{2k/(k+1)} \times(2k+1)^{-1/(k+1)} . \tag{32}$$

Therefrom, two basis sets which are essentially different lead to identical results when the VT is fulfilled (independently of the fact that $C_k\neq C_k^B$). As an immediate consequence, we can expect that $\langle H\rangle$ will behave in the manner denoted by Eqs. (21) and (31) whenever $\phi(x)$ possesses n zeros (n large) and satisfies the VT. These results enable one to conclude not only that Eq. (6) will be satisfied but that

$$\lim_{n,m\to\infty}\left[\frac{\bar{E}_n}{\bar{E}_m}-\frac{E_n}{E_m}\right]=0 \tag{33}$$

regardless of which basis set is employed to calculate $\bar{E}_n$ and $\bar{E}_m$ provided, of course, that the functions ϕ obey the VT. Furthermore, with these functions it is possible to estimate properly the relative transition frequencies

$$\bar{R}_{i,j}^{n,m}=\frac{\bar{E}_n-\bar{E}_m}{\bar{E}_i-\bar{E}_j}\cong R_{i,j}^{n,m}=\frac{E_n-E_m}{E_i-E_j} \tag{34}$$

in those cases where n, m, i, and j are large enough.

In order to verify these conclusions, we employ the quartic oscillator ($k=2$). Owing to the fact that the g dependence of $E_n(a_0)$ and $E_n(b_0)$ is the correct one, we restrict ourselves to displaying the behavior of the approximate eigenvalues with the quantum number n. In Table I, we show the energies $E_n(a_0)$ and $E_n(b_0)$ calculated via Eqs. (18) and (29) together with the exact values E_n given by Reid.[12] The quotients $E_n(a_0)/E_n$ and $E_n(b_0)/E_n$ are close enough to one (especially for the former case), which clearly demonstrates that the SVM allows one to approximate in a satisfactory way the calculation of any eigenstate. However, the property of the SVM that we are particularly interested in is self-evident when one considers the ratios

$$E_n(a_0)/E_{n-1}(a_0)$$

and

$$E_n(b_0)/E_{n-1}(b_0) .$$

For large n values, such ratios are practically identical to the exact ones. The ratio

$$E_n(a_0)/E_{n-1}(a_0)$$

coincides with E_n/E_{n-1} up to the fourth figure for $n\geq 5$.

According to expectations, the relative frequencies $\bar{R}_{i,j}^{n,m}$ are also in excellent agreement with the exact values (see Table II). This behavior is not due to a fortuitous cancellation of errors. The SVM predicts the proper variation of $\bar{E}_n$ with n, for n large enough. This remarkable property of the SVM could be very useful, for example, in vibrational spectroscopy.

Since the exact and trial functions satisfy the relation

$$E_n=g(k+1)\langle n\,|\,x^{2k}\,|\,n\rangle , \tag{35}$$

it follows at once that the appropriate average values of x^{2k} show the correct behavior with respect to n and g. A natural inquiry consists in asking about the degree of exactness of variational eigenvalues for other $2k$ oscillators. In order to make this point clear, we present in Table III the coefficients C_k and C_k^B, together with the semiclassical ones C_k^{WKB} (Refs. 7,8) and the ratios C_k/C_k^{WKB} and C_k^B/C_k^{WKB}. Results show that, for the four cases considered,

$$\bar{E}_n<E_n^{\mathrm{WKB}} \quad \text{for } n \text{ large} .$$

Table III also shows, that $\{\phi_n^0\}$ yields better results when $k<5$, while ϕ_n^B permits a better approximation when $k\geq 5$. This particular behavior can be explained because, when k is large, the potential gx^{2k} is more like that of the particle in a box model than that of the harmonic-oscillator model.

TABLE I. Energy eigenvalues of the quartic oscillator ($g=1$).

n	$E_n(a_0)$	$E_n^B(b_0)$	E_n	$E_n(a_0)/E_n$	$E_n(b_0)/E_n$	$E_n(a_0)/E_{n-1}(a_0)$	$E_n(b_0)/E_{n-1}(b_0)$	E_n/E_{n-1}
0	1.0817	1.1909	1.0604	1.0201	1.1231			
1	3.8474	4.2173	3.7997	1.0126	1.1099	3.5568	3.5413	3.5833
2	7.4370	8.0721	7.4557	0.9975	1.0827	1.9330	1.9140	1.9622
3	11.5739	12.2709	11.6447	0.9939	1.0538	1.5563	1.5202	1.5619
4	16.1383	16.7879	16.2618	0.9924	1.0324	1.3944	1.3681	1.3965
5	21.0607	21.5889	21.2384	0.9916	1.0165	1.3160	1.2860	1.3060
6	26.2948	26.6501	26.5285	0.9913	1.0046	1.2491	1.2344	1.2491
7	31.8069	31.9481	32.0986	0.9909	0.9953	1.2100	1.1988	1.2100
8	37.5714	37.4646	37.9230	0.9907	0.9879	1.1815	1.1727	1.1815
9	43.5676	43.1843	43.9812	0.9906	0.9819	1.1598	1.1527	1.1598
10	49.7789	49.0940	50.2563	0.9905	0.9769	1.1427	1.1368	1.1427
11	56.1913	55.1827	56.7342	0.9904	0.9727	1.1288	1.1240	1.1289
12	62.7928	61.4406	63.4030	0.9904	0.9690	1.1175	1.1134	1.1175
13	69.5732	67.8592	70.2524	0.9903	0.9659	1.1080	1.1045	1.1080
14	76.5234	74.4309	77.2732	0.9903	0.9632	1.0999	1.0968	1.0999
15	83.6356	81.1490	84.4575	0.9903	0.9608	1.0929	1.0903	1.0930
16	90.9026	88.0075	91.7981	0.9902	0.9587	1.0869	1.0845	1.0869
17	98.3182	95.0009	99.2886	0.9902	0.9568	1.0816	1.0795	1.0816
18	105.8765	102.1243	106.9233	0.9902	0.9551	1.0769	1.0750	1.0769
19	113.5724	109.3730	114.6969	0.9902	0.9536	1.0727	1.0710	1.0727
20	121.4012	116.7430	122.6046	0.9902	0.9522	1.0689	1.0674	1.0689
21	129.3584	124.2304	130.6421	0.9902	0.9509	1.0655	1.0641	1.0656
22	137.4400	131.8317	138.8051	0.9902	0.9498	1.0625	1.0612	1.0625
23	145.6424	139.5435	147.0901	0.9902	0.9487	1.0597	1.0585	1.0597

IV. ANHARMONIC OSCILLATORS

For anharmonic oscillators with a Hamiltonian operator

$$H=p^2+x^2+gx^{2k}, \tag{36}$$

the condition (10) also leads to a minimum which is given by the following equations:

$$E_n(t)=(t+t^{-1})(n+0.5)+gt^k\langle x^{2k}\rangle, \quad t=a_0^2, \tag{37}$$

$$t^{k+1}-t^{k-1}-q=0, \quad q\equiv kg\langle x^{2k}\rangle(n+0.5)^{-1}. \tag{38}$$

The eigenfunctions of H^0 were chosen as trial functions $\phi_n(x)$. For large g (or n) values, it is deduced at once that

$$t\cong q^{1/(k+1)}+(k+1)^{-1}q^{-1/(k+1)}. \tag{39}$$

Substituting (39) in (37) and retaining up to the two largest terms, we obtain

$$E_n(t)\cong(n+0.5)\times[k^{-1}(k+1)q^{1/(k+1)}+q^{-1/(k+1)}]. \tag{40}$$

When n is large enough,

$$q\cong gk(2k)!(k!)^{-2}2^{-k}(n+0.5)^{k-1} \tag{41}$$

and Eq. (40) becomes

$$E_n(t)\cong a_k(n+0.5)^{2k/(k+1)}g^{1/(k+1)}+b_k(n+0.5)^{2/(k+1)}g^{-1/(k+1)}, \tag{42}$$

where

$$a_k=(k+1)k^{-1}b_k^{-1}, \tag{43}$$

$$b_k=\{(k!)^2 2^k k^{-1}[(2k)!]^{-1}\}^{1/(k+1)}. \tag{44}$$

TABLE II. Relative frequencies for the quartic oscillator ($g=1$).

	$R_{23,20}^{23,22}$	$R_{23,21}^{23,22}$	$R_{22,20}^{23,22}$	$R_{22,21}^{23,22}$
Eq. (29)	0.3382	0.5036	0.5111	1.0145
Eq. (18)	0.3384	0.5037	0.5114	1.0149
Exact[10]	0.3389	0.5037	0.5114	1.0149

TABLE III. Coefficients C_k for several oscillators.

k	C_k	C_k^{WKB}	C_k/C_k^{WKB}	C_k^B	C_k^B/C_k^{WKB}
2	2.163 374	2.185 069	0.9901	2.018 077	0.9236
3	2.206 501	2.264 971	0.9742	2.123 853	0.9377
4	2.215 734	2.309 757	0.9593	2.189 099	0.9478
5	2.213 356	2.338 265	0.9466	2.233 455	0.9552

For the quartic anharmonic oscillator ($k=2$), the asymptotic formula (42) adopts the following form:

$$E_n(t)=2.163\,374(n+0.5)^{4/3}g^{1/3} +0.693\,361(n+0.5)^{2/3}g^{-1/3} . \quad (45)$$

The preceding expression is very similar to that deduced from the WKB method[7–9].

$$E_n^{\mathrm{WKB}}\cong 2.185\,069(n+0.5)^{4/3}g^{1/3} +0.675\,5458(n+0.5)^{2/3}g^{-1/3} . \quad (46)$$

This agreement explains the similarity between variational and exact values in the whole range of n and g values.

The suitable dependence of $E_n(t)$ with g is not really surprising because the variational functions $\phi_n(a_0,x)$ satisfy the VT and the Hellmann-Feynman theorem (HFT), and it is well known that such theorems determine this particular dependence.[11] However, the special point that had not been discussed previously, and that we wish to bring out in this work, consists of the fact that the SVM yields the proper asymptotic behavior of E_n. In a more precise manner: Equation (42) assures us that Eqs. (6) and (23) will be satisfied. Equation (42) is also useful for estimating in an approximate fashion the eigenvalues of any anharmonic oscillator when the quantum number n is sufficiently large. It is hoped that the conclusions presented up to now are independent of the chosen basis set.

We will use the basis set corresponding to the particle in a box model in order to verify such independence. A simple and direct calculation gives us the following result for the variational eigenvalues (for large g and n values):

$$E_n(b_0)\cong a_k^B(n+1)^{2k/(k+1)}g^{1/(k+1)} +b_k^B(n+1)^{2/(k+1)}g^{-1/(k+1)} , \quad (47)$$

where

$$a_k^B=(k^{1/(k+1)}+k^{-k/(k+1)}) \times(2k+1)^{-1/(k+1)}\left[\frac{\pi}{2}\right]^{2k/(k+1)} , \quad (48)$$

$$b_k^B=\frac{1}{3}\left[\frac{2k+1}{k}\right]^{1/(k+1)}\left[\frac{\pi}{2}\right]^{2/(k+1)} . \quad (49)$$

As a particular case, when $k=2$ we obtain a very similar expression to (45) and (46), but with numerical coefficients which are slightly smaller in both terms:

$$E_n(b_0)\cong 2.018\,077(n+1)^{4/3}g^{1/3} +0.611\,325(n+1)^{2/3}g^{-1/3} . \quad (50)$$

The dependence of $E_n(a_0)$ with g was formerly verified by Killingbeck[6] numerically for the ground state of the quartic anharmonic oscillator ($k=2$). Hence, we shall restrict ourselves to verify our conclusions with regard to the relationship between $E_n(a_0)$ and n. In Table IV, we present the variational eigenvalues computed for $k=2$ and $g=1$ from Eqs. (37) and (38) [$E_n(a_0)$] together with the asymptotic formula (45) (E_n^{asymp}) and the exact results (E_n) reported previously in Ref. 13. The ratio $E_n(a_0)/E_n$ clearly shows that the SVM allows one to estimate the eigenvalues of the quartic anharmonic oscillator with a maximum error of about 1%. With the sole exception of the ground state, the same results are obtained via formula (45). These results clearly demonstrate the usefulness of Eq. (42). In agreement with the model discussed in Sec. III the approximate ratios $\bar{E}_n/\bar{E}_{n-1}$ are close to the exact ratio when $n>5$. This behavior suggests that, for this case, the SVM permits one to calculate the relative frequencies with a high degree of accuracy. Since anharmonic oscillators are frequently employed for studying molecular vibrations, the conclusions derived in this section would be of utility in this field. We have shown by way of Eq. (42) that $E_n(t)$ reproduces in a satisfactory manner the behavior of E_n when g is large. If g is small enough, so that $q\ll 1$, then Eqs. (37) and (38) describe the correct conduct of E_n also:

$$E_n(t)\cong 2n+1+g\langle x^{2k}\rangle+O(g^2) . \quad (51)$$

TABLE IV. Energy eigenvalues for the quartic anharmonic oscillator ($g=1$).

n	$E_n(a_0)$	E_n^{asymp}	E_n	$E_n(a_0)/E_n$	E_n^{asymp}/E_n	$E_n(a_0)/E_{n-1}(a_0)$	$E_n^{\text{asymp}}/E_{n-1}^{\text{asymp}}$	E_n/E_{n-1}
0	1.4033	1.2953	1.3924	1.0078	0.9303			
1	4.6782	4.6232	4.6488	1.0063	0.9945	3.3337	3.5692	3.3387
2	8.6470	8.6176	8.6550	0.9991	0.9957	1.8484	1.8640	1.8618
3	13.1095	13.0946	13.1568	0.9964	0.9953	1.5161	1.5195	1.5201
4	17.9677	17.9623	18.0756	0.9940	0.9937	1.3706	1.3717	1.3739
5	23.1619	23.1634	23.2974	0.9942	0.9942	1.2891	1.2896	1.2889
6	28.6514	28.6581	28.8353	0.9936	0.9939	1.2370	1.2372	1.2377
7	34.4059	34.4166	34.6408	0.9932	0.9935	1.2008	1.2009	1.2013
8	40.4019	40.4160	40.6904	0.9929	0.9933	1.1743	1.1743	1.1746
9	46.6207	46.6375	46.9650	0.9927	0.9930	1.1539	1.1539	1.1542
10	53.0469	53.0660	53.4491	0.9925	0.9928	1.1378	1.1378	1.1381
11	59.6673	59.6885	60.1295	0.9923	0.9927	1.1248	1.1248	1.1250
12	66.4709	66.4938	66.9950	0.9922	0.9925	1.1140	1.1140	1.1142
13	73.4480	73.4725	74.0359	0.9921	0.9924	1.1050	1.1050	1.1051
14	80.5902	80.6160	81.2435	0.9920	0.9923	1.0972	1.0972	1.0974
15	87.8899	87.9170	88.6103	0.9919	0.9922	1.0906	1.0906	1.0907
16	95.3405	95.3686	96.1296	0.9918	0.9921	1.0848	1.0848	1.0849
17	102.9359	102.9651	103.7953	0.9917	0.9920	1.0797	1.0797	1.0797
18	110.6707	110.7007	111.6018	0.9917	0.9919	1.0751	1.0751	1.0752
19	118.5399	118.5708	119.5442	0.9916	0.9919	1.0711	1.0711	1.0712
20	126.5389	126.5706	127.6178	0.9915	0.9918	1.0675	1.0675	1.0675
30	212.8884	212.9255	214.7797	0.9912	0.9914			
40	309.0250	309.0652	311.8315	0.9910	0.9911			
50	413.2499	413.2921	417.0563	0.9909	0.9910			
100	1025.7900	1025.8371	1035.5442	0.9906	0.9906			

Consequently, we conclude that the insertion of a scaling factor in the trial function adjusts the behavior of the eigenvalues in the complete range of g values. Recently, Bozzolo and Plastino[14] presented a new and interesting method to study a perturbed harmonic oscillator with a Hamiltonian operator

$$H=H^0+gV\ . \tag{52}$$

The procedure followed by these authors consists in relating the eigenstates Ψ_n of H and ϕ_n^0 of H^0 by means of a mapping operator F_n:

$$\Psi_n=\exp(iF_n)\phi_n^0\ . \tag{53}$$

When $V(x)$ is even, $F_n(x)$ has the following expression:

$$F_n=i\sum_{j=1}^{\infty}h_{nj}(A^{\dagger 2j}-A^{2j})\ , \tag{54}$$

where $A^\dagger$ and A are the creation and annihilation operators

$$A^\dagger=p+ix,\quad A=p-ix \tag{55}$$

and $\{h_{nj}\}$ are variational parameters.

Retaining only the first term in the expansion (54)

$$F_n=ih_n(A^{\dagger 2}-A^2)\ , \tag{56}$$

Bozzolo and Plastino[14] obtained an excellent approximation for the first two states of several perturbed oscillators and for the complete range of values corresponding to the perturbation parameter g. The success of this method can be explained immediately, because it coincides with the SVM when F_n has the form (56). In such a case,

$$iF_n=-2ih_n(xp+px)=\frac{i}{2}(\ln a)(xp+px)\ ,$$
$$a=\exp(-4h_n)\ . \tag{57}$$

Hence we see that a or h_n can be used as variational parameters.

V. FURTHER COMMENTS

Results presented in this work show clearly that the possibilities of the SVM are not restricted to providing an upper bound for the first two states of

the even anharmonic oscillators, but allow one to estimate accurately the change of eigenvalues with g and n for the whole range of variation of such parameters. Apparently, this property does not depend on the chosen basis set. We believe that a rigorous mathematical demonstration could yield a deeper knowledge about eigenfunctions and eigenvalues associated with anharmonic oscillators. These relevant aspects of the SVM have been demonstrated only for Hamiltonians with a general form (4), but there are certain evidences that their validity may be more general.

Our assertion that $\bar{E}_n$ depends on n and g in a correct manner means that Eq. (6) is fulfilled (and a similar one for $g \rightarrow \infty$). However, it is necessary to point out that the VT and HFT properly determine this dependence, but they cannot afford the exact value of the coefficient C_k. This coefficient depends on the chosen basis set (as shown in Secs. III and IV). Naturally, when this set is more close to that one corresponding to the model under study, then the accuracy is greater in the estimate of C_k. The marked usefulness of the SVM does not lie in the possibility of an individual estimate of the eigenvalues, but in the calculation of relative quantities, such as $R_{i,j}^{m,n}$. Furthermore, this method is very easy to be applied to a wide number of problems. We deem that results presented here possess a real theoretical interest because they plainly show the important role that plays the VT in the determination of the functional dependence of the eigenvalues with respect to the quantum number.

Finally, we wish to point out that scaling transformations have a marked utility even in problems with wholly different characteristics to those discussed here. Recently, they have been applied with a great success to quantum systems that obey nontrivial boundary conditions, such as those of Dirichlet and von Neumann[15] and for models with a potential that has a discontinuity.[16] In both cases, the introduction of a scaling factor in the trial function which is variationally optimized permits one to reproduce the essential aspects of the physical problem.

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