Energy eigenvalues of double-well oscillator with mixed quartic and sextic anharmonicities

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The renormalized hypervirial-Padé scheme has been employed to determine energy eigenvalues of a double-well oscillator with mixed quartic and sextic anharmonicities and the special cases obtained from its potential by taking either anharmonicity as zero. The renormalization parameters calculated from two analytical expressions (one of these being suggested as an improvement of the earlier prescription) are found to be inadequate, while the approach in which this parameter is treated as a variable quantity works well. The results for a wide range of anharmonicity values are compared with the findings of other workers and the agreement is good to superb. It turns out that the technique applied here is effectual when the wells are not very deep. Discussion of the dependence of the renormalization parameter and the energies on the quantities defining the double-well potential and also on the quantum number is also included.

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I. INTRODUCTION

The double-well potentials obtained by adding anharmonic terms to $-\frac{1}{2}m\omega^2x^2$ can be used for modeling of two-state systems. Some of the problems to which the double-well anharmonic-oscillator (DWAO) model has been applied are the interpretation of the infrared spectra of the NH_3 molecule, infrared and Raman spectra of the hydrogen-bonded systems, inversion characteristics of isomers, structural phase transitions, polarizability of perovskite ferroelectrics, formation of noble-gas monolayers on a graphite substrate, macroscopic quantum coherence in superconducting Josephson devices, switching and storage devices in computers, and so on [1–9]. Besides, the Brownian particle in a bistable potential has been used as a model in explaining the chemical reactions, second-order phase transitions, ligand migration of biomolecules, etc. [10,11]. In the theory of these problems, the most important characteristics are related to the separation between the two lowest-lying energy levels as it defines the tunneling rate through the double-well barrier.

Although, generally, an oscillator interacts with the surroundings, in some cases, particularly when the number density of the oscillators is low, the effects of dissipation can be ignored. This has, in fact, sustained interest in determining the energy eigenvalues of anharmonic oscillators as well as double-well anharmonic oscillators. This type of approach has now been strengthened in view of recent experiments leading to successful isolation of single quantum oscillators from the dissipation mechanism and thus facilitating investigation of the dynamics of individual systems under appropriate conditions [12–14].

The DWAO that has quite frequently been employed to interpret the experimental data listed above is

$$V(x)=m\left(-\tfrac{1}{2}\omega^2x^2+\tfrac{1}{4}\alpha x^4\right) . \tag{1.1}$$

In light of the experience gained from successful modeling based on anharmonic oscillators, an obvious step in the direction of improvement in the precision of the description of bistable systems is to add a sextic term to Eq. (1.1), yielding

$$V(x)=m\left(-\tfrac{1}{2}\omega^2x^2+\tfrac{1}{4}\alpha x^4+\tfrac{1}{6}\beta x^6\right) . \tag{1.2}$$

Obviously, (1.2) reduces to (1.1) for $\beta=0$ and to the sextic double-well oscillator for $\alpha=0$.

Gorringe and Leach [8] have presented an ansatz for finding the exact solution to the Schrödinger equation for the potential given by Eq. (1.2) and have tabulated energies corresponding to some selected values of α and β. Also, Chaudhuri and Mondal [15] have used a modified Hill determinant method to obtain energy eigenvalues for a few α and β combinations. In addition, the energies of the two DWAO's obtained by $\beta=0$ and $\alpha=0$ have been found for different magnitudes of anharmonicity parameters by various workers employing Wick-ordered Borel summation [16], modified Hill determinants [15,17], scaled harmonic basis technique [18], supersymmetry quantum mechanics [7,19,20], two-step approximation procedure [21]. Taylor-series expansion [22], maximum entropy theorem [23], exact solution formalisms [3,24], and some other ingenious methods [25–27].

In view of these facts, we have carried out a detailed investigation of the energy eigenvalues of double-well oscillators with quartic, sextic, and mixed quartic-sextic anharmonicities over a wide range of α and β values. We have achieved our objective using the renormalized hypervirial Padé technique [28–30], which have not been exploited by any worker for determination of the energies of DWAO's. The specific goals we set before us are the following: (i) to study the efficacy of Killingbeck's [28,29] variational approach based on the renormalized hypervirial method in the calculation of energies of DWAO's with respect to the values of ω^2, α, and β and of the quantum number n of the state; (ii) to look for an analytic expression for the renormalization parameter used in (i) and to check its usefulness in simplifying the algorithm for

the computation work; (iii) to investigate the dependence of the variational parameter of (i) on the values of ω^2, α, β, and n; (iv) to know the extent to which the use of the Padé approximants, which have been found by using Killingbeck's algorithm [31], improves upon the results of (i); (v) to compare the outcome of the above computations with the findings of various workers, who have used other methods for some of the ω^2, α, β, and n values considered here; and (vi) to bring out the effect of ω^2, α, and β on the energy eigenvalues for a particular type of DWAO.

The outcome of the efforts with the above-mentioned aims and the discussion of the concomitant issues constitute the content of this paper.

II. RECURRENCE RELATIONS IN THE FRAMEWORK OF THE RENORMALIZED HYPERVIRIAL FORMALISM

In order to keep the first-order contribution from the sextic term in Eq. (1.2) of the same order as the second-order effect of the quartic term and also to circumvent any possible complications arising from the presence of two independent anharmonicity parameters α and β in the recurrence relations, we use a perturbation parameter λ in place of α and substitute $\beta=\lambda^2\eta$, so that (1.2) is rewritten in terms of single-perturbation parameter λ as

$$V(x)=m\left(-\tfrac{1}{2}\omega^2x^2+\tfrac{1}{4}\lambda x^4+\tfrac{1}{6}\lambda^2\eta x^6\right) . \tag{2.1}$$

Renormalizing $V(x)$ and hence the corresponding Hamiltonian by adding and subtracting the harmonic term $\frac{1}{2}m\lambda Kx^2$, we get a new Hamiltonian:

$$H=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\tfrac{1}{2}m(\omega')^2x^2+m\lambda\left[\frac{1}{4}x^4-\frac{1}{2}Kx^2\right]+\frac{1}{6}m\lambda^2\eta x^6 , \tag{2.2}$$

where

$$\omega'=(-\omega^2+\lambda K)^{1/2} \tag{2.3}$$

is the new increased frequency. Using the hypervirial theorem [32], we get an expression for the exact energy E_n in terms of the expectation value $\langle x^N\rangle_n$ of the state:

$$\begin{aligned}E_n\langle x^N\rangle_n=&\frac{1}{2}m[(\omega')^2-\lambda K]\frac{N+2}{N+1}\langle x^{N+2}\rangle_n\\&+\frac{1}{4}m\lambda\frac{N+3}{N+1}\langle x^{N+4}\rangle_n\\&+\frac{1}{6}m\lambda^2\eta\frac{N+4}{N+1}\langle x^{N+6}\rangle_n\\&-\frac{\hbar^2}{8m}N(N^2-1)\langle x^{N-2}\rangle_n .\end{aligned} \tag{2.4}$$

Expanding E_n and $\langle x^N\rangle_n$ as a power series in λ, we have

$$E_n=\sum_{j=0}^{\infty}E_n^{(j)}\lambda^j \tag{2.5}$$

and

$$\langle x^N\rangle_n=\sum_{p=0}^{\infty}C_p^{(N)}\lambda^p . \tag{2.6}$$

Here

$$E_n^{(0)}=(n+\tfrac{1}{2})\hbar\omega' \tag{2.7}$$

and

$$C_p^{(0)}=\delta_{op} . \tag{2.8}$$

Substituting (2.5) into (2.4) and equating the coefficients of the same power of λ on the two sides of the resulting equation, we have the recurrence relation for the expansion coefficients $C_p^{(N)}$, viz.,

$$C_p^{(N+2)}=\frac{2}{(N+2)m(\omega')^2}\left[(N+1)\sum_{j=0}^{\infty}E_n^{(j)}C_{p-j}^{(N)}+\frac{1}{2}mK(N+2)C_{p-1}^{(N+2)}-\frac{1}{4}m(N+3)C_{p-1}^{(N+4)}-\frac{1}{6}m\eta(N+4)C_{p-2}^{(N+6)}+\frac{\hbar^2}{8m}N(N^2-1)C_p^{(N-2)}\right] . \tag{2.9}$$

Next, according to the Hellmann-Feynman theorem [32],

$$\frac{\partial E_n}{\partial\lambda}=\left\langle\frac{\partial H}{\partial\lambda}\right\rangle_n , \tag{2.10}$$

which, together with (2.2), (2.5), and (2.6) and on equating the coefficients of equal powers of λ on both the sides, gives

$$E_n^{(j)}=\frac{m}{j}\left[-\frac{1}{2}KC_{j-1}^{(2)}+\frac{1}{4}C_{j-1}^{(4)}+\frac{\eta}{3}C_{j-2}^{(6)}\right] . \tag{2.11}$$

Thus, determining the expansion coefficients from Eqs. (2.9) and (2.8), we can find $E_n^{(j)}$ in a hierarchical manner and hence E_n can be calculated from (2.5).

III. DETERMINATION OF RENORMALIZATION PARAMETER

In his work, Killingbeck has treated K as a variable parameter to get the best converged value of E_n. However, Chaudhuri and Mondal [15] have argued for finding an analytic expression for K by equating to zero the coefficients of $(a^\dagger)^2$ and a^2 in the Hamiltonian expressed in terms of the creation and annihilation operators. In

this section we first consider this approach for obtaining a condition giving K, then find a modified expression to improve upon this condition, and also comment upon the variational method.

A. Chaudhuri and Mondal prescription

In terms of the creation and annihilation operators, the Hamiltonian (2.2) reads

$$H=\frac{1}{4}\hbar\omega'\left[1-\frac{\omega^2}{(\omega')^2}\right]+\frac{3\hbar^2\lambda}{16m(\omega')^2}+\frac{5\hbar^3\lambda^2\eta}{16m^2(\omega')^3}+\left[\frac{1}{2}\hbar\omega'\left[1-\frac{\omega^2}{(\omega')^2}\right]+\frac{3\hbar^2\lambda}{4m(\omega')^2}+\frac{15\hbar^3\lambda^2\eta}{8m^2(\omega')^3}\right]a^\dagger a$$
$$+\left[-\frac{1}{4}\hbar\omega'\left[1+\frac{\omega^2}{(\omega')^2}\right]+\frac{3\hbar^2\lambda}{8m(\omega')^2}+\frac{15\hbar^3\lambda^2\eta}{16m^2(\omega')^3}\right][(a^\dagger)^2+a^2]$$
$$+\left[\frac{\hbar^2\lambda}{16m(\omega')^2}+\frac{5\hbar^3\lambda^2\eta}{16m^2(\omega')^3}\right][(a^\dagger)^4+a^4]+\left[\frac{3\hbar^2\lambda}{8m(\omega')^2}+\frac{15\hbar^3\lambda^2\eta}{8m^2(\omega')^3}\right](a^\dagger)^2a^2$$
$$+\left[\frac{\hbar^2\lambda}{4m(\omega')^2}+\frac{5\hbar^3\lambda^2\eta}{4m^2(\omega')^3}\right][(a^\dagger)^3a+(a^\dagger)a^3]$$
$$+\frac{\hbar^3\lambda^2\eta}{48m^2(\omega')^3}[(a^\dagger)^6+6(a^\dagger)^5a+15(a^\dagger)^3a^2+20(a^\dagger)^3a^3+15(a^\dagger)^2a^4+6a^\dagger a^5+a^6]\ . \tag{3.1}$$

Here we have used Eq. (2.3) to get the expression in ω'. Putting the coefficients of $(a^\dagger)^2$ and a^2 equal to zero, we get

$$4m^2(\omega')^4+4m^2\omega^2(\omega')^2-6m\hbar\lambda\omega'-15\hbar^2\lambda^2\eta=0\ , \tag{3.2}$$

which can be solved for ω' and hence K for known values of ω, λ, and η. Obviously, the K value so found is independent of n, and we identify it by using subscript c with K, viz., K_c.

If we take $\eta=0$, Eq. (3.2) becomes the condition giving K_c for the quartic case. This reads

$$2m(\omega')^3+2m\omega^2\omega'-3\hbar\lambda=0\ . \tag{3.3}$$

B. Second-order perturbation-theory approach

With the intention of generalizing the result of Eq. (3.2) to obtain n dependence, we first note that for the Hamiltonian [Eq. (3.1)] the expectation value with respect to the harmonic-oscillator state $|n\rangle$ is given by

$$\langle n|H|n\rangle=\left[n+\frac{1}{2}\right]\frac{\hbar\omega'}{2}\left[1-\frac{\omega^2}{(\omega')^2}\right]+\frac{3\hbar^2\omega}{16m(\omega')^2}(2n^2+2n+1)+\frac{5\hbar^3\lambda^2\eta}{48m^2(\omega')^3}(4n^3+6n^2+8n+3)\ . \tag{3.4}$$

Treating ω' as a variational quantity and deciding to determine it in such a way that $\langle n|H|n\rangle$ becomes minimum, we have

$$4(2n+1)m^2[(\omega')^4+\omega^2(\omega')^2]-6(2n^2+2n+1)m\hbar\lambda\omega'-5(4n^3+6n^2+8n+3)\hbar^2\lambda^2\eta=0\ . \tag{3.5}$$

Taking $n=0$ in (3.5), we get Eq. (3.2). Thus we observe that the procedure laid down in Ref. [15] amounts to determining $\langle 0|H|0\rangle$ with ω' as a variational parameter and finally finding it corresponding to the requirement $d\langle 0|H|0\rangle/d\omega'=0$. Consequently, the expression in ω' given by (3.5) is the condition to be fulfilled by the variational parameter corresponding to the quantum number n. Once again, $n=0$ leads to a condition for the case of a double-well oscillator with quartic anharmonicity.

But we know that $\langle n|H|n\rangle$ represents the diagonal elements of the matrix for H, and hence by considering (3.4), we are essentially evaluating E_n to the second order in perturbation, ignoring the contribution of the nondiagonal elements in the expression

$$E_n=\langle n|H|n\rangle+\sum_{m=n}(H_{nm})^2\Big/(E_n^{(0)}-E_m^{(0)})\ . \tag{3.6}$$

So, to improve upon the K parameter determined from (3.5), we find out E_n by considering the complete expression in (3.6). This gives us

$$E_n=\left[n+\frac{1}{2}\right]\frac{\hbar\omega'}{2}\left[1-\frac{\omega^2}{(\omega')^2}\right]+\frac{3\hbar^2\lambda}{16m(\omega')^2}(2n^2+2n+1)\left[2+\frac{\omega^2}{(\omega')^2}\right]-(2n+1)\frac{\hbar\omega'}{16}\left[1+\frac{\omega^2}{(\omega')^2}\right]^2$$
$$-\frac{\hbar^3\lambda^2}{128m^2(\omega')^5}(34n^3+51n^2+59n+21)+\frac{5\hbar^3\lambda^2\eta}{48m^2(\omega')^3}(4n^3+6n^2+8n+3)\ . \tag{3.7}$$

Differentiating E_n with respect to ω' and equating to zero the expression so obtained, we finally get

$$24(2n+1)m^2(\omega')^2[(\omega')^2+\omega^2]^2-96(2n^2+2n+1)m\hbar\lambda[(\omega')^3+\omega^2\omega'] \\ -40(4n^3+6n^2+8n+3)\hbar^2\lambda^2\eta(\omega')^2+5(34n^3+51n^2+59n+21)\hbar^2\lambda^2=0 . \quad (3.8)$$

Obviously, we can solve this sextic equation in ω' to know ω' and hence K for a particular set of values of ω, λ, η, and n. In order to distinguish the K determined by the second-order perturbation treatment from the other K values, we use a prime on it. Putting $\eta=0$ in Eq. (3.21) gives us condition for the case of a double-well oscillator with quartic anharmonicity. This reads

$$24(2n+1)m^2(\omega')^2[(\omega')^2+\omega^2]^2-96(2n^2+2n+1)m\hbar\lambda[(\omega')^3+\omega^2\omega']+5(34n^3+51n^2+59n+21)\hbar^2\lambda^2=0 . \quad (3.9)$$

C. Variational method

As mentioned earlier, Killingbeck recommended treating K as a variational quantity in the final expression for E_n to be chosen in such a way that the best number of stable digits is obtained for its value. His approach has been shown to be fully qualified for the calculation of energy values of anharmonic oscillators [30,33,34].

IV. CALCULATIONS AND NUMERICAL RESULTS

The determination of the expansion coefficients $C_p^{(N)}$ from the recurrence relation (2.9) shows that

$$C_p^{(2M+1)}=0 , \quad (4.1)$$

where $p,M=0,1,2,3,\ldots$. The calculations for the energies have been performed by truncating the series summation in (2.5) at $j=32$. However, the listed results correspond to the case for which the largest possible number of digits converged. In addition, the computations have been carried out with double precision, though the values of the energy are being given up to the digit for which the stability was the best. It may be mentioned that all the results being reported here are in units corresponding to $\hbar=m=1$.

In order to see the relative efficacy of the three methods for the determination of the renormalization parameter in giving precise energy eigenvalues, we carried out computations for $n=0$ and 1 for a few typical cases of the three types of double-well oscillators using K_c, K', and K values. However, the results for only the quartic anharmonicity are projected in Table I. A perusal of this table shows that (i) generally, $K>K'>K_c$; (ii) while the K_c approach fails in most cases, the K' approach is inadequate for $\alpha<\omega^2$; (iii) use of K' produces better convergence than that of K_c, but the energy values determined with K are the most accurate and, hence, reliable; and (iv) for a particular ω^2, the number of stable digits in the energy value increases with an increase in the values of α and n. The conclusions drawn in the other two cases are essentially the same as mentioned above, except that the convergence even with K is poor for $\omega^2>\alpha,\beta$.

The superiority of the variational approach over the method using the two analytical expressions is understandable because these expressions have been obtained from perturbation theory—K' is found by including the

TABLE I. Comparison of energy eigenvalues for some representative quartic double-well oscillators obtained from K_c and K' values and by treating K as a variational parameter.

ω^2	α	n	K_c	$E(K_c)$	K'	$E(K')$	K	$E(K)$
1.0	0.4	0	3.09	a	3.38	a	7.5	−0.154
		1	3.09	a	4.13	0.1	7.5	0.142 76
	40.0	0	0.39	1.0	0.47	1.4	1.5	1.371 566 9
		1	0.39	a	0.66	4.99	1.5	4.989 416 52
	400.0	0	0.18	3.0	0.22	3.1	0.6	3.069 478 40
		1	0.18	a	0.30	11.0	0.6	11.033 081 0
5.0	2.0	0	2.66	a	2.60	a	9.0	−2.1
		1	2.66	a	2.74	a	12.5	−1.8
	400.0	0	0.18	a	0.22	2.9	0.6	2.943 549 56
		1	0.18	a	0.31	10.7	0.7	10.721 123 666 1

[a]Oscillatory and divergent.

nondiagonal elements in the second-order perturbation and, as such, is an improvement over K_c, where only diagonal elements are considered. In contrast, in the variational method we look for the most stable value in the number obtained in computation.

In view of the above observations, we have listed in Tables II–IV results based on the variational approach for double-well oscillators with quartic, sextic, and mixed quartic-sextic anharmonicities, respectively. However, the knowledge of K' has been exploited to choose the initiating value of K because $K > K'$. Also, for $(\omega')^2$ to be positive, (2.3) shows that $K > \omega^2/\lambda$. Also included in these tables are the energy values found from the Padé approximants $E(P)$ to the series expansions with the K parameter. These computations have been carried out by keeping the number of terms in the sequence as 34. But the energy values given in the tables are the best converged ones. With a view to compare the present findings with those of earlier workers, the available results having a maximum number of stable digits are also projected in these tables.

V. DISCUSSION AND CONCLUSIONS

From the entries of Tables II–IV, we note the following.

(i) For the values of ω^2, α, β, and n listed in these tables, the renormalized hypervirial method yields reasonably good values of the energy. However, the convergence of the series is relatively poor if the anharmonicity parameter α or β is less than ω^2, and this aspect becomes more prominent with an increase of ω^2 and n values. In fact, this approach failed for large values of n and ω^2 pertaining to the situation $\omega^2 > \alpha, \beta$. Accordingly, such results are not displayed in the tables. Nonetheless, the number of stable digits obtained for $\alpha, \beta \gg \omega^2$ is quite heartening. For example, in the case of a quartic double-well oscillator, the energy eigenvalues for $\alpha = 400.0$ for all ω^2 and n have been found to be convergent to nine or more significant figures. In the sextic oscillator this number is five for $\beta = 600.0$, and in the mixed quartic and sextic oscillator the convergence is best for $\alpha = 400.0$ and $\beta = 600.0$. This feature of the results is understandable

TABLE II. Calculated energy eigenvalues for some quartic double-well anharmonic oscillators for various states. (O represents other values.)

n	ω^2	α	K	$E(K)$	$E(P)$	$E(O)$
0	1.0	0.4	7.5	−0.154	−0.154 126	0.4709[a]
		2.0	4.0	0.328 827	0.328 826 503	0.328 826 502 595[b]
		4.0	3.0	0.514 780 41	0.514 780 415 53	
		40.0	1.5	1.371 566 9	1.371 566 851 96	1.377 816 88[a]
		400.0	0.6	3.069 478 40	3.069 478 403 20	3.070 103 41[a]
	1.6	0.4	14.5	−0.96	−0.83	−0.816 75[c]
		1.6	4.0	0.103 20	0.103 200 94	0.103 25[c]
	5.0	2.0	9.0	−2.1	−1.78	−1.705 071 380 62[b]
		400.0	0.6	2.943 549 56	2.943 595 566 4	
	7.429 336 31	4.0	7.5	−2.1	−1.78	−1.761 382[d]
1	1.0	0.4	7.5	0.142 76	0.142 765 1	0.767 76[a]
		2.0	4.0	1.417 268 1	1.417 268 101 06	1.417 268 101 06[b]
		4.0	3.0	2.020 552 12	2.020 552 122 0	
		40.0	1.5	4.989 416 52	4.989 416 525 31	4.995 666 52[a]
		400.0	0.6	11.03 308 10	11.033 081 008 438	11.033 706 01[a]
	1.6	0.4	10.0	−0.76	−0.748 66	−0.748 75[c]
		1.6	4.5	0.875 119 7	0.875 119 810 80	0.875[c]
	5.0	2.0	12.5	−1.8	−1.623	−1.625 337 681 14[b]
		400.0	0.7	10.727 236 661	10.727 236 662 01	
2	1.0	0.4	8.5	1.0099	1.0102	1.634 85[a]
		2.0	4.0	3.081 950	3.081 950 63	
		4.0	3.5	4.190 715	4.190 715 85	
		40.0	1.5	9.888 492	9.888 492 495	9.894 742 35[a]
		400.0	0.6	21.694 055	21.694 054 888	21.694 679 67[a]
38	1.0	2.0	12.0	138.160 094 732	138.160 094 731 658 5	138.160 094 733[b]
	5.0	2.0	12.5	122.183 482 2	122.183 482 182 290 4	122.183 482 182 25[e]
		400.0	2.0	827.326 346 209	827.326 346 208 819 5	
39	1.0	2.0	12.0	143.033 637 294	143.033 637 294 269 7	143.033 637 294[b]
	5.0	2.0	12.5	126.791 650 1	126.791 650 143 763 1	126.791 650 143 763[e]
		400.0	2.0	856.158 489 152	856.158 489 152 173 0	

[a]Reference [16].
[b]Reference [18].
[c]Reference [3].
[d]Reference [23].
[e]Reference [22].

TABLE III. Energy eigenvalues of few double-well oscillators with sextic anharmonicity. (O represents other values).

n	ω^2	β	K	$E(K)$	$E(P)$	$E(O)$
0	1.0	0.03	140.5	−1.7	−1.2	−1.027 124 45[a]
		0.12	64.0	−0.273	−0.258	−0.2575[b]
		0.3	39.5	−0.025	−0.022 12	−0.022 212 05[c]
		3.0	9.0	0.408	0.408 324	
		6.0	6.5	0.545	0.545 437 96	0.545 379 45[a]
		60.0	2.0	1.136	1.136 678 93	1.136 678 9[a]
		600.0	0.6	2.111	2.111 458	2.111 458 2[a]
	2.0	0.03	616.0	−1.0	−3.5±0.1	
		0.3	40.0	−0.68	−0.62	
		6.0	7.0	0.396	0.396 779	
		60.0	2.0	1.060	1.060 800 7	
		600.0	0.7	2.0690	2.069 988	
1	1.0	0.03	156.0	−0.7	−1.0122	−1.005 617 8[a]
		0.3	31.0	0.503	0.5032	0.503 152[c]
		3.0	9.5	1.7975	1.7975	
		6.0	6.5	2.2703	2.270 305	2.270 305 0[a]
		60.0	2.0	4.416	4.416 339	4.416 395 3[a]
		600.0	0.7	8.0621	8.062 15	8.062 152[a]
	2.0	0.3	46.0	−0.38	−0.411	
		6.0	6.5	1.9451	1.945 05	
		60.0	2.0	4.2427	4.242 63	
		600.0	0.7	7.9666	7.965 96	
2	1.0	3.0	11.0	4.080	4.0796	
3	1.0	3.0	12.0	6.9314	6.9322	
4	1.0	3.0	13.5	10.2521	10.251 72	
5	1.0	3.0	14.0	13.981	13.981 73	

[a]Reference [17].
[b]Reference [24].
[c]Reference [15].

TABLE IV. Comparison of the calculated energies for double-well oscillators with mixed quartic and sextic anharmonicities for different values of α and β as obtained by us and other workers.

n	ω^2	α	β	K	$E(K)$	$E(P)$	$E(O)$
0	1.0	4.0	3.0	6.0	0.638 138	0.638 138 724	
		400.0	600.0	1.0	3.296 709 6	3.296 709 679 874	
	2.0	4.0	3.0	6.0	0.500 00	0.499 999 999	0.500[a]
		−4.0	3.0	−7.0	−0.59	−0.49	−0.499 993 5[b]
	10.0	4.0	3.0	14.0	−1.70	−1.499	−1.5[a]
	14.0	4.0	3.0	14.0	−6.0	−3.6±0.2	−3.617[a]
1	1.0	4.0	3.0	6.0	2.5025	2.502 513 714 8	
		400.0	600.0	1.0	12.010 205	12.010 204 796 94	
	2.0	4.0	3.0	6.5	2.1865	2.186 500 529	2.187[a]
		−4.0	3.0	−14.0	−0.3	−0.08	−0.077 046 5[b]
	10.0	4.0	3.0	24.5	−1.4	−1.138	−1.138[a]
	14.0	4.0	3.0	25.5	−4.4	−3.55	−3.532[a]
2	1.0	4.0	3.0	6.5	5.270	5.269 587	
		400.0	600.0	1.0	24.038 20	24.038 193 464	
	2.0	4.0	3.0	7.5	4.872	4.871 82	4.872[a]
	10.0	4.0	3.0	15.0	1.74	1.7	1.672[a]
	14.0	4.0	3.0	40.5	−2.1	c	0.335[a]
3	1.0	4.0	3.0	8.5	8.61	8.606 836 50	
		400.0	600.0	1.0	38.231	38.228 363 454	
	2.0	4.0	3.0	14.0	8.13	8.130 954	8.131[a]
	10.0	4.0	3.0	25.5	4.5	4.1097	4.110[a]
	14.0	4.0	3.0	56.5	0.3	2.1	1.967[a]

[a]Reference [8].
[b]Reference [15].
[c]The Padé approximants were highly oscillatory in nature.

because $(\omega')^2$ is small for large ω^2 and small α, but large if α is also large.

(ii) For particular values of ω^2 and n, K decreases with an increase in α or β, but αK always increases. For example, in the case of a quartic double-well oscillator, K decreases from 7.5 to 0.6 as α increases from 0.4 to 400.0 for $\omega^2=1.0$ and $n=0$. However, the product αK varies from 3.0 to 240.0. Similarly, from Table IV we note that K is 6.0 for $\omega^2=1.0$, $\alpha=400.0$, and $\beta=300.0$ for $n=0$.

The variation of K with n for same ω^2 and same anharmonicity parameters shows different trends in different types of double-well oscillators. In the case of quartic anharmonicity, K does not show significant variation with n for the same ω^2 and α, though it increases for very large n. E.g., for $\omega^2=1.0$ and $\alpha=2.0$, K is 4.0 for $n=0$, 1, and 2 and becomes 12.0 for $n=39.0$. For the double-well oscillator with sextic anharmonicity, an increase in K with n for the same ω^2 and β values is a little more clear. For example, for $\omega^2=1.0$ and $\beta=3.0$, it increases from 9.0 to 14.0 when n varies from 0 to 5.0. In contrast with this, the variation in K with n for a quartic-sextic double well is not that visible.

As regards the dependence of K on the value of ω^2 for same n, α, or β, it generally increases with an increase in ω^2, though the variation is different for different types of systems. For large values of α and β, K is essentially independent of ω^2 because $(\omega')^2=-\omega^2+\lambda K\simeq\lambda K$ whether $\omega^2=1$ or 5.

(iii) In most of the cases, the Padé approximants to the energy improve upon the precision of the values, except for $\omega^2=2.0$, $\alpha=0$, and $\beta=0.03$ for $n=0$ and for $\omega^2=1.0$, $\alpha=4.0$, and $\beta=3.0$ for $n=3.0$

(iv) As regards the comparison of the present results with the findings of other workers, we note that in almost all cases the agreement is very good when $\omega^2<\alpha$ or β, but is not very encouraging for $\omega^2>\alpha$ or β. Nonetheless, the degree of precision of the results obtained makes us believe that all the present values for $\omega^2<\alpha$ or β must be correct. The agreement of E_0 for $\omega^2=1.0$, $\alpha=0.0$, and $\beta=0.12$ with the exact value reported by Chhajlany and Malnev [24] is indeed heartening. But still we cannot generalize it to comment upon the discrepancies between our results and those of others for $\omega^2>\beta$ or α. It may also be mentioned that the degree of accuracy obtained by the present technique does not seem to depend upon the parity of the state. This is in contrast with the conclusion drawn by Hodgson and Varshni [22], for a quartic double-well oscillator, in which case the present technique has yielded larger but the same number of stable digit for E_{38} and E_{39} listed in Table II.

(v) Since the renormalized hypervirial Padé approach has not worked well for the case of deep wells (large ω^2), we have not obtained nearly degenerate energy states, a special feature of the DWAO's. The dependence of E_n on α or β (increase with anharmonicity) and on ω^2 (decrease with increase in ω^2) is as expected.

To conclude, we observe that the renormalized hypervirial Padé method in which K is treated as a variational parameter is quite successful in giving the accurate energy values for double-well oscillators with quartic, sextic, and mixed quartic-sextic anharmonicities provided $\omega^2<\alpha,\beta$.

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