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Hypervirial perturbation calculations for a spiked oscillator

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Abstract : The renormalized hypervirial perturbation method is used to compute the energy levels for a spiked harmonic oscillator $V(x) = x^2 + \lambda / x^{\alpha}$, where α is a real positive parameter Results are produced for a wide range of parameters α , ($10 \leq \lambda \leq 10^6$) and of state numbers. Numerical results are compared for the special cases α = 1, 5/2

Keywords : Hypervirial perturbation theory, spiked oscillator, energy level calculation

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1. Introduction

The study of the spiked harmonic oscillator (SHO) has evoked much interest because of its varied applications in chemical physics, nuclear physics and particles physics [1–6]. The literature available on the spiked harmonic oscillator is rather limited, when compared with that for the anharmonic oscillator of the type

$$H = -\frac{d^2}{dx^2} + x^2 + \lambda x^{2N} \quad N = 2, 3 \ldots\ldots . \tag{1}$$

The spiked harmonic oscillator system is defined by the quantum Hamiltonian

$$H = -\frac{d^2}{dx^2} + x^2 + \lambda x^{-\alpha} \tag{2}$$

defined in the one-dimensional half space [0, ∞], the eigenfunctions obeying Dirichlet boundary conditions [7, 8]. The Hamiltonian is characterized by means of two parameters,

λ which plays the role of a coupling constant, and $\alpha \geq 0$ which controls the type of singularity of the potential at the origin [9].

The Hamiltonian given by eq. (2) has been the subject of intensive study in the last two decades. In the literature, a variety of techniques have been used to investigate the eigenvalues and other properties of the SHO. Nearly all previous calculations have been limited to a few excited states; for instance Detwiler and Klauder [1] made variational studies of the ground state of the spiked harmonic oscillator and found upper bounds for the eigenvalue corrections which are proportional to $\lambda \ln \lambda$ when $\alpha = 3$, and proportional to $\lambda^{1/(\alpha-2)}$ when $\alpha > 3$. Afterwards, Harrell [2] developed a special perturbation theory called singular perturbation theory, and obtained the first terms of the small λ expansion, which turned out to be a nonpower series expansion. Aguilera-Navarro *et al* [7] have applied a variational procedure and a large coupling perturbative calculation for the ground state energy. A perturbative study was carried out by the workers [8] in the two extremes of weak and strong coupling. Employing the Rayleigh-Ritz large-order perturbative expansions, Aguilera-Navarro *et al* [9] have been able to analyze the problem around the three regions $\lambda \to \infty$, $\lambda \to 0$, $\lambda \to -\infty$, for the ground state of the nonsingular spiked harmonic oscillator, for the case $\alpha = 1$. More recently Miller [10] has applied a nonperturbative algorithm (iterative technique) for obtaining the eigenvalue for (SHO). Estévez-Bretón and Estévez-Bretón [11] have derived an exact analytical ground state solution valid for the special case $\alpha = 2$.

In different context, the Hamiltonian given by eq. (2) has been investigated by Killingbeck [12] who used numerical algorithms to integrate the Schrödinger equation, based on finite differences to compute the ground state energy for small values of λ, for two values of $\alpha = 4, 6$. Also Korsch and Laurent [13] used the Milne method to find the energy for the case $\alpha = 4, 6$.

In the present work, we wish to point out that the hypervirial perturbation theory is used to study and calculate energy eigenvalues of the spiked oscillator for small and large values of λ, for a wide range of values of α.

Our calculation deal with several values of α, since the method used makes this extension easy to perform. Our main object is to demonstrate that the hypervirial approach is able to work and produce results even for large values of λ, α and the state number n. For purposes of clarity, this paper is divided into three sections. Section 2 gives the theory, Section 3 describes the formalism of the renormalized series method, and Section 4 gives the numerical results and their discussion.

2. Theory

To calculate energy eigenvalues for the (SHO), we considered the Schrödinger equation

$$\left[\frac{d^2}{dx} + x^2 + \lambda x^{-\alpha}\right] \psi(x) = E\psi(x). \tag{3}$$

The shape of the interaction potential for large values of λ is very different from the shape in the case of small λ values. Instead of having just a spike very close to the origin, the potential for large λ resembles a wide valley extending from $x = 0$ to $x = \infty$ with a minimum in the middle.

For the special case $\alpha = 2$, the Schrödinger eqation (3) may be solved exactly [14],

$$E^{\alpha=2}(\lambda) = 2n + 3 + 2l \tag{4}$$

where $$\lambda = l(l+1). \tag{5}$$

If we insert $l = \dfrac{\sqrt{1+4\lambda} - 1}{2}$ in eq. (4), we get the following form for the energy.

$$E_n^{\alpha=2} = 2 + 4n + 2\sqrt{\lambda}$$

$$\left[1 + \frac{1}{8\lambda} - \frac{}{\overline{128\lambda^2}} + \frac{}{\overline{1024\lambda^3}} - \frac{}{\overline{32768\lambda^4}} + \frac{}{\overline{262144\lambda^5}} - \frac{21}{4194304\lambda^6} + \ldots\right] \quad \lambda > \frac{1}{4}. \tag{6}$$

In the absence of other reported results, we have devised some internal checks on the reliability of our results; for example the closed forms above for the energy provide checks on our calculations for the case $\alpha = 2$.

Reviews of various numerical perturbative and non-perturbative calculations for the (SHO) can be found in references [7-9] which suggested use of variational and perturbative methods for the (SHO) by expanding the potential about its minimum to calculate the energy eigenvalues. Here we treat more general (SHO) problems, by considering higher power indices (α = 3/2, 5/2, 7/2 .....), higher values of the state number n and higher λ values ($5 \leq \lambda \leq 10^6$). We expand $V(x)$ around its minimum. Let x_m and $V(x_m)$ be the values of x and $V(x)$, respectively, at the minimum.

Let $y = x - x_m$; the expansion of $V(x)$ around $y = 0$ can be written as a Taylor series.

$$V(y) = V(x_m) + (\alpha+2)y^2 + \sum_{I=3}^{20} (-1)^I \frac{2}{\alpha}(\alpha)_I \beta^{I-2} \frac{y^I}{I!}, \tag{7}$$

where $(\alpha)_I$ is the Pochhammer symbol and

$$\beta = \frac{1}{x_-}. \tag{8}$$

The coefficients given by eq. (7) alternate in sign; the coefficients take (+ sign) for even I values, and (– sign) for odd I values. We have expanded the potential as given by eq. (7) to the limit in which any term beyond that limit makes no difference to our results. For our calculations, this limit was reached for (I = 20).

The central idea of this work is to expand the potential $V(x)$ in a Taylor series about its minimum value, and solve the resulting perturbed oscillator problem by hypervirial perturbation theory. The potential is expanded around the right-hand minimum, while the new coordinate $y = x - x_m$ covers the full real axis. When λ is large, the potential minimum occurs at a large value of x, so that the wave function centered at x_m does not penetrate far into the left-hand potential peaks; obviously this is not the case for small λ. The highest power of y appearing in the potential is 20. The expanded potential $V(y)$ of eq. (7) is of mixed parity type. It is clear from eq. (7) that we can regard the first two terms as the unperturbed terms and the other terms as the perturbation.

3. Formulation of the problem

The hamiltonian for the potential described by eq. (2) is

$$H = -\frac{d^2}{dy^2} + V(y). \tag{9}$$

Here we use units $\hbar = m = 1$. The potential $V(y)$ given by (7) can be rewritten in terms of the perturbation parameter $\underline{\lambda}$ as

$$V(y) = \sum_{I=0}^{20} \underline{\lambda} V(I)\, y^I \quad \underline{\lambda} = 1 \tag{10}$$

with the coefficients given by eq. (7). The sum $\sum_{I=0}^{20} (-1)^I \frac{2}{\alpha}(\alpha)_I \frac{\beta^I}{I!}$ is replaced by $\underline{\lambda} V(I)$. Starting from the hamiltonian given by eq. (9) and using the basic relations for commutators

$$\left[\frac{d}{dy}, H\right] = \frac{dV}{dy}, \tag{11}$$

$$\left[y^N, H\right] = \frac{N}{2}(N-1)y^{N-2} + N y^{N-1} \frac{d}{dy}, \tag{12}$$

$$\left[y^N \frac{d}{dy}, H\right] = y^N \frac{dV}{dy} + \frac{N}{2}(N-1)y^{N-2}\frac{d}{dy} + 2Ny^{N-1}(V-H), \tag{13}$$

the diagonal hypervirial requirement that $< \left| y^N \frac{d}{dy}, H \right] >$ shall vanish for the eigenstates of eq. (7) lead to the result.

$$2E(N+1)\left\langle y^N \right\rangle = \sum_{I=0}^{20} \underline{\lambda} V(I)\ (2N+2+I)\ \left\langle y^{N+1} \right\rangle - \frac{N}{4}(N^2-1)\left\langle y^{N-2} \right\rangle \tag{14}$$

The Hellmann-Feynman theorem provides a further relationships between the energy E and the expectation values $\langle y^N \rangle$. Let us assume that the energy E and expectation values $\langle y^N \rangle$ can be expanded in power series of the perturbation parameter λ as

$$E = \sum E(J)\, \underline{\lambda}^J, \tag{15}$$

$$\langle y^N \rangle = \sum R(N, M) \underline{\lambda}^M. \tag{16}$$

In order to improve the convergence properties of the perturbation series, we use a rearrangement of terms in the potential given by (7). To illustrate this technique, it is necessary to write the potential appearing in eq. (7) in renormalized form

$$V(y) = V(x_m) + [\mu - \lambda K]\, y^2 + \underline{\lambda} \sum_{I=3}^{20} V(I) y^I, \tag{17}$$

where μ is given the numerical value

$$\mu = (\alpha + 2) + \underline{\lambda} K\,. \tag{18}$$

The use of the renormalization parameter K is helpful in improving convergence. If we use the perturbation expansions (15) and (16) in the hypervirial relation given by eq. (14), we obtain the recurrence relation

$$(2N+2) \sum_{o}^{M} E(J) R(N, M-J) = -\frac{N}{2}\left[N^2 - 1\right] R(N-2,\, M) - (2N+4)$$

$$[\mu R(N+2, M) - KR(N+2,\, M-1)] + \sum_{I=3}^{20} V(I)\,(2N+2+I)$$

$$R(N+I, M-1). \tag{19}$$

Applying the Hellmann-Feynman theorem in the form

$$\frac{\partial E}{\partial \underline{\lambda}} = \left\langle \frac{\partial H}{\partial \underline{\lambda}} \right\rangle = \left\langle \frac{\partial V}{\partial \underline{\lambda}} \right\rangle, \tag{20}$$

we obtain a recurrence relation for the energy coefficients of the form

$$(M+1)\, E\,(M+1) = \sum_{I=3}^{20} V(I)\, R(1, M) - KR(2, M). \tag{21}$$

The unperturbed energy corresponding to the SHO can be expressed as

$$E(0) = V\,(x_m) + (2n+1)\sqrt{\mu} \quad (n = 0,\ 1,\ 2,\ \ldots\ldots). \tag{22}$$

The zero-order contribution to E is given by the first term in eq. (22) and next contribution comes from the harmonic oscillator term, the second term in (22). The SHO series have

even and odd powers of the perturbation parameter $\underline{\lambda}$. The actual series for the energy has the form

$$E(K) = E(0) + \underline{\lambda}E(1) + \underline{\lambda}^2E(2) + \underline{\lambda}^3E(3) + \underline{\lambda}^4E(4) \tag{23}$$

From the recurrence relations (19) and (21) together with the unperturbed energy (22) and the initial coefficient value $R(0, 0) = 1$, we can calculate sequentially the perturbation series for the $\langle y^N \rangle$ and the energy.

4. Results and Discussion

The renormalized series method has been used for calculating the eigenvalues of the (SHO) given by eq. (2). Eigenvalues for different values of λ, α and state number n are listed in Tables (1–4).

Table 1. Ground state energy eigenvalues of the spiked harmonic oscillator for $\alpha = 1, 5/2$. For comparison, the second lines in the first and second columns display the energies corresponding to Refs. 9 and 8, respectively. The empty spaces mean that the corresponding eigenvalues are not be reported.

λ	$E_{\alpha=1}$	M	K	$E_{\alpha=5/2}$	M	K
0.5	3.3	8	14	3.6	10	27
				3.848553		
1	4.1	9	15	4.3	8	26
	4.057906			4.317311		
2	4.94	10	14	4.9	12	22
3	5.86	9	12	5.53	15	21.5
4	6.63	11	8	5.92	14	19
5	7.377	11	10	6.295	18	20
	7.384031741			6.296472		
8	9.377	14	10	7.222	16	17.5
10	10.577	10	8	7.735	18	15
	10.57748343			7.735111		
25	17.9283	15	8	10.4886	17	10
50	27.40514	15	5	13.4724	16	8.2
75	35.360350	14	3	15.6989	13	7
100	42.46291809	12	1	17.541989	16	5.4
				17.541889		
150	55.09654352325	13	1	20.575833	17	4
200	66.37422526412	19	1	23.086306	17	3.5
300	88.43224389401	17	1	27.2179594	33	8
400	104.33633594703	18	8	30.63609298	38	8
500	120.79206109643	17	1	33.605710885	46	10
750	157.74209512062	18	1	39.8172869302	68	12
1000	190.72330743978	16	1	44.9554847996	52	8
				44.955485		

In Table 1 numerical results are compared for two special cases $\alpha = 1,\ 5/2$ for the ground state energy eigenvalues for several values of λ, $(0.5 \leq \lambda \leq 10^3)$. It is clear from the Table 1 that there is some agreement between our results and the previous published results [7,9].

Table 2. The energy for the ground and excited states of the spiked oscillator for four values of α, over a wide range values of λ. The empty spaces mean that the corresponding eigenvalues cannot be calculated by our technique.

n	λ	$\alpha = 1/2$	$\alpha = 3/2$	$\alpha = 5/2$	$\alpha = 7/2$
0	5	7.93	6.96	6.29	6.1
	10	12.19	9.37	7.74	7.2
	100	67.25660691	29.3971	17.5422	12.67
	1000	415.88978565801	104.410223884	44.9554847996	26.108849
	5000	1502.98720233231	259.0784470059	89.69174923454	44.9890390239
	10^4	2165.68031939241	384.07821353971	121.282856042479	57.20834699402
	10^5	16495.4300708630	1426.57990603771	333.685605689407	129.071238218737
	10^6	104070.732071571	5312.60615971726	924.715125454449	295.092262512018
1	5	11.2	10.7	10.5	10.5
	10	15.52	13.13	11.9	11.4
	100	70.447816	33.156557	21.764	17.31
	1000	419.056597675	108.15657318	49.1863749	30.7322
	5000	1506.15072948168	262.8219865100	93.928518942	49.64028525
	10^4	2618.84331453422	387.82113922046	125.5211584788	61.867940951
	10^5	16498.59246220739	1430.32190436784	337.92667180376	133.74797411045
	10^6	104073.8943672486	5316.34790861919	928.957198239358	299.776690735924
2	5				
	10	19.2	17.2	16.2	15.6
	100	73.666548	36.936	26.06	22.5
	1000	422.22790766514	119.0743425	53.40675614	35.30463
	5000	1509.31550336201	266.567378827	98.159734395	54.257196
	10^4	2622.00702624843	391.56531985602	129.75529689958	66.49974191
	10^5	16501.7549672131	1434.06424267388	342.166186613224	138.411643985016
	10^6	104077.056680942	5320.08974896653	933.198706164038	304.455250571815
3	5				
	10				
	100	76.92	40.74	30.14	26.4
	1000	425.4038	115.663	57.621	39.84
	5000	1512.48152	270.31461	102.38567	58.8437
	10^4	2625.171454072	395.31074436	133.985422	71.10623
	10^5	16504.91758586865	1437.80692014302	346.404170972921	143.06279166
	10^6	104080.21901265201	5323.83168070048	937.439651994369	309.128051709891
4	5				
	10				
	100	80.19	44.52	34.29	31.3
	1000	428.584	119.425	61.83	44.34
	5000	1515.6488	274.0637	106.6066	63.4037
	10^4	2628.336598	399.05741	138.21168	75.6896
	10^5	16508.08031816236	1441.54993596524	350.64064531398	147.70192735
	10^6	104083.38136237757	5327.57370376231	941.68003847566	313.7952007643

Table 2. *(Cont'd).*

n	λ	α = 1/2	α = 3/2	α = 5/2	α = 7/2
5	5				
	10				
	100	83.5	48.4	38.7	35.6
	1000	431.768636674	123.185569	66.0191	49.16
	5000	1518.81729130003	277.8144331	110.822637	67.94402
	10^4	2631.50245619404	402.80528129976	142.4341902319	80.252022
	10^5	16511.2431640827	1445.29328933321	354.875629655027	152.3295303566
	10^6	104086.5437301188	5331.31581809333	945.919868332854	318.456801386269

Table 3. The energy for the ground and excited states of the spiked oscillator for four values of α, over a wide range values of λ. The empty spaces mean that the corresponding eigenvalues cannot be calculated by our technique.

α	λ	E_0	E_1	E_2	E_3
3	10	7.249	11.63	16.4	22.3
	100	14.6414	19.045	23.382	28.69
	500	25.7990039	30.22795	34.6252	39.024
	1000	33.31676152	37.7554906	42.166094	46.5542
4	10	6.64	11.52	16.2	22.4
	100	11.276	16.11	21.58	24.9
	500	17.4764	22.2455	26.98	31.97
	1000	21.369519	26.15539	30.886	35.651
5	10	6.29	11.4	15.9	21.6
	100	9.469	15.09	21.1	28.4
	500	13.422	18.54	23.92	29.82
	1000	15.7647	20.834	26.017	31.523
6	10	5.9			
	100	8.46	14.4	21.1	28.9
	500	11.151	16.94	23.31	27.3
	1000	12.724	18.19	24.21	30.81

In Tables 2 and 3, we have calculated the energy eigenvalues for the ground state and many excited states for several values of α ($\frac{1}{2} \leq \alpha \leq 6$) over a wide range values of λ ($5 \leq \lambda \leq 10^6$). The most studied (SHO) is $\alpha = 5/2$ for ground state only [7,10]. Our calculations deal with several values of α and many excited states, since the method used makes this extension easy to perform.

Currently there are no other eigenvalue-results available by any other method for the cases such as $\lambda = 500$, 1000 and $\alpha = 7/2$; consequently, it is not possible to infer the accuracy of the full set of our present results by direct comparison. However, for some special cases, it is possible to check our calculations; for example at $\alpha = 2$, the results were checked to high accuracy against those obtained by exact solution (6). Table 4 presents a selected set of energies for several sets of the perturbation parameter λ ($10 \leq \lambda \leq 10^3$) for four energy levels E_0, E_1, E_2, E_3. The agreement between the numerical and exact results is seen to

be good. Especially for larger values of λ, the difference between the numerical and exact results decreases *i.e.*

$$|E_{\text{numerical}} - E_{\text{exact}}| \cong 0 \tag{24}$$

as is clear from the listed results in Table 4.

Table 4. The comparison of the renormalized series numerical calculation with exact calculation from eq. (6). The values of the renormalization parameter K are given. M is the order of the perturbation expansion with which we obtain convergence.

n	λ	$E_{\text{numerical}}$	M	K	E_{exact}	$\lvert E_{\text{num}} - E_{\text{exa}} \rvert$
0	10	8.49	10	18	8.4031242374	0.8687576260D–01
	50	16.1780	30	24	16.1774468788	0.5531212000D–03
	100	22.0249	45	18	22.0249843945	0.8439450000D–04
	250	33.63858441	64	16	33.6385840391	0.3708999969D–06
	500	46.732538504	60	15	46.7325384927	0.1129999561D–07
	1000	65.2534584038	58	12	65.2534584035	0.2999911430D–09
1	10	12.8	8	20	12.4031242374	0.4800879714D+00
	50	20.197	26	15	20.1774468788	0.1968397121D–01
	100	26.0261	20	10	26.0249843945	0.1117575728D–02
	250	36.6386001	23	7	37.6385840391	0.1725318712D–04
	500	50.732538925	37	6	50.7325384927	0.4325225801D–06
	1000	69.2534584155	34	5	69.2534584035	0.1215288137D–07
2	10	17.2	9	40	16.4031242374	0.7968757626D+00
	50	24.18	16	12	24.1774468788	0.5761214444D–01
	100	30.0254	19	20	30.0249843945	0.1141560550D–01
	250	41.63888	54	11	41.6385840391	0.2959609000D–03
	500	54.732546486	54	12	54.7325384927	0.7993299995D–05
	1000	73.253458612	54	10	73.2534584035	0.2084999977D–06
3	10	21.2	10	20	20.4031242374	0.8544475337D+00
	50	28.19	16	15	24.1774468788	0.2064556248D–01
	100	34.08	15	20	34.0249843945	0.5501560550D–01
	250	45.6411	33	18	45.6385840391	0.2515960900D–02
	500	58.732629	55	14	58.7325384927	0.9050730000D–04
	1000	77.2534608	50	10	77.2534584035	0.2396499994D–05

Our results for the spiked harmonic oscillator have the following consequences :

First the renormalized series method works very well even for higher values of λ, α and state number n.

Second, the renormalized series converges well (with a proper value of K) for high values of λ, but not for low values of λ. Our work indicates the great importance of a good choice of the renormalization parameter K in order to get the best convergence. To select the correct convergence energy, we require stability against the various values of renormalization

parameter K. The general consideration that governs our choice is that as λ increases the values of K decreases.

Third, our numerical investigations of the spiked oscillator show that applicability of the renormalized series method is limited to large values of λ; this behavior is clear from our results in Tables 1–4. When applicable, the renormalized series approach has been shown to be very effective and more simple than standard matrix diagonalization, which would require the computation of standard matrix elements of the various powers of x^N. The hypervirial method gives the $\langle y^N \rangle$ and E values for a selected state directly.

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