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Self-interacting one-dimensional oscillators

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Abstract. Energy eigenvalues and $\langle x^2 \rangle_n$ for the oscillators having potential energy $V(x) = (\omega^2 x^2/2) + \lambda < x^{2r} > x^{2s}$ have been determined for various values of λ, r, s and n using renormalized hypervirial–Padé scheme. In general, the results show an improvement over the findings of earlier workers. Variation of the evaluated quantities and of the renormalization parameter with λ, r, s and n has been discussed. In addition, this potential has been employed as an illustrative example of the applicability of alternative formalism of perturbation theory developed by Kim and Sukhatme (*J. Phys.* **A25** 647 (1992)).

Keywords. Self-interacting oscillators; energy eigenvalues; perturbation theory.

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1. Introduction

There are a number of important and interesting situations in physical and biological studies where the interaction between the system and its surroundings influence not only the former but also the latter. This results in the modification of environmental field so that the interaction potential acting on the system also depends upon its own state ψ_n and is, therefore, written as $V(\psi_n)$. Accordingly, the time-independent Schrödinger equation for the system becomes non-linear and reads [1–3];

$$H(\psi_n)\psi_n = [H_0 + V(\psi_n)]\psi_n = E_n\psi_n \tag{1}$$

with H_0 as the Hamiltonian for the isolated system. A typical example of such a self-dependent system is one-dimensional oscillator described by the Hamiltonian ($\hbar = m = 1$)

$$H = -(1/2)(\mathrm{d}^2/\mathrm{d}x^2) + (\omega^2 x^2/2) + \lambda \langle x^{2r} \rangle x^{2s}, \tag{2}$$

where both r and s are integers. Obviously, when $r = s = 1$, (2) becomes Hamiltonian of a self-interacting harmonic oscillator whose force constant is linearly dependent on the mean square of displacement of vibration, and $r \geqslant 1$, $s \geqslant 2$ correspond to the self-interacting anharmonic oscillators whose anharmonicity depends on $\langle x^{2r} \rangle$. Also for $\omega = 0$, $r \geqslant 1$, $s \geqslant 2$ we have the self-dependent oscillators with extremely large magnitudes of anharmonicity – the so-called infinite-field limit of the oscillators. Furthermore, for $r = 0$ and $s = 2$ or 3 we get the special cases of well-studied quartic or sextic anharmonic (when $\omega \neq 0$) and pure quartic or sextic ($\omega = 0$) oscillators.

Since (1) cannot be solved exactly, some iteration and approximation methods have been used to determine the energy eigenvalues. An adaptation of Rayleigh–Schrödinger

perturbation theory (RSPT) has been put forward for this purpose and applied to the problem of a molecule in a polarizable medium [1,3,4]. Surján [3] also pointed out limitations of iterative method, configuration interaction approach and variational technique for solving the time-independent non-linear Schrödinger equation. However, since perturbation theory suffers from the uncertainty about its convergence, particularly for large perturbations, Cioslowski [5] employed an extension of connected moments expansion to obtain the solution for (1) and illustrated it by finding the values of energy and mean square displacements of vibration $\langle x^2 \rangle$ for the ground state ($n = 0$) of self-interacting harmonic oscillator for different magnitudes of λ. Vrscay [2] analyzed the perturbation expansion for (2) using hypervirial and Hellmann–Feynman theorems and performed numerical calculations to determine lower and upper bounds to energy for different values of r and $s = 2$ corresponding to $\omega = 0$ as well as $\omega \neq 0$ employing a renormalized RSPT wherein summation was carried out by the Padé approximants method.

Killingbeck [6–8] presented a variational parameter-based renormalized hypervirial Padé scheme (RHPS) that yields very accurate energy eigenvalues (and also $\langle x^2 \rangle$ values) in a simple manner for anharmonic oscillators. We examined the extent to which this technique is successful in finding the energies and the expectation values of x^2 for self-interacting harmonic and anharmonic oscillators and this communication is an outcome of the effort for a wide range of values of r, s, λ and n. We shall discuss in the sequel the dependence of energy, $\langle x^2 \rangle$ and the variational parameter on various quantities.

It is pertinent to mention that Kim and Sukhatme [9] have developed an alternative formalism for Rayleigh–Schrödinger perturbation theory (ARSPT) for a one-dimensional problem described by linear Schrödinger equation. Being an expansion in the powers of perturbation parameter, this leads to the same results as RSPT but without requiring cumbrous sums over intermediate eigenstates and also reduces to the logarithmic perturbation theory of Au and Aharonov [10]. We have also obtained expression for energy of the self-interacting oscillators in the framework of this approach and compared the results with the findings of RHPS.

2. Renormalized hypervirial-Padé calculations

2.1 *Theoretical framework*

Following Killingbeck's [6–8] prescription, the Hamiltonian (2) is renormalized by adding and subtracting $(\lambda K x^2/2)$ so that denoting $(\omega^2 + \lambda K)^{1/2}$ by ω', we get

$$H = (-1/2)(\mathrm{d}^2/\mathrm{d}x^2) + (\omega'^2 x^2/2) + \lambda \langle x^{2r} \rangle x^{2s} - (\lambda K x^2/2). \tag{3}$$

Using the hypervirial theorem together with the relevant commutation relations, expanding E_n and $\langle x^N \rangle_n$ as

$$E_n = \sum_{j=0}^{\infty} E_n^{(j)} \lambda^j, \tag{4}$$

$$\langle x^N \rangle_n = \sum_{k=0}^{\alpha_s} C_k^{(N)} \lambda^k, \tag{5}$$

and equating coefficients of the same powers of λ on the two sides of the resulting equation, we obtain the recurrence relation

$$C_p^{(N+2)} = [(2(N+1))/((N+2)\omega'^2)] \sum_{j=0}^{p} E_n^{(j)} C_{p-j}^{(N)} + (K/\omega'^2) C_{p-1}^{(N+2)}$$
$$- [((2(N+s+1))/((N+2)\omega'^2)] \sum_{k=0}^{p-1} C_{p-k-1}^{(2r)} C_k^{(N+2s)}$$
$$+ [(N-1)N(N+1)/4(N+2)\omega'^2] C_p^{(N-2)}. \tag{6}$$

Here

$$C_p^{(0)} = \delta_{0p} \tag{7}$$

and

$$E_n^{(0)} = (n+1/2)\omega'. \tag{8}$$

The $E_n^{(j)}$ for $j \geqslant 1$ are related with $C_p^{(N)}$ by using the Hellmann–Feynman theorem and this gives us

$$E_n^{(j)} = (1/j)\left[(-K/2)C_{j-1}^{(2)} + \sum_{k=0}^{j-1} (k+1) C_k^{(2r)} C_{j-k-1}^{(2s)}\right]. \tag{9}$$

Equations (8) and (9) when substituted in (4) give E_n in terms of K and $C_j^{(N)}$ and the latter are determined from (6) in a hierarchial manner. Similarly, substitution of (6) in (5) with $N = 2$ leads to the formula for evaluation of $\langle x^2 \rangle_n$. It may be pointed out that the product terms $C_{p-k-1}^{(2r)} C_k^{(N+2s)}$ in (6) and $C_k^{(2r)} C_{j-k-1}^{(2s)}$ in (9) allow the calculation to treat the term $\lambda \langle x^{2r} \rangle x^{2s}$ in (3) directly, without any need for iteration of any kind.

2.2 *Numerical results and discussion*

In order to execute the computations the parameter K is determined in such a way that maximum number of stable digits in the value is obtained from the final expression for E_n for a particular state. Also it is found that

$$C_P^{(2M+1)} = 0 \tag{10}$$

for $p, M = 0, 1, 2, 3, \cdots$, which is a consequence of even power terms in the potential. The computations for energy as well as $\langle x^2 \rangle_n$ have been executed with double precision and by terminating the series summation in (4) at $j = 32$; though in some cases, particularly those for which λ is large, summation had to be extended up to $j = 52$ (or even 80) to obtain proper convergence. However, in all cases the values being reported correspond to a situation for which the maximum number of digits was stable. The energy values so determined (E_n) and those improved upon by finding Padé approximants, $E_n(P)$, to the series expansion with chosen K parameters are listed in tables 1–3 for different values of r, s, n, ω and λ. Also projected in these tables are the relevant $\langle x^2 \rangle_n$ obtained by performing sum in (5) by the Padé approximants. With a view to compare our results with those of other workers, their values have also been included in these tables. It may be mentioned that the entries in the tables have been kept up to such an unrealistic number of significant figures just to emphasize the degree to which results of the present calculations can be trusted.

Table 1. A comparison of the energy and $\langle x^2 \rangle_0$ values for the ground state of the oscillator described by $H = (-1/2)(d^2/dx^2) + (\omega^2 x^2/2) + \lambda \langle x^2 \rangle x^2$ for $\omega = 1$ and different values of λ, in units corresponding to $\hbar = m = 1$ with the findings $E_0(C)$ and $\langle x^2 \rangle_0(C)$ of Cioslowski [5].

λ	K	E_0	$E_0(P)$	$E_0(C)$	$\langle x^2 \rangle_0$	$\langle x^2 \rangle_0(C)$
0·01	0·0	0·5024814959720006	0·5024814959720006	0·502482	0·4975307588519251	0·497531
0·05	0·0	0·5120601501075252	0·5120601501075252	0·512060	0·4882238931256487	0·488224
0·10	0·0	0·5233402659023011	0·5233402659023011	0·523340	0·4777006782938250	0·477701
0·50	0·5	0·5957439419765593	0·5957439419765594	0·595744	0·4196433776070806	0·419643
1·0	0·5	0·6623589786223730	0·6623589786223730	0·662359	0·3774388331233464	0·377439
100·0	0·5	2·3564	2·356698839		0·10608058858	
1000·0	0·5	5·02	5·016638		0·04983388	
10000·0	0·5	10·44	10·7737		0·0232058	

Table 2. Calculated energy eigenvalues and $\langle x^2 \rangle$ for the ground state of the self-interacting anharmonic oscillators (2) with $\omega = 1$, $s = 2$ and different values of r and λ. $E_0(V)$ are the results from Vrscay [2] where the actual entries are the lower bounds and the upper bounds are obtained by using k digits in parenthesis in place of the k digits in the lower bounds.

r	λ	K	E_0	$E_0(P)$	$E_0(V)$	$\langle x^2 \rangle_0$
0·0	0·1	5·5	0·559146327183519	0·5591463271835196	0·559146327183519(21)	0·4125253683836503
	0·5	3·5	0·696175820764	0·696175820765145	0·696175816(25)	0·3058136507175871
	1·0	3·0	0·8037706513	0·80377065123426	0·8037705(7)	0·2571498214428097
	5·0	1·5	1·224587036	1·2245870360590	1·224578(94)	0·1614549608918456
	10·0	1·5	1·50497240777	1·504972407778891	1·50495(9)	0·1300220425511937
	100·0	0·5	3·1313842	3·13138416493688	3·13126(47)	0·061562164077664
	1000·0	0·5	6·69422085	6·694220850504031	6·6939(44)	0·02869929544012135
	10000·0	0·5	14·39770	14·397995343518	14·397(8)	0·01333357844469

1·0	0·1	2·0	0·5297174305616420	0·5297174305616415	0·529717430561641	0·4499704234328627
	0·5	1·0	0·597374410	0·597374410316	0·5973744110315(6)	0·3743483196796829
	1·0	1·0	0·6490584853	0·64905848544106 3	0·64905848 54(5)	0·3344821496075 80
	5·0	0·5	0·8415397	0·8415396038 4427	0·8415395 9(61)	0·2438211434 48
	10·0	0·5	0·96303	0·96303104203	0·9630310 0(6)	0·2094291392
	100·0	0·5	1·597	1·599640	1·599659 0(6)	0·12205
	1000·0	0·5	2·707	2·707	2·780180(82)	0·069494
	10000·0	0·5	6·0	4·639	4·907511(5)	0·0450
2·0	0·1	2·0	0·5363246515445	0·5363246515444485	0·5363246515444448(9)	0·4407528022802836
	0·5	1·0	0·600620224	0·6006198960748 95	0·6006198959(61)	0·3715050862911 12
	1·0	1·0	0·6444	0·6443961975632	0·644396 19(20)	0·3376646000 42
	5·0	1·0	0·79	0·792923	0·792897 0(5)	0·261287
	10·0	1·0	0·899	0·880389	0·880525(7)	0·23173
	100·0	1·0	1·222	1·2670	1·30394(5)	0·160
	1000·0	0·5	2·0	1·795	2·00811(4)	0·1051
	10000·0	0·5	5·7	2·747	3·14556(62)	0·07914
3·0	0·1	2·5	0·556719	0·55671875183	0·5567187 5180(6)	0·4152979506405128
	0·5	2·5	0·62	0·6272901429	0·6272896(905)	0·3499805931
	1·0	2·5	0·64	0·67021397	0·670209(17)	0·32087514
	5·0	2·5	0·851	0·8028	0·8042(4)	0·2576
	10·0	1·5	0·94	0·876	0·8788(91)	0·23244
	100·0	1·5	1·094	1·0432	1·2164(78)	0·1795
	1000·0	1·5	2·5	1·4308	1·7346(77)	0·104
	10000·0	1·5	7·7	2·3	2·511(7)	0·0562

Table 3. Energies and $\langle x^2 \rangle_n$ values for the $\omega = 0, \lambda = 1$ oscillators for different r, s, and n. $E_n(V)$ are the lower bounds of energy reported by Vrscay [2] wherein replacement of last k digits in the entries by the k digits in the parenthesis gives the upper bound.

s	r	n	K	E_n	$E_n(P)$	$E_n(V)$	$\langle x^2 \rangle_n$
2·0	0·0	0	3·0	0·667986259	0·66798625915577	0·66795(801) 0·667986*	0·28733756676175
		1	3·0	2·3936440163	2·393644016483	2·39347(84) 2·393644*	0·715605073742
		2	3·0	4·69679538	4·69679538694	4·6961(76) 4·696795*	0·987930252944
	1·0	0	1·0	0·48906	0·4890639276	0·4890636(40)	0·3924590130
		1	1·5	2·201	2·201546766	2·2009(28)	0·7780456130804
		2	2·5	4·682	4·68255850243	4·67(71)	0·99093396317
	2·0	0	1·0	0·50	0·494648	0·49464(5)	0·38802808008
		1	1·5	2·3	2·28795366	2·27(31)	0·74866193012
		2	2·0	5·1	5·1373329972	4·9(5·7)	0·90321305788
3·0	0·0	0	7·5	0·68041	0·680703		0·258929
		1	8·5	2·5800	2·57972		0·603946
		2	9·5	5·394	5·3943		0·7601
	1·0	0	3·0	0·518	0·5196		0·3392
		1	3·5	2·32	2·333		0·6678
		2	4·5	5·1	5·112		0·804
	2·0	0	1·5	0·51	0·508		0·347
		1	2·5	2·3	2·341		0·667
		2	3·0	5·0	5·340		0·768

*Energy eigenvalues of other workers reported by Vrscay.

Perusing through the computational data displayed in the three tables, we arrive at the following conclusions:

(1) In self-interacting oscillators and the infinite-field limit oscillators (tables 1 and 3) wherever comparison with the findings of other workers is possible, our results for $E_n(P)$ as well as $\langle x^2 \rangle_n$ are more accurate. This prompts us to infer that other values found by RHPS are also quite reliable for these categories of oscillators. As far as self-interacting anharmonic oscillators with $s = 2$ (table 2) are concerned, $E_0(P)$ are an improvement over the results of Vrscay for $r = 1{\cdot}0$ for λ up to 10·0 and for $r = 2{\cdot}0, 3{\cdot}0$ for λ up to 1·0, in addition to being so for $r = 0$ for all λ. However, in all other cases, the convergence of $E_0(P)$ is worse than the two bounds of energy reported by Vrscay. Furthermore, such a comparison is not possible for $\langle x^2 \rangle_0$ as these values have not been determined by Vrscay. Nonetheless, the extent to which these sums are convergent, they too must be correct.

(2) For self-interacting oscillators, the renormalization parameter K is zero for λ up to 0·1 and 0·5 for λ values ranging from 0·5 to 10,000. Thus, for very low λ values even ordinary hypervirial-Padé or simple hypervirial method is successful. In the case of anharmonic oscillators whether ω is 0 or not, K does not vary significantly or monotonically with λ, r or n. For a particular set of values of s and r, it decreases with increase in n; and for specific values of r and n, K increases if s is increased.

(3) If we consider a particular type of oscillator with $\omega \neq 0$ then the ground state energy increases while $\langle x^2 \rangle_0$ decreases with increase in the contribution of the perturbation term, i.e., in the value of λ. For a particular λ, the values of E_0 and $\langle x^2 \rangle_0$ for $r = 0$ are, respectively, higher and lower than the corresponding values for $r \neq 0$ cases though for $r = 1, 2, 3$ the variations of E_0 as well as $\langle x^2 \rangle_0$ with r do not exhibit a well defined trend. In the case of $\omega = 0$, $\lambda = 1$ oscillators there is no definite trend in the variation of E_n and $\langle x^2 \rangle_n$.

3. ARSPT

In the framework of perturbation theory, the interaction

$$V(\psi_n) = \lambda \langle x^{2r} \rangle x^{2s} \tag{11}$$

is treated as a perturbation and since it depends upon $\psi_n(x)$, similar to ψ_n and E_n this too is expressed as a power series in the perturbation parameter λ. Thus, following Surján and Ángyán [1], Surján [3] and Kim and Sukhatme [9], we write

$$\psi_n(x) = \psi_n^{(0)}(x)[1 + \lambda f_n^{(1)} + \lambda f_n^{(2)} + \cdots], \tag{12}$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots, \tag{13}$$

and

$$V(\psi_n) = \lambda V_n^{(1)}(x) + \lambda^2 V_n^{(2)}(x) + \cdots. \tag{14}$$

Here, the wavefunctions are taken to be real because we are concerned with one-dimensional bound state situation with local confining potential [11, 12]. From (11), (12) and (14) we have

$$V_n^{(1)}(x) = x^{2s} \int_{-\infty}^{\infty} \psi_n^{(0)^2}(x')(x')^{2r} \mathrm{d}x' \tag{15}$$

Table 4. A comparison of the ground state energy for the Hamiltonian (2) with $r = 1$ determined by ARSPT (E_0) and RHPS $E_0(P)$. All entries are in the units corresponding to $\hbar = m = \omega = 1$.

	$s = 1$		$s = 2$	
λ	0·1	1·0	0·1	1·0
E_0	0·5225	0·5000	0·5361	−0·5547
$E_0(P)$*	0·5233	0·6624	0·5297	0·6491

*$E_0(P)$ values have been rounded off to four significant figures.

and

$$V_n^{(2)}(x) = 2x^{2s} \int_{-\infty}^{\infty} (x')^{2r} \psi_n^{(0)^2}(x') f_n^{(1)}(x') \mathrm{d}x'. \tag{16}$$

Following the customary procedure, we get

$$E_n^{(1)} = \int_{-\infty}^{\infty} V_n^{(1)}(x) \psi_n^{(0)^2}(x) \mathrm{d}x, \tag{17}$$

and

$$E_n^{(2)} = -\int_{-\infty}^{\infty} [E_n^{(1)} f_n^{(1)}(x) - V_n^{(2)}(x) - V_n^{(1)}(x) f_n^{(1)}(x)] \psi_n^{(0)^2}(x) \mathrm{d}x \tag{18}$$

with

$$f_n^{(1)}(x) = -2 \int^{x} [\mathrm{d}x'/\psi_n^{(0)^2}(x')] \int_{-\infty}^{x'} [E_n^{(1)} - V_n^{(1)}(x'')] \psi_n^{(0)^2}(x'') \mathrm{d}x''. \tag{19}$$

With a view to compare the results obtained by using ARSPT with those of RHPS we have determined ground state energy for the self-interacting oscillators with $r = 1$, $s = 1, 2$ keeping $\omega = 1$. We have for $r = 1, s = 1$

$$E_0 = 0{\cdot}5[1 + (\lambda/2) - (\lambda^2/2)] \tag{20}$$

and for $r = 1$, $s = 2$

$$E_0 = 0{\cdot}5[1 + (3\lambda/4) - (183\lambda^2/64)]. \tag{21}$$

The values found for $\lambda = 0{\cdot}1$ and $1{\cdot}0$ by two methods are compared in table 4. As expected the E_0 values differ significantly from $E_0(P)$ and the deviation is higher for higher s and λ.

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