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Eigenvalues of kp^{2m} anharmonic oscillator

Awele Maduemezia

Department of Physics, University of Ibadan, Ibadan, Nigeria

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Abstract. The first four energy levels of the anharmonic oscillator $H = p^2+q^2-kp^{2M}$ are numerically evaluated for the M values 2, 3, 4, up to the tenth order of perturbation theory, and for $M = 1$, for all orders of perturbation theory. A recursion formula derived in a recent paper of the author on applications of hypervirial and Hellmann–Feynman theorems is used. The results indicate that for $M > 1$, the perturbation expansion in k is divergent. The ratios of absolute values of successive terms of the perturbation series form a monotonically increasing sequence, in agreement with an earlier result of Bender and Wu. The rate of divergence of this sequence of ratios is small. Furthermore, for $k = 10^{-9}$, the individual values of the ratios are small—less than 10^{-4}. Thus for sufficiently small k values, and for the purpose of practical calculations, the energy expansion in k effectively behaves like a convergent series up to very high orders of perturbation theory. The case $M = 1$ reduces to a harmonic oscillator. The perturbation series for this case converges to the exact solution, $(2N+1)(1-k)^{1/2}$, for the state N.

1. Introduction

In a recent paper (Maduemezia 1973, to be referred to as M1) a perturbative scheme using the hypervirial and Hellmann–Feynman theorems was developed for the linear anharmonic oscillator with a velocity-dependent anharmonic term. The hamiltonian for such a system is written $H = p^2+q^2-kp^D$, where $k = hf/(4mc^2)$, f is the oscillator frequency, h is Planck's constant and m is the particle mass.

It was assumed in M1 that the energy was expressible as a convergent power series in k, k being a small number. This assumption is really not essential. All that is needed is the development of a formal power series in k. For such an expansion to be of practical use, however, the convergence of the series would be essential. One might mention in passing that since the variables p and q enter the harmonic oscillator hamiltonian symmetrically (in the units chosen), the system defined by the above hamiltonian behaves in a similar way, as far as the energy spectrum is concerned, to the one defined by the hamiltonian $H = p^2+q^2-kq^D$. What is said for one should therefore apply to the other.

Bender and Wu (1969) investigated the ground state of the quartic anharmonic oscillator within the framework of quantum field theory. As a result of their numerical computation, they suggest, as do also Biswas *et al* (1973), that the perturbation series in k is divergent for all k, though each term of the series is finite.

Since the closed formula given in M1 is exact and is easily programmable on a computer, we decided to investigate any finer structure that the results of these previous authors may possess. We do this by evaluating the energy levels of the ground state and of the first three excited states for the first ten orders of perturbation theory, and for three even values of the order of anharmonicity D. The value $k = 10^{-9}$ is chosen. This value is nine orders of magnitude larger than the value $3{\cdot}5 \times 10^{-18}$ that one would use if m is the proton mass and f is a radio frequency of the value 3·2 MHz. Another value one could use is $k = 10^{-3}$, corresponding to $hf = 10$ MeV; $mc^2 = 1000$ MeV, which are orders of magnitude that feature in low-energy nuclear physics.

The calculation was performed on a Hewlett–Packard (programmable) calculator, model 9830A. An IBM 360/25 processor is also available here, but we find that the Hewlett–Packard machine has the one advantage that its calculating range extends down to $9{\cdot}99999999999 \times 10^{-99}$ compared to $5{\cdot}4 \times 10^{-79}$ for the IBM 360/25. This is important since it is essential that we be able to let the eigenvalues become as small as possible, but not necessarily zero, in order to see the finer structures of the perturbation series. The attendant limitation on computer memory means that we cannot go far beyond tenth-order perturbation theory.

2. The recursion formula

The main formula derived in M1 may, with minor changes in notation, be written

$$R(a+1, i) = \frac{a}{4(a+1)}\Bigg[4E(0)R(a-1, i) - 4\sum_{r=1} R(a-1, i-r)R(n, r-1)H(i-r^-) + \left(\frac{4a+2n}{a}\right)R(n-1+a, i-1)H(i-1^-) + (a-1)(a-2)R(a-3, i)\Bigg], \tag{1}$$

where $R(0,j) = \delta_{j0}$; $H(i-j^-) = 0$, if $i < j$, and $+1$, if $i \geqslant j$. $E(0) = 2N+1$, $N = 0, 1, 2, \ldots$, and the rth order correction to the energy is given by

$$k^r E(r) = -k^r r^{-1} R(n, r-1), \qquad r \geqslant 1. \tag{2}$$

Putting the order of anharmonicity $n = 2M$, we note that equation (1) is a recursion relation which relates any $R(B, J)$ to such $R(A, I)$ for which $I < J$. We also note that in this relationship, all A that occur on the right-hand side are even (odd) if B is even (odd). Since we are primarily interested in finding the eigenvalue corrections given by equation (2), it suffices to consider only *even* values of B. We accordingly make the following changes in notation: we denote $R(2K, 0)$ by $Q(K)$ for all K, and $R(2K, I)$ by $P(K, I)$ for all K, and for $I > 0$. We then obtain

$$E(J+1)\begin{cases} = -Q(M) & \text{for } J = 0, \\ = -(J+1)^{-1}P(M, J) & \text{for } J \geqslant 1. \end{cases} \tag{3}$$

We now make the substitutions $(a-3) = 2B$, $B = -1, 0, 1, 2, \ldots$, and $Q(0) = 1$ in equation (1), and obtain the following three computer-oriented forms:

$$Q(B+2) = \frac{2B+3}{4(B+2)}[2E(0)Q(B+1) + (2B+1)(B+1)Q(B)], \tag{4}$$

$$P(B+2, 1) = \frac{2B+3}{2(B+2)}\Bigg(E(0)P(B+1, 1) - Q(B+1)Q(M) + \frac{2B+3+M}{2B+3}Q(M+B+1) + \tfrac{1}{2}(B+1)(2B+1)P(B, 1)\Bigg), \tag{5}$$

$$P(B+2,J) = \frac{2B+3}{2(B+2)}\left(E(0)P(B+1,J) - P(B+1,J-1)Q(M) - \frac{Q(B+1)P(M,J-1)}{J}\right.$$
$$+\tfrac{1}{2}(2B+1)(B+1)P(B,J) - \sum_{R=2}^{J-1}\frac{P(B+1,J-R)P(M,R-1)}{R}$$
$$\left.+\frac{2B+3+M}{2B+3}P(M+B+1,J-1)\right), \qquad J > 1. \tag{6}$$

The result of the evaluation of equations (3)–(6) is given in tables 1–4 for the three cases $M = 2, 3, 4$. In these tables, $H(J)$ stands for the term $k^J E(J)$ in the expansion $E = \Sigma_{J=0}\, k^J E(J)$, J being the order of perturbation theory.

Table 1. First- to tenth-order energy corrections for the state $N = 0$ with degrees of anharmonicity $2M = 4$, 6 and 8. $k = 10^{-9}$; $H(J) = k^J E(J)$.

$2M$	$E(J)$	$E(J)/E(J-1)$	$H(J)$	$H(J)/H(J-1)$
4	−7·5000E−01		−7·5000E−10	
	−1·3125E+00	1·7500E+00	−1·3125E−18	1·7500E−09
	−4·5703E+00	3·4821E+00	−4·5703F−27	3·4821E−09
	−2·5411E+01	5·5599E+00	−2·5411E−35	5·5599E−09
	−1·8709E+02	7·3627E+00	−1·8709E−43	7·3627E−09
	−1·6997E+03	9·0848E+00	−1·6997E−51	9·0848E−09
	−1·7950E+04	1·0561E+01	−1·7950E−59	1·0561E−08
	−2·1622E+05	1·2046E+01	−2·1622E−67	1·2046E−08
	−2·9085E+06	1·3452E+01	−2·9085E−75	1·3452E−08
	−4·3306E+07	1·4889E+01	−4·3306E−83	1·4889E−08
6	−1·8750E+00		−1·8750E−09	
	−2·7305E+01	1·4563E+01	−2·7305E−17	1·4563E−08
	−1·1913E+03	4·3630E+01	−1·1913E−24	4·3630E−08
	−1·0033E+05	8·4223E+01	−1·0033E−31	8·4223E−08
	−1·3662E+07	1·3617E+02	−1·3662E−38	1·3617E−07
	−2·7356E+09	2·0024E+02	−2·7356E−45	2·0024E−07
	−7·5813E+11	2·7713E+02	−7·5813E−52	2·7713E−07
	−2·7835E+14	3·6715E+02	−2·7835E−58	3·6715E−07
	−1·3092E+17	4·7035E+02	−1·3092E−64	4·7035E−07
	−7·6809E+19	5·8668E+02	−7·6809E−71	5·8668E−07
8	−6·5625E+00		−6·5625E−09	
	−1·0549E+03	1·6075E+02	−1·0549E−15	1·6075E−07
	−7·7565E+05	7·3526E+02	−7·7565E−22	7·3526E−07
	−1·5430E+09	1·9893E+03	−1·5430E−27	1·9893E−06
	−6·4304E+12	4·1675E+03	−6·4304E−33	4·1675E−06
	−4 8675E+16	7·5696E+03	−4·8675E−38	7·5696E−06
	−6·0700E+20	1·2470E+04	−6·0700E−43	1·2470E−05
	−1·1620E+25	1·9143E+04	−1·1620E−47	1·9143E−05
	−3·2368E+29	2·7857E+04	−3·2368E−52	2·7857E−05
	−1·2586E+34	3·8884E+04	−1·2586E−56	3·8884E−05

3. The case of quadratic perturbation, 2M = 2

For $M = 1$, the hamiltonian becomes

$$H = (1-k)p^2 + q^2. \tag{7}$$

Table 2. First- to tenth-order energy corrections for the state $N = 1$ with degrees of anharmonicity $2M = 4$, 6 and 8. $k = 10^{-9}$; $H(J) = k^J E(J)$.

2*M*	*E*(*J*)	*E*(*J*)/*E*(*J*−1)	*H*(*J*)	*H*(*J*)/*H*(*J*−1)
4	−3·7500E+00		−3·7500E−09	
	−1·0313E+01	2·7500E+00	−1·0313E−17	2·7500E−09
	−4·4648E+01	4·3295E+00	−4·4648E−26	4·3295E−09
	−3·1693E+02	7·0983E+00	−3·1693E−34	7·0983E−09
	−3·1817E+03	1·0039E+01	−3·1817E−42	1·0039E−08
	−3·9039E+04	1·2270E+01	−3·9039E−50	1·2270E−08
	−5·4305E+05	1·3911E+01	−5·4305E−58	1·3911E−08
	−8·3396E+06	1·5357E+01	−8·3396E−66	1·5357E−08
	−1·3950E+08	1·6727E+01	−1·3950E−73	1·6727E−08
	−2·5196E+09	1·8062E+01	−2·5196E−81	1·8062E−08
6	−1·3125E+01		−1·3125E−08	
	−3·6832E+02	2·8062E+01	−3·6832E−16	2·8062E−08
	−2·4785E+04	6·7292E+01	−2·4785E−23	6·7292E−08
	−3·0688E+06	1·2382E+02	−3·0688E−30	1·2382E−07
	−5·7207E+08	1·8641E+02	−5·7207E−37	1·8641E−07
	−1·4690E+11	2·5679E+02	−1·4690E−43	2·5679E−07
	−4·9641E+13	3·3792E+02	−4·9641E−50	3·3792E−07
	−2·1426E+16	4·3162E+02	−2·1426E−56	4·3162E−07
	−1·1543E+19	5·3874E+02	−1·1543E−62	5·3874E−07
	−7·6127E+21	6·5951E+02	−7·6127E−69	6·5951E−07
8	−5·9063E+01		−5·9063E−08	
	−1·9889E+04	3·3675E+02	−1·9889E−14	3·3675E−07
	−2·3396E+07	1·1763E+03	−2·3396E−20	1·1763E−06
	−6·5714E+10	2·8087E+03	−6·5714E−26	2·8087E−06
	−3·5289E+14	5·3701E+03	−3·5289E−31	5·3701E−06
	−3·2505E+18	9·2109E+03	−3·2505E−36	9·2109E−06
	−4·7599E+22	1·4644E+04	−4·7599E−41	1·4644E−05
	−1·0448E+27	2·1949E+04	−1·0448E−45	2·1949E−05
	−3·2802E+31	3·1397E−04	−3·2802E−50	3·1397E−05
	−1·4188E+36	4·3254E+04	−1·4188E−54	4·3254E−05

The system is harmonic. With the following scaling:

$$\begin{aligned} H &= h(1-k)^{1/2}, \\ p &= P(1-k)^{-1/2}, \\ q &= Q(1-k)^{1/2}, \end{aligned} \tag{8}$$

the hamiltonian becomes $h = P^2+Q^2$, with $[Q, P] = i$, as before. Hence h has eigenvalues $2N+1, N = 0, 1, 2, \ldots,$ and so H has the eigenvalues $(2N+1)(1-k)^{1/2}$, $N = 0, 1, 2, \ldots.$

We may compare this result with the perturbation theory result given by equations (3)–(6) for $M = 1$. We obtain

$$E(1) = -Q(1) = -\tfrac{1}{2}E(0) = -\tfrac{1}{2}(2N+1), \tag{9}$$

Table 3. First- to tenth-order energy corrections for the state $N = 2$ with degrees of anharmonicity $2M = 4$, 6 and 8. $k = 10^{-9}$; $H(J) = k^J E(J)$.

$2M$	$E(J)$	$E(J)/E(J-1)$	$H(J)$	$H(J)/H(J-1)$
4	−9·7500E+00		−9·7500E−09	
	−3·8437E+01	3·9423E+00	−3·8437E−17	3·9423E−09
	−2·0580E+02	5·3543E+00	−2·0580E−25	5·3543E−09
	−1·7433E+03	8·4705E+00	−1·7433E−33	8·4705E−09
	−2·2333E+04	1·2811E+01	−2·2333E−41	1·2811E−08
	−3·5844E+05	1·6050E+01	−3·5844E−49	1·6050E−08
	−6·4052E+06	1·7870E+01	−6·4052E−57	1·7870E−08
	−1·2338E+08	1·9262E+01	−1·2338E−64	1·9262E−08
	−2·5395E+09	2·0583E+01	−2·5395E−72	2·0583E−08
	−5·5552E+10	2·1875E+01	−5·5552E−80	2·1875E−08
6	−4·6875E+01		−4·6875E−08	
	−2·3054E+03	4·9182E+01	−2·3054E−15	4·9182E−08
	−2·2878E+05	9·9236E+01	−2·2878E−22	9·9236E−08
	−4·0974E+07	1·7910E+02	−4·0974E−29	1·7910E−07
	−1·0567E+10	2·5789E+02	−1·0567E−35	2·5789E−07
	−3·5649E+12	3·3737E+02	−3·5649E−42	3·3737E−07
	−1·5090E+15	4·2328E+02	−1·5090E−48	4·2328E−07
	−7·8400E+17	5·1956E+02	−7·8400E−55	5·1956E−07
	−4·9270E+20	6·2844E+02	−4·9270E−61	6·2844E−07
	−3·7007E+23	7·5111E+02	−3·7007E−67	7·5111E−07
8	−2·6906E+02		−2·6906E−07	
	−1·7780E+05	6·6081E+02	−1·7780E−13	6·6081E−07
	−3·3275E+08	1·8715E+03	−3·3275E−19	1·8715E−06
	−1·3481E+12	4·0514E+03	−1·3481E−24	4·0514E−06
	−9·5455E+15	7·0808E+03	−9·5455E−30	7·0808E−06
	−1·0856E+20	1·1373E+04	−1·0856E−34	1·1373E−05
	−1·8800E+24	1·7318E+04	−1·8800E−39	1·7318E−05
	−4·7451E+28	2·5239E+04	−4·7451E−44	2·5239E−05
	−1·6806E+33	3·5418E+04	−1·6806E−48	3·5418E−05
	−8·0867E+37	4·8117E+04	−8·0867E−53	4·8117E−05

$$E(2) = -\tfrac{1}{2}P(1,1) = -\tfrac{1}{8}E(0) \qquad (10)$$

$$E(J+1) = -(J+1)^{-1}P(1,J), \qquad J > 1 \qquad (11)$$

$$= -(J+1)^{-1}\left(\frac{(2J-1)P(1,J-1)}{2J}\right). \qquad (12)$$

ie,

$$E(3) = -\tfrac{1}{16}E(0), \qquad E(4) = -\tfrac{5}{128}E(0),$$

and so forth. We can see immediately that $E(0)$, $E(1)$, $E(2)$, $E(3)$, and $E(4)$ are the first five terms of the series $E(0)(1-k)^{1/2}$, which has been shown above to be the exact solution of the eigenvalue problem. By evaluating the equations (3) to (6) to any order, we can see that the perturbation series does indeed converge to this exact solution. This is a useful check on the validity of the perturbation theoretic methods developed in this paper and in M1.

Table 4. First- to tenth-order energy corrections for the state $N = 3$ with degrees of anharmonicity $2M = 4$, 6 and 8. $k = 10^{-9}$; $H(J) = k^J E(J)$.

2M	E(J)	E(J)/E(J−1)	H(J)	H(J)/H(J−1)
4	−1·8750E+01		−1·8750E−08	
	−9·8438E+01	5·2500E+00	−9·8438E−17	5·2500E−09
	−6·4629E+02	6·5655E+00	−6·4629E−25	6·5655E−09
	−6·4187E+03	9·9316E+00	−6·4187E−33	9·9316E−09
	−9·9719E+04	1·5536E+01	−9·9719E−41	1·5536E−08
	−2·0072E+06	2·0128E+01	−2·0072E−48	2·0128E−08
	−4·4612E+07	2·2226E+01	−4·4612E−56	2·2226E−08
	−1·0499E+09	2·3535E+01	−1·0499E−63	2·3535E−08
	−2·6028E+10	2·4791E+01	−2·6028E−71	2·4791E−08
	−6·7847E+11	2·6066E+01	−6·7847E−79	2·6066E−08
6	−1·1813E+02		−1·1813E−07	
	−9·3589E+03	7·0229E+01	−9·3589E−15	7·9229E−08
	−1·3227E+06	1·4133E+02	−1·3227E−21	1·4133E−07
	−3·3078E+08	2·5008E+02	−3·3078E−28	2·5008E−07
	−1·1620E+11	3·5131E+02	−1·1620E−34	3·5131E−07
	−5·1611E+13	4·4414E+02	−5·1611E−41	4·4414E−07
	−2·7721E+16	5·3713E+02	−2·7721E−47	5·3713E−07
	−1·7654E+19	6·3682E+02	−1·7654E−53	6·3682E−07
	−1·3185E+22	7·4687E+02	−1·3185E−59	7·4687E−07
	−1·1466E+25	8·6962E+02	−1·1466E−65	8·6962E−07
8	−8·4656E+02		−8·4656E−07	
	−1·0208E+06	1·2058E+03	−1·0208E−12	1·2058E−06
	−2·9716E+09	2·9111E+03	−2·9716E−18	2·9111E−06
	−1·7439E+13	5·8688E+03	−1·7439E−23	5·8688E−06
	−1·6596E+17	9·5164E+03	−1·6596E−28	9·5164E−06
	−2·3759E+21	1·4316E+04	−2·3759E−33	1·4316E−05
	−4·9303E+25	2·0751E+04	−4·9303E−38	2·0751E−05
	−1·4414E+30	2·9236E+04	−1·4414E−42	2·9236E−05
	−5·7798E+34	4·0099E+04	−5·7798E−47	4·0099E−05
	−3·0987E+39	5·3613E+04	−3·0987E−51	5·3613E−05

4. Conclusion

We first note that in tables 1–4, the entries for $M = 2$, $J = 1, 2$ and $N = 0$ to 3, namely

$$E(1) = -7{\cdot}5000\text{E}-01, \qquad E(2) = -1{\cdot}3125\text{E}+00;$$

$$E(1) = -3{\cdot}7500\text{E}+00, \qquad E(2) = -1{\cdot}0313\text{E}+01;$$

$$E(1) = -9{\cdot}7500\text{E}+00, \qquad E(2) = -3{\cdot}8437\text{E}+01;$$

$$E(1) = -1{\cdot}9750\text{E}+01, \qquad E(2) = -9{\cdot}8438\text{E}+01,$$

agree with the results given in Maduemezia (1973) for first- and second-order perturbation theory.

For $M = 1$, the perturbation is quadratic. The dynamical system is harmonic, and we see from the previous section that the perturbation theoretic solution converges to the exact solution.

From the last column of tables 1–4, we see that for $2M$ greater than 2, the perturbation power series in k is slowly divergent. This divergence is in agreement with the result of Bender and Wu (1969). The smallness of the individual entries in this last column also indicates that the series effectively behaves like a convergent one up to order ten. If we view the divergence in the sense of energy corrections becoming unduely large, we can see that this would become manifest only at very high orders.

The divergence of the perturbation series must be seen as an expression of the basic structural instability of the harmonic oscillator (see eg Zeeman 1972) when subjected to (p, q)-dependent perturbations, however small.

Nevertheless, to the extent that the series does behave like a convergent one if one works up to order ten, and to the extent that higher-order terms are expected mutually to annihilate each other, it makes sense to use the perturbation series for physically meaningful calculations.

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