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# The anharmonic oscillator $-d^2/dx^2 + x^2 + b/x^4 + c/x^6$ for extreme values of the anharmonicity constants

R Guardiolat and J Rost

† Departamento de Física Atómica y Nuclear, Universidad de Valencia Estudi General, Avda. Dr Moliner 50, 46100-Burjasot, Valencia, Spain

t Departamento de Física Teórica Universidad de Valencia Estudi General, and IFIC, Centre Mixt Universitat de Valencia-CSIC, Avda. Dr Moliner 50, 46100-Burjasot, Valencia, Spain

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Abstract. The  $bx^{-4} + cx^{-6}$  anharmonic perturbation to the harmonic oscillator is studied in two extreme regimes: large anharmonicity constants, corresponding to b large, c large or both large, and small anharmonicity constants. In the former case, a large order strong coupling expansion in terms of an *ad hoc* expansion parameter is constructed. In the latter case, the lowest order corrections to the unperturbed energies are obtained. Elementary solutions as well as the consequences of the self-transformation of the Hamiltonian are also analysed.

### 1. Introduction

The spiked harmonic oscillator described by the Hamiltonian

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^2 + \frac{b}{x^4} + \frac{c}{x^6} \tag{1}$$

has quite appealing properties which make the determination of its ground state energy a challenging problem. This Hamiltonian is defined in the  $[0,\infty]$  half-space with Dirichlet boundary conditions. In order to have a discrete spectrum at least c must be a positive number.

The study of such a singular potential has relevance in connection with the imaginary time formulation of quantum mechanics and its relation with diffusion theory. They give rise to the so-called *Klauder phenomenon* [1-3], which consists in that once the singular part of the potential is turned on, its effects are not completely turned off. In the so-called diffusion Monte Carlo method [4], which step-by-step integrates the Schrödinger equation for a many-body system by using an stochastic algorithm, special care has to be taken in the regions where the interaction is strongly repulsive or strongly attractive to avoid a blow up of the population of walkers. This is normally taken into account by using an importance sampling driving function with appropriate cusp conditions [4].

Our Hamiltonian has a short-distance behaviour of the same kind as the familiar Lennard-Jones interactions, widely used to describe quantum fluids at zero temperature. In the variational description of such extended systems [5, 6], one requires, as the adequate Jastrow correlation factor [7], a bound-state like solution of the twobody system with special healing properties at long distances. With regard to another many-body theory, the so-called quantum thermodynamics perturbation theory [8, 9], based on the low-density expansion of the ground state energy of the many-body system [10], is of interest to determine the zero-energy scattering solution of the two-particle interaction [11].

The main point to be stressed with respect to the potential in equation (1) is that one never deals with *small* perturbations. More precisely, even for very small values of both c and b, the effect of the anharmonicities cannot be considered as a perturbation because they dramatically change the wavefunction near the origin. The required change of the wavefunction, even if restricted to a small region of the space (when b and c are small) has to be such that it makes finite the otherwise infinite matrix elements of the potential.

On the other hand, when either b or c is large, the anharmonic terms do compete with the harmonic potential  $x^2$  and again none of the terms of the interaction may be considered negligible or small. As a consequence, the ground state energy appears in these two extreme limits as an expansion in terms of non-integral powers of *ad hoc* effective coupling constants.

From the mathematical point of view, this problem is a non-trivial generalization of the simple spiked oscillator problem. With this name one usually refers to the anharmonic oscillator

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^2 + \frac{\lambda}{x^{\alpha}}.$$
(2)

Detwiler and Klauder [12] realized that problems of this kind, or with similar behaviour, had very special properties in the small coupling regime. Later, Harrell [13] was able to construct a special perturbation theory, called *singular* perturbation theory, to determine the leading term of the ground state energy for small  $\lambda$ , which turned out to depend on non-integral powers of the coupling parameter. Moving to the other extreme, the strong coupling regime, Aguilera-Navarro *et al* [14] found the expansion of the ground state energy. This expansion contains a term diverging with  $\lambda$ , plus a constant term and plus an expansion in terms of non-integral and negative powers of  $\lambda$ .

In a different context, Hamiltonians of the kind in equations (1) and (2) have also raised some interest with regard to the numerical algorithms used to integrate the Schrödinger equation; in particular, those based on finite differences [15]. The abnormal behaviour of the ground state energy as a function of the integration step has been assigned [15] to the particularly singular character of the interaction, for small values of the anharmonicity constants.

There are still two other properties to be mentioned with regard to this problem. First, this Hamiltonian transforms into itself under the change  $x \rightarrow 1/x$  [18, 19]. Secondly, this Hamiltonian possesses infinite sets of *elementary* solutions, i.e. solutions which may be written as the product of an exponential times a polynomial containing positive and/or negative powers of x [18]. These elementary solutions appear only for specific values of the anharmonicity constants.

The expansion of the wavefunction involving both positive and negative powers of x has proven to be a very precise tool for the determination of the ground state energy. The method requires the solution of Hill-determinantal equations and has been termed [19] an *almost non-numerical* method. However, although based on an

algebraic analysis, it seems inappropriate to determine the analytic dependence of the energy in terms of the coupling parameters.

The two approaches mentioned, namely the singular perturbation theory and the strong coupling perturbation method, require some modifications for their application to our problem equation (1), particularly the determination of the relevant expansion parameter. It is the main purpose of this work to adapt these special perturbation expansions to our more general case.



Figure 1. The ground state energy and the first excited state energy corresponding to c = 0.001 as a function of b.

In order to show the kind of results we want to analyse we present in figure 1 the behaviour of the two lowest eigenvalues of the Hamiltonian of equation (1) for a fixed and small value of c = 0.001 as a function of b in the range (-0.2, 0.2). These eigenvalues were computed by using the simplest finite-differences method based on the replacement of the second derivative operator by the second differences operator divided by the integration step squared,  $D^2 \rightarrow \delta^2/h^2$ , combined with the Richardson extrapolation method (see [16, 17]). The abrupt change of the ground state energy at a value of b around -0.1 is really surprising because, in a very small interval the energy jumps from values close to the unperturbed energy, 3, to large and negative values. In contrast, the first excited state does not show this abrupt change.

The paper is organized as follows. In section 2 we present a brief discussion of the elementary solutions. Section 3 is devoted to the determination of the leading corrections to the unperturbed energy in the small coupling limit, and in two different regimes corresponding to the dominance of one of the anharmonicities over the other. Section 4 is devoted to the strong coupling regime. Two tasks are solved in this section: the determination of the relevant expansion parameter (a combination of b and c) and the explicit construction of the perturbative expansion. Section 5 describes and exploits the relationships which result from the transformation of the Hamiltonian into itself, allowing for the extension of the domain of validity of the perturbative expansions. A summary of the results and their limitations is presented in the last section. We have also included two appendixes which describe the technicalities required for our study.

## 2. Elementary solutions

According to the structure of the Hamiltonian, equation (1), the wavefunction will be dominated by the exponential term

$$f = \exp\left(-\frac{x^2}{2} - \frac{\sqrt{c}}{2x^2}\right) \tag{3}$$

which takes care of the  $x \to \infty$  part of the interaction as well as the leading  $x \to 0$  part, corresponding to  $c/x^6$ .

Consider the action of the full Hamiltonian equation (1) on a generic trial function

$$\psi_1 = x^p f \tag{4}$$

given by

$$\frac{1}{\psi_1}(H-E)\psi_1 = (2p+1-E) + \frac{(2\sqrt{c}-p^2+p)}{x^2} + \frac{b+(3-2p)\sqrt{c}}{x^4}.$$
 (5)

The right-hand side of this equation is null for the following values of b, c and E (set 1)

$$E = 2p + 1 \qquad 2\sqrt{c} = p(p-1) \qquad b = (2p-3)\sqrt{c} \tag{6}$$

with the exception of p = 0 and p = 1, which correspond to a null coupling, and also of the interval [0, 1] which will correspond to a non-normalizable trial function. Otherwise, p may be any real, positive or negative number. Note that the trial function has no nodes (apart from the zeros at the origin and infinity), so that it represents the ground state wavefunction.

A second set of solutions may be generated by considering a slightly more complicated wavefunction

$$\psi_2 = (x^p + ax^{p+q})f. \tag{7}$$

Now the Schrödinger equation may only be satisfied if q = 0, q = 2 or q = 4 (negative values may also be formally considered, but in practice they will represent the same set of functions). The case q = 0 may be ruled out, because it will just reproduce set 1. The case q = 4 is a particular case of the more general situation described later (set 3), so that only the case q = 2 represents a new set of solutions. The possible solutions corresponding to a normalizable wavefunction and without extra nodes (i.e. with a positive) are the solutions of the set of equations (set 2)

$$E = 5 + 2p$$
  

$$2\sqrt{c} = (p^{2} + p + 5) + \sqrt{12p^{2} + 12p + 25}$$
  

$$b = (2p - 3)\sqrt{c}.$$
(8)

There may be two solutions for  $\sqrt{c}$ , but only the solution written in equation (7) with a positive sign in front of the square root symbol corresponds to a positive value of

a in equation (7), i.e. has no nodes. In this case there are no excluded regions in p, which may have any real value.

One can continue by trying other forms for the trial function, with three, four, etc. terms. The next set corresponds to the three-term ansatz  $x^p(1 + a_1x^2 + a_2x^4)f$ , and the solutions are (set 3)

$$E = 2p + 9$$
  

$$b = (2p - 3)\sqrt{c}$$
  

$$8c^{3/2} - 4(3p^2 + 9p + 46)c + 2(3p^4 + 18p^3 + 71p^2 + 132p + 216)c^{1/2}$$
  

$$- p(p^5 + 9p^4 + 25p^3 + 15p^2 - 26p - 24) = 0.$$
 (9)

Again p may be positive or negative. After a numerical investigation of these equations we have not found any excluded region. Note however that only one of the roots of the cubic equation for  $c^{1/2}$  fulfils the two conditions of being positive and corresponding to a solution without nodes. The equations (9) have several particular cases corresponding to the roots of the independent term of the last equation. All these solutions correspond to integer values of p, and are

$$p = 1, -4 \qquad 2\sqrt{c} = 29 + \sqrt{401}$$

$$p = -1, -2 \qquad 2\sqrt{c} = 20 + \sqrt{260}$$

$$p = 0, -3 \qquad 2\sqrt{c} = 23 + \sqrt{313}$$
(10)

with the corresponding values of b and E from the first two equations of (9).



Figure 2. Curves connecting the parameter pairs (b, c) corresponding to the elementary solution sets described in the text. There is a complex structure near c = 0 in the line labelled 1 which cannot be appreciated in this figure.

Figure 2 shows in the plane (b, c) the curves connecting the elementary solutions for the three mentioned sets. Note that there is a small region around b = 0 and c = 0 with a strange behaviour which cannot be appreciated in this figure, which will be discussed later. The elementary solutions may serve as a test for other approximate methods. However, they are not useful for studying the small coupling limit, even if this looks reasonable. In the small coupling regime one seeks for solutions whose energy is slightly different from 3, the unperturbed energy. Focusing on set 1 this would correspond to  $p = 1 + \epsilon$ ,  $\epsilon > 0$ , and correspondingly, at the lowest order in  $\epsilon$ ,

$$E = 3 + 2\epsilon \qquad c = \epsilon^2/4 \qquad b = -\epsilon/2. \tag{11}$$

However, there is yet another solution with small values for b and c, namely the case  $p = -\epsilon$ ,  $\epsilon > 0$ , where

$$E = 1 - 2\epsilon \qquad c = \epsilon^2/4 \qquad b = -3\epsilon/2. \tag{12}$$

Certainly it is quite surprising that so a small change, from  $b = -\epsilon/2$  to  $b = -3\epsilon/2$ , is able to change the energy from 3 to 1. One may conclude that the origin in the plane (b, c) is a complex point and that our problem has a singular behaviour for small values of the anharmonicity constants.

#### 3. The small coupling expansion

It is convenient to start this section with a brief description of Harrell's investigation on the spiked harmonic oscillators [13], focusing on the case  $x^2 + c/x^6$ . For small values of c Harrell found that the ground state wavefunction should be expressed as the product of the unperturbed harmonic oscillator function  $u_0 = x \exp(-x^2/2)$ times a correcting factor W(x, c) given by

$$W(x,c) = K_{1/4} (c^{1/2} x^{-2}/2) / x^{1/2}$$
(13)

where K is the modified Bessel function. The shape of the correcting factor may be analysed by using the limiting forms of the modified Bessel function for very small (large x) and very large (small x) values of its argument. The corresponding limits are

$$\lim_{x \to \infty} W(x,c) = \pi c^{-1/8} / \Gamma(3/4)$$
(14)

and

$$\lim_{x \to 0} W(x,c) = \sqrt{\pi x} c^{-1/4} \exp(-\sqrt{c}/2x^2)$$
(15)

so that the unperturbed wavefunction is modified only in a small region around the origin. By using this ansatz Harrell obtained the lowest order correction to the energy

$$E(c) \approx 3 + \frac{2\Gamma(3/4)c^{1/4}}{\Gamma(5/4)\pi^{1/2}} \approx 3 + 1.525\,519\,5c^{1/4}$$
(16)

Finally, we should mention another appealing characteristic of Harrell's work. It is that he did not in fact require the full expression of the correcting factor W(x, c) to compute the relevant matrix elements. In fact only the limiting forms were needed. So he bypassed the formidable task of evaluating the integrals involving the unperturbed wavefunction, the correcting factor and the various parts of the Hamiltonian. Unfortunately we cannot use Harrell's approach in our more involved problem with two spikes,  $1/x^4$  and  $1/x^6$ .

We have used an alternative method, valid when the  $x^{-4}$  anharmonicity is much less important than the  $x^{-6}$  anharmonicity. It consists of a variational calculation with the non-orthogonal basis

$$\Psi_N = \mathcal{N}_N x^{3-2N} \exp(-x^2/2 - \sqrt{c}/2x^2)$$
(17)

where  $\mathcal{N}_N$  is a convenient scaling factor given by  $\mathcal{N}_1 = 1$  and  $\mathcal{N}_N = c^{N/2-5/8}$ . The state N = 1 corresponds to the unperturbed oscillator ground state wavefunction corrected at short distances by the exponential factor of equation (15). In principle N should take positive and negative integer values, cf [19] but we have found that negative values of N do not contribute to the leading energy correction.

To establish the form of the energy dependence on the perturbation parameters it is convenient to consider the simplest variational calculation involving only the N = 1state. The expectation value of the Hamiltonian turns out to be (see appendix A for more details)

$$\langle \Psi_1 | H | \Psi_1 \rangle = \frac{\sqrt{\pi}}{4} [3 + 8c^{1/4} + 4c^{1/2} + 2bc^{-1/4}] \exp(-2c^{1/4})$$
 (18)

and the norm

$$\langle \Psi_1 | \Psi_1 \rangle = \frac{\sqrt{\pi}}{4} (1 + 2c^{1/4}) \exp(-2c^{1/4}).$$
 (19)

Then the lowest order correction in c is proportional to  $c^{1/4}$ , as expected, and the lowest order correction in b is proportional to the unexpected combination  $b/c^{1/4}$ . As far as we are building the  $x^{-4}$  perturbation on top of the  $x^{-6}$  one, our result will only be valid when

$$c \ll 1 \qquad b \ll c^{1/2} \tag{20}$$

where b may be negative, whereas c must be obviously positive.

This suggests to define new expansion parameters

$$\eta = c^{1/4} \qquad \sigma = b/c^{1/2} \tag{21}$$

and to expand everything up to first order in  $\eta$  and  $\sigma$ . There remains at this order

$$E \approx 3 + 2\eta + 2\sigma\eta. \tag{22}$$

The coefficient 2 of  $\eta$  in this equation should be compared with Harrell's exact result 1.5255, so that we are probably on the right path to obtaining a good description. To improve the values of the leading correcting terms we just solve the generalized eigenvalue equation

$$\det\langle \Psi_N | H - E | \Psi_M \rangle = 0 \tag{23}$$

at the lowest orders in  $\eta$  and  $\sigma$ . All technical details are omitted, for inclusion in appendix A. Table 1 lists the values of  $\alpha$  and  $\beta$  describing the small coupling regime as

$$E \approx 3 + \alpha c^{1/4} + \beta b/c^{1/4}$$
(24)

for various sizes of the basis, up to ten states. In the table we also include the exact value of  $\alpha$  from Harrell [13] as well as the value of  $\beta$ . The latter has been determined by a numerical integration of the Schrödinger equation for  $c = 10^{-4}$  and  $b = \pm 1 \times 10^{-3}$  up to  $\pm 4 \times 10^{-3}$  and afterwards computing the derivative with respect to  $\sigma$ . The integration of the Schrödinger equation was carried out, as explained in the introduction, by using the simplest finite-differences algorithm and then using the Richardson extrapolation method to increase the precision of the result. Note that because of the singular character of the potential the use of higher order integration rules (like the Numerov method) will not produce more precise results than the simple rule used here [20].

Looking to the evolution of the values of  $\alpha$  and  $\beta$  with the number of basis states one realizes that the expansion is acceptable but nevertheless it converges very slowly towards the exact values. This reflects the inadequacy of the basis. In fact, the basis states do satisfy the long distance behaviour of the small coupling solution, equation (14) but they do not represent faithfully the small distance behaviour, equation (15).

A better starting state could be

$$\Psi_a = x \sqrt{\frac{x}{g\eta + x}} \exp\left[-\left(\frac{x^2}{2}\right) - \left(\frac{\eta^2}{2x^2}\right)\right]$$
(25)

where  $\eta = c^{1/4}$ . This wavefunction has the proper limiting dependence on x, both near the origin and at large distances, when g has the value

$$g = \frac{\pi}{\Gamma^2(3/4)} \approx 2.092\,099\,24. \tag{26}$$

Let us first obtain the upper bound to  $\alpha$ , equation (24), related to this wavefunction. This requires the evaluation of the norm as well as the expectation value of the Hamiltonian equation (1) at b = 0, at the leading order in  $\eta$ .

The expectation value of the Hamiltonian requires the computation of the integral

$$\left\langle \Psi_{a} \left| -\frac{\mathrm{d}^{2}}{\mathrm{d}x^{2}} + x^{2} + \frac{\eta^{4}}{x^{6}} \right| \Psi_{a} \right\rangle = \int_{0}^{\infty} \mathrm{d}x \exp\left[ -x^{2} - \frac{\eta^{2}}{x^{2}} \right] \left[ 3x^{2} - 2g\eta x + \eta^{2}(g^{2} + 2) - \frac{2g\eta^{3}}{x + \eta g} - \frac{(4g^{4}\eta^{2} + 3g^{2} - 4)\eta^{2}}{4(x + g\eta)^{2}} + \frac{3g^{3}\eta^{3}}{4(x + g\eta)^{3}} \right]$$

$$(27)$$

at the first order in  $\eta$ . The small  $\eta$  limit of the first three integrals of the square bracket are easily evaluated by using the method described in appendix A. For the remaining three integrals it is convenient to make the change of variables  $x \to \eta/t$ . This results in

$$\left\langle \Psi_{a} \left| -\frac{\mathrm{d}^{2}}{\mathrm{d}x^{2}} + x^{2} + \frac{\eta^{4}}{x^{6}} \right| \Psi_{a} \right\rangle \approx \frac{3\sqrt{\pi}}{4} - g\eta - \frac{(3g^{2} - 4)\eta}{4} \\ \times \int_{0}^{\infty} \frac{\exp(-t^{2})\mathrm{d}t}{(1 + gt)^{2}} + \frac{3g^{3}\eta}{4} \int_{0}^{\infty} \frac{\exp(-t^{2})t\mathrm{d}t}{(1 + gt)^{3}}.$$

$$(28)$$

The value of the square of the normalization at lowest order in  $\eta$  is much simpler,

$$\langle \Psi_a | \Psi_a \rangle \approx \frac{\sqrt{\pi}}{4} - \frac{g\eta}{2}.$$
 (29)

By combining equations (28) and (29) one may obtain the value of  $\alpha$  of the expansion of the ground state energy, equation (24). Once g is substituted by its value, equation (26), and the integrals appearing in equation (28) are evaluated numerically, the small c limit

$$E(b=0) \approx 3 + 1.555\,04c^{1/4} \tag{30}$$

is obtained which is very close to the exact result of Harrell [13] quoted in the last row of table 1.

**Table 1.** The various upper bounds for the coefficients  $\alpha$  and  $\beta$  of the small coupling expansion corresponding to equation (24) for several values of the dimension of the space. The last row, labelled 'Exact', includes the value of Harrell [13] for  $\alpha$ , and the numerical approximation for  $\beta$ .

Nmax	α	β
1	2	2
2	1.8182	1.6860
3	1.7518	1.5722
4	1.7157	1.5108
5	1.6923	1.4713
6	1.6757	1.4483
7	1.6632	1.4222
8	1.6532	1.4056
9	1.6451	1.3922
10	1.6384	1.3809
Exact	1.5255	0.9605

The perturbative correction related to the  $b/x^4$  terms may also be computed in a similar way. The relevant matrix element is

$$\langle \Psi_a | x^{-4} | \Psi_a \rangle = \int_0^\infty \frac{1}{x(g\eta + x)} \exp\left(-x^2 - \frac{\eta^2}{x^2}\right) \,\mathrm{d}x. \tag{31}$$

After the change of variables  $x \to \eta/t$ , there remains, at the leading order in  $\eta$ , the value

$$\langle \Psi_a | x^{-4} | \Psi_a \rangle \approx \eta \int_0^\infty \frac{\mathrm{d}x \, \exp(-t^2)}{(1+gt)}. \tag{32}$$

Again the integral is computed numerically, and the final expansion of the ground state energy with this approximate wavefunction in the  $c \rightarrow 0$  limit with  $b \ll c^{1/2}$ , turns out to be

$$E \approx 3 + 1.555\,04c^{1/4} + 1.068\,56b/c^{1/4} \tag{33}$$

a result very close to the expansion quoted in the last row of table 1. We should mention, however, that it is not clear how to improve this calculation based on the wavefunction  $\Psi_a$ , equation (25), in an analogous way to the one used at the beginning of this section with the basis of equation (17).

Let us now consider the other small coupling regime, namely when the  $x^{-4}$  perturbation is much more important than the  $x^{-6}$  perturbation. In this case, the correcting function W has a simple form [13], and the leading form of the wavefunction valid for small b and c = 0 is

$$\Psi = x \exp\left(-\frac{x^2}{2} - \frac{\sqrt{b}}{x}\right) \tag{34}$$

the energy being

$$E \approx 3 + 4\sqrt{b/\pi}.\tag{35}$$

To compute the correction due to the  $x^{-6}$  anharmonicity we may again use the variational principle, to leading order in the relevant parameter

$$\lambda = 2\sqrt{b}.\tag{36}$$

The norm is simply  $\sqrt{\pi}/4$ . In order to compute the expectation value of the perturbation,  $\langle \Psi | x^{-6} | \Psi \rangle$ , we split the integration interval into two parts

$$I_{\rm a} = \int_0^{q\lambda} x^{-4} \exp(-x^2 - \lambda/x) \,\mathrm{d}x$$
(37)

anđ

$$I_{\rm b} = \int_{q\lambda}^{\infty} x^{-4} \exp(-x^2 - \lambda/x) \,\mathrm{d}x \tag{38}$$

q being a free parameter. One then has the following lower and upper bounds

$$\exp(-q^2\lambda^2)\int_0^{q\lambda} x^{-4}\exp(-\lambda/x)\,\mathrm{d}x \leqslant I_a \leqslant \int_0^{q\lambda} x^{-4}\exp(-\lambda/x)\,\mathrm{d}x \tag{39}$$

and

$$\exp(-1/q)\int_{q\lambda}^{\infty} x^{-4}\exp(-x^2)\,\mathrm{d}x \leqslant I_b \leqslant \int_{q\lambda}^{\infty} x^{-4}\exp(-x^2)\,\mathrm{d}x. \tag{40}$$

The integrals bounding  $I_a$  may be computed analytically, and it is also quite easy to get the leading term in  $\lambda$  of the integrals bounding  $I_b$ , with the result

$$\frac{1}{\lambda^3} \left[ e^{-1/q} \left( 2 + \frac{2}{q} + \frac{1}{q^2} \right) + \frac{1}{3q^3} \right] \ge I_a + I_b \ge \frac{1}{\lambda^3} e^{-1/q} \left( 2 + \frac{2}{q} + \frac{1}{q^2} + \frac{1}{3q^3} \right).$$
(41)

Choosing q to take the value which maximizes the lower bound and the value which minimizes the upper bound (note that the values of q for the lower and upper bounds

may be different), with the fortunate result that both limits are the same and equal to  $2/\lambda^3$ , so that in this regime we have

$$E \approx 3 + 4\sqrt{\frac{b}{\pi}} + \frac{1}{\sqrt{\pi}} \frac{c}{b^{3/2}}$$
 (42)

provided that

$$b \ll 1 \qquad c \ll b^2 \tag{43}$$

with both b and c positive.

The main results of this section are the two small coupling regimes given by equation (24) with the conditions of equation (20), and equation (42) in the domain determined by equation (43). Note, however, that there exists still a *third case* corresponding to the regime where both perturbations are of the same importance. This case will be discussed in section 5.

## 4. The strong coupling expansion

The shape of the interaction potential for large values of b, or large values of c, or both large, is very different from the shape in the case of small anharmonicity parameters. Instead of having just a spike very close to the origin, now the potential resembles a wide valley extending from x = 0 up to  $x = \infty$  with a minimum in the middle. Again none of the terms of the potential may be considered as small in the sense of perturbation theory.

To compute the ground state energy we may follow a method borrowed from the 1/N expansion of Witten [21], where N is the number of dimensions of the space, for the study of the hydrogen atom. This method was successfully applied [14] to the simple spiked oscillator  $x^2 + \lambda/x^{\alpha}$ , as well as to the anharmonic  $x^N$  potential in an N-dimensional space [22]. The basic idea underlying this strong coupling expansion is to seat down at the minimum of the potential (which will correspond to a global shift of the energy), then construct a one-dimensional harmonic oscillator centred at this point with a shape parameter related to the second derivative of the full potential at the minimum and, finally, compute the effect of the rest of the interaction by means of an almost standard perturbation theory. The minimum of our potential is located at  $x = x_m$  satisfying the equation

$$x^8 - 2bx^2 - 3c = 0. (44)$$

For both c > 0 and b > 0 we have the bounds on  $x_m$ 

$$x_{\rm m}^8 > 3c$$
  $x_{\rm m}^6 > 2b$  (45)

i.e.  $x_m$  will be a large number for b or c large. The value of the potential at the minimum is given by

$$V(x_{\rm m}) = \frac{4x_{\rm m}^2}{3} \left(1 + \frac{\gamma}{4}\right) \tag{46}$$

where we have introduced the parameter

$$\gamma = b/x_{\rm m}^6. \tag{47}$$

For b > 0 and c > 0, one has  $\gamma < 1/2$ . The second derivative is

$$V''(x_{\rm m}) = 16(1 - \gamma/2) \tag{48}$$

and the remaining derivatives are given by the closed formula

$$V^{(N)}(x_{\rm m}) = \frac{(-1)^N (6)_N}{3x_{\rm m}^{N-2}} \left( 1 - \gamma \left( 2 - \frac{60}{(N+4)(N+5)} \right) \right) \tag{49}$$

where  $(z)_N$  is the Pochhammer symbol.

Following the steps described earlier we change variable by moving to a new origin of coordinates located at  $x_m$ , so that for  $t = x - x_m$  there results the equivalent problem

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}t^2} + \frac{E_{-2}}{\lambda^2} + \alpha^2 t^2 + \sum_{k=1}^{\infty} \lambda^k C_k t^{k+2}$$
(50)

where  $E_{-2}$  is the minimum potential energy, equation (46),

$$E_{-2} = (4+\gamma)/3 \tag{51}$$

the oscillator constant  $\alpha$  is

$$\alpha = 2\sqrt{2-\gamma} \tag{52}$$

and the constants defining the perturbation are

$$C_{k} = \frac{(-1)^{k} (6)_{k+2}}{3(k+2)!} \left( 1 - \gamma \left( 2 - \frac{60}{(k+6)(k+7)} \right) \right).$$
(53)

We have introduced the *relevant* coupling constant

$$\lambda = 1/x_{\rm m}.\tag{54}$$

The ground state energy of the new Hamiltonian will have a diverging term  $E_{-2}\lambda^{-2}$ , the sub-index -2 reflecting the fact that this quantity is proportional to  $\lambda^{-2}$ , plus the zero-point motion of the harmonic oscillator,

$$E_0 = \alpha \tag{55}$$

which is of the order zero in the effective coupling constant, plus all the perturbative corrections corresponding to the last term in the Hamiltonian. Due to parity considerations only even powers of  $\lambda$  contribute to the ground state energy (but odd powers contribute to the wavefunction corrections). In conclusion, the ground state energy is given by the expansion

$$E = E_{-2}\lambda^{-2} + E_0 + \sum_{k, \text{ even} \ge 2} E_k \lambda^k$$
(56)

in terms of the effective coupling constant  $\lambda = 1/x_{\rm m}$ .

It is convenient to make some comments on this expansion of the energy. The anharmonicity parameters b and c appear almost only through the combination corresponding to  $x_m$ . There is also a residual dependence on b and c through the other parameter  $\gamma$  but the range of variation of this quantity is small (from 0 to  $\frac{1}{2}$  for positive b and c) and does not play a relevant role in the convergence of the expansion.

The actual dependence of  $x_m$  on b and c may be written down by solving equation (44). This is actually a quartic equation in  $x_m^2$ , but the resulting expression is too cumbersome to be of any practical interest. In actual calculations it is better to solve this equation by using the time-honoured substitution method due to Bernouilli,

$$x_{\rm m}^{(0)} = (3c)^{1/8} \tag{57}$$

$$x_{\rm m}^{(n)} = [3c + 2b(x_{\rm m}^{(n-1)})^2]^{1/8}$$
(58)

which converges very quickly.

Even if we have paid special attention to the case in which both b and c are positive, the method can also be applied to negative values of b. Note, however, that c must always be positive. The only condition to have in mind for the application of the strong coupling expansion is that  $x_m$  must be large.

**Table 2.** The comparison of the strong coupling expansion with some exact results. Each column corresponds to an elementary solution of one of the sets described in section 1. For each solution we list the values of the parameters b and c, the exact value of the energy and the value  $x_{\rm m}$  of the minimum of the interaction. The last rows include the strong limit expansion, and the label of the first column indicates the number of terms considered in the strong coupling expansion.

Set	Set 1	Set 1	Set 2	Set 2	Set 3
Ь	1	9	7	45	-24.5125
с	1	9	49	225	600.8623
E(exact)	5	7	7	11	11
xm	1.254 88	1.7321	1.7837	2.4274	2.4942
0	4.875 229	6.915 322	6.989 695	10.956 593	10.982 859
2	5.069 840	7.021 248	7.006 559	11.006 935	10.003 993
4	4.961 81	6.995 461	6.995791	10.998 913	10.998 942
6	5.015 19	7.000 204	7.002916	11.000 121	11.000 315
8	5.007 04	7.000 690	6.997 789	11.000 021	10.999 898
10	4.967 986	6.999 415	7.001814	10.999 975	11.000 033
12	5.054 252	7.000 205	6.998 435	11.000 012	10.999 991
14	4.957 805	7.000 189	7.001 343	10.999 996	11.000 000
16	4.900 698	6.999 563	6.999 002	10.999 998	11.000 002
18	5.560 719	7.000 386	7.000 256	11.000 002	10.999 996
20	3.588 351	7.000 867	7.001 452	10.999 997	11.000.004

The calculation of the coefficients  $E_k$  of the strong coupling expansion is described in appendix B. We show in table 2 some comparisons of the strong coupling expansion with exact results for the ground state energy. For this comparison we have selected some cases corresponding to the sets of elementary solutions described in section 2, including also negative values of b. In all cases the value of  $x_m$  is not too large, ranging from 1.25 to 2.50, so that the comparison is not the most favourable. Nevertheless, the results of the strong coupling expansion are very good, with the only exception in the case b = c = 1 where the expansion shows symptoms of instability. Of course this series should have some radius of convergence which cannot be determined unless one has a closed expression for the coefficients.

## 5. The self-transformation of the Hamiltonian

By changing  $x \to 1/x$  in equation (1), and afterwards introducing a new wavefunction as the old one divided by x, there results the differential equation

$$-\frac{d^{2}\Psi}{dx^{2}} + cx^{2}\Psi - \frac{E}{x^{4}}\Psi + \frac{1}{x^{6}}\Psi = -b\Psi.$$
(59)

In order to obtain an equation formally equivalent to equation (1) it is still necessary to scale the new independent variable x by the quantity  $c^{-1/4}$ , so as to remove the coefficient c from the harmonic potential. Then this gives the same starting Hamiltonian with a new set of parameters related to the starting set of parameters by the equations

$$\hat{b} = -c^{1/2}E$$
  $\hat{c} = c$   $\hat{E} = -bc^{-1/2}$ . (60)

The meaning of these substitution rules is fairly obvious: if the eigenvalue E is known for given values of b and c, then the eigenvalue corresponding to the set of parameters  $\hat{b}$  and  $\hat{c}$  as given by the first two equations (60) is  $\hat{E}$  as computed by means of the last equation of set (60).

These replacement rules can be used to transform the previous weak coupling and strong coupling formulae, so as to get specific equations relating the energy to the anharmonicity parameters, with a different domain of validity. Special care is needed so as to use the perturbative expansions in their strict domain of validity, otherwise the inversion may lead to nonsense results.

For example, to invert the expansion given in equation (24), and in addition to consider the restrictions given in equation (20), care has to be taken so that the next neglected term (which is proportional to  $c^{1/2}$ ) is much smaller than the last considered term, which is proportional to  $b/c^{1/4}$ . Then for a small enough value of c, the corresponding b must lie in a strip delimited by the conditions

$$c \gg b^2 \gg c^{3/2}.\tag{61}$$

These two conditions in turn delimit the domain of the transformed coupling constants. In this case there results the new weak coupling expansion

$$E \approx \frac{1}{\beta} (\alpha + 3c^{-1/4} + bc^{-3/4})$$
(62)

which is valid for small c and for values of b in a small interval centred around  $-c^{1/2}(3 + \alpha c^{1/4})$ . The size of this interval is quite small, but the derivative of the energy with respect to b is very large, i.e.

$$\mathrm{d}E/\mathrm{d}b \approx c^{-3/4}/\beta. \tag{63}$$

In other words, it is still a fairly large domain.



Figure 3. The small coupling expansions for the ground state energy. Line 1 corresponds to equation (24), and line 2 to equation (42). The lines 3 and 4 are the transform of equations (24) and (42), respectively. The continuous curve represents the numerically computed values of the energy.

It is not possible to invert the other small coupling expansion, corresponding to equation (42), because this gives a transcendental equation. However, it is still possible to compute the energies and domains corresponding to the transformation equations. This is shown in figure 3, which corresponds to c = 0.001 and b in the interval (-0.2, 0.2). In addition to the numerically determined values of ground state energy, there appear four other almost straight lines. The line near b = 0, labelled 1, corresponds to the weak coupling expansion given in equation (24). Its transformed equation is the line near b = -0.1, labelled 3. The line 2, centred near b = 0.15, corresponds to the other small coupling expansion equation (42), and is transformed into line 4, which is the almost vertical line at the left of the figure. We note that the last two cases do not strictly fulfil the required restrictions given in equation (20). This is the reason for the small differences between the numerically determined eigenvalue and the perturbative expansion.

In conclusion, by using the small coupling expansions and the transformation equations (60), we may cover all the domain around c = b = 0.

The transformation equations may also be used in the case of the strong coupling expansion, but in this case it is again not possible to get a closed formula because the dependence on the anharmonicity parameters is quite involved. Note, however, that the transformation allows to extend the domain of validity of the strong coupling expansion to large and negative values of b, as implied by the first of equations (60).

Finally, let us simply mention that the (b, c) lines corresponding to the elementary solutions transform into themselves, so that no new information is obtained from these solutions.

#### 6. Summary

In this paper we have determined the analytic behaviour of the ground state energy of the  $x^2 + b/x^4 + c/x^6$  anharmonic oscillator corresponding to several regimes of the anharmonicity constants:

(i) For  $c \ll 1$  and  $b \ll c^{1/2}$  the leading terms are

$$E \approx 3 + \alpha c^{1/4} + \beta b/c^{1/4} \tag{64}$$

where  $\alpha = 2\Gamma(3/4)/\pi^{1/2}\Gamma(5/4)$ , [13], and several approximate values for  $\beta$  are shown in table 1 and in equation (33).

(ii) For  $b \ll 1$  and  $c \ll b^2$  the leading terms are

$$E \approx 3 + 4(b/\pi)^{1/2} + c/\pi^{1/2}b^{3/2}.$$
(65)

These results do not directly cover all the accesible region around b = c = 0. However, the use of the self-transforming property of the Hamiltonian covers all the area around null values of the anharmonicity constants.

Finally, we have determined the analytic behaviour of the ground state energy for large values of the anharmonicity constants. This in turn implies large values of  $x_m$ , the abscisa of the minimum of the potential. The ground state energy depends on b and c mainly through  $x_m$ . The expansion has a term diverging as  $x_m^2$ , then a constant term and finally an expansion in powers of  $1/x_m^2$ . Again the use of the self-transforming property of the Hamiltonian permits the extension of the validity domain for large values of c to large and negative values of b, covering in this way all the region around the point  $c = \infty$ .

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#### Appendix A. The calculation of the small coupling expansion

The question is to solve the generalized eigenvalue equation (23) corresponding to the Hamiltonian equation (1) in the non-orthogonal basis given in equation (17). Moreover, we are interested only in the lowest orders of the parameters  $\eta$  and  $\sigma$  introduced in section 3. The matrix elements of interest are

$$\begin{aligned} \langle \Psi_k | H - W | \Psi_j \rangle &= \mathcal{N}_k \mathcal{N}_j \int_0^\infty \exp(-x^2 - \eta^2 / x^2) [(7 - 4j - W) x^{6-2(k+j)} \\ &+ (2\eta^2 - 4j^2 + 10j - 6) x^{4-2(k+j)} + \eta^2 (4j - 3 + \sigma) x^{2-2(j+k)}] \, \mathrm{d}x. \end{aligned}$$
(A1)

The relevant integrals are of the generic form

$$I_{p} = \int_{0}^{\infty} x^{p} \exp(-\nu x^{2} - \mu/x^{2}) \,\mathrm{d}x \tag{A2}$$

for even values of p, which may be generated from  $I_0$ ,

$$I_0 = (\sqrt{\pi}/2) \exp(-2\sqrt{\mu\nu})/\sqrt{\nu}$$
(A3)

by computing derivatives with respect to  $\nu$  (for p > 0) or  $\mu$  (for p < 0) and substituting afterwards  $\nu \to 1$  and  $\mu \to \eta^2$ . Then the determinant of the matrix is computed and solved in terms of the eigenvalue W.

This process may be easily carried out with the help of an algebraic code. We used REDUCE [23] to carry out this algebraic calculation and the resulting program is so simple and short that we prefer to write it down instead of attempting to explain all technical details related to this computation. The code is listed at the end of this appendix.

The correspondence of the variables in the code with our current notation is

$$Y \to \eta$$

$$S \to \sigma$$

$$N \to \nu$$

$$M \to \mu$$
(A4)

The procedure INTEGRAL computes  $I_p$  as described earlier. Note that all integrals have been scaled by fixing  $I_0 = 1$ , which is called AUX in the code. The procedure NORM defines the scaling factors  $\eta^{2j-5/2}$  as outlined in section 3, their role being to avoid negative powers of  $\eta$  in front of the matrix elements. Next there is a long statement (14 lines) which evaluates the matrix elements. It contains two chained DO-loops, their indices corresponding to the labels of the states. The assignment to the variable ZZZ is a plain translation of equation (A1). The only tricky point is related to the asymptotic rules Y\*\*2=0 and S\*\*2=0. This is a special instruction of REDUCE which will skip all terms depending on powers of Y and S greater than or equal to 2. The individual pieces needed to compute a given matrix element contain positive and negative powers of high degrees on  $\eta$  and  $\sigma$ , but once the combination called ZZZ is evaluated it is regular, and the leading powers in  $\eta^0$  and  $\eta^1$  may be extracted. Once simplified ZZZ and stored in H(k, j), the rules must be *cleared* for the next computation. The rest of the code is self-explanatory.

#### Algorithm

%Before inputting this package define ND with a numeric value % Algorithm to define the basic integrals AUX:=1/(SQRT(N)\*EXP(2\*SQRT(N\*M))); PROCEDURE INTEGRAL(P); IF P=0 THEN 1 ELSE IF P>0 THEN SUB(N=1,SUB(M=Y\*\*2,(-1)\*\*(P/2)\*DF(AUX,N,P/2)/AUX)) ELSE SUB(N=1,SUB(M=Y\*\*2,(-1)\*\*(-P/2)\*DF(AUX,M,-P/2)/AUX)) ; %

```
% Scaling of states to avoid powers of Y in the denominator
PROCEDURE NORM(K);
IF K=1 THEN 1 ELSE Y^{**}(2^{*}K-5/2);
%
B:=S*Y**2;
% Note that C \approx Y^{**4}
%
% Matrix elements
MATRIX H(ND.ND):
FOR K:=1 STEP 1 UNTIL ND DO FOR J:=K STEP 1 UNTIL ND DO
BEGIN
% W is the eigenvalue. First compute with all powers of Y
ZZZ:=(7 - 4*J-W)*INTEGRAL(6-2*(K+J))
+(2*Y*2-4*J**2+10*J-6)*INTEGRAL(4-2*(K+J))
+(4*J*Y**2-3*Y**2+B)*INTEGRAL(2-2*(K+J));
ZZZ:=ZZZ*NORM(J)*NORM(K);
% Then remove unwanted powers in Y and S
LET Y**2=0; LET S**2=0;
H(K,J):=ZZZ;
CLEAR S**2; CLEAR Y**2;
% And the symmetric term
H(J,K):=H(K,J);
END:
% Generalized eigenvalue equation
LET Y**2=0; LET S**2=0;
EQUATION:=DET(H);
% Solve it
EOUATION:=SUB(W=3+A*Y,EQUATION);
% After this substitution the leading term is null, and the rest
% is linear in A. so
A:=-SUB(A=0,EQUATION)/SUB(A=0,DF(EQUATION,A));
% Finally, expand in powers of S
A:=SUB(S=0,A)+S*SUB(S=0,DF(A,S));
% End of the algorithm
```

# Appendix B. The calculation of the strong coupling expansion

The purpose of this appendix is the determination of the series expansion of the ground state energy of the Hamiltonian given in equation (50) in powers of the strong coupling constant  $\lambda$ . With the change of variable  $t \to x/\sqrt{\alpha}$  and after removing the *t*-independent term, there remains the Hamiltonian

$$h = -\frac{d^2}{dx^2} + \sum_{k=0}^{\infty} \lambda^k D_k x^{k+2}$$
(B1)

where

$$D_k = C_k \alpha^{-(k+4)/2}$$
  $k = 1, ..., \infty$  (B2)

and  $D_0 = 1$ . We are searching for the expansion of the ground state energy of h in powers of  $\lambda$ , i.e.

$$E = \sum_{0}^{\infty} E_k \lambda^k.$$
(B3)

The most immediate way to proceed is to use a modified version of the familiar Rayleigh-Schrödinger perturbation theory, as in [14]. There are, however, other more efficient methods based on the polynomial character of the perturbation potential.

One such method consists of extending the algorithm used by Bender and Wu [24], also known as Dalgarno's F-functions method [25], for the computation of the small coupling expansion of the  $x^4$  anharmonic oscillator. The wavefunction is written as

$$\psi(x) = \exp(-x^2/2) \sum_{n=0}^{\infty} \lambda^n p_n(x)$$
 (B4)

where  $p_x(x)$  are polynomials of degree 3n whose coefficients are recursively determined, together with the coefficients  $E_n$ , after a direct substitution of the wavefunction in the Schrödinger equation.

However, the most efficient way to treat our perturbed oscillator is to use the hypervirial perturbation theory [16]. This method is based on the relation

$$2E\langle f'\rangle = \langle fV' + 2f'V\rangle - \langle f'''\rangle/2 \tag{B5}$$

between expectation values taken with respect to any exact eigenstate of the full Hamiltonian. We will focus on the ground state. In equation (B5) f is an arbitrary function of x, provided the expectation values are defined (not infinity). By choosing  $f = x^{N+1}$ , with  $N \ge -1$ , one obtains the set of equations

$$2(N+1)E\langle x^N \rangle = \sum_{k=0}^{\infty} (2N+k+4)D_k \langle x^{N+2+k} \rangle - N(N^2-1)\langle x^{N-2} \rangle/2.$$
 (B6)

The next step is to expand both the energy and the moments in terms of the coupling constant  $\lambda$ ,

$$E = \sum_{p=0}^{\infty} E_k \lambda^k \tag{B7}$$

and

$$\langle x^r \rangle = \sum_{p=0}^{\infty} A_{r,k} \lambda^k.$$
(B8)

The coefficients  $E_k$  and  $A_{n,k}$  are the quantities to be determined. Some of them have known values.  $E_0$  is the unperturbed harmonic oscillator energy,

$$E_0 = 1.$$
 (B9)

The normalization of the wavefunction requires

$$A_{0,k} = \delta_{0k} \tag{B10}$$

and from the known values of the moments of  $x^r$  with respect to the unperturbed harmonic oscillator ground state wavefunction we obtain

$$A_{2k+1,0} = 0 \tag{B11}$$

and

$$A_{2k,0} = \frac{(2k-1)!!}{2^k}.$$
(B12)

By substituting the  $\lambda$  expansions in equation (B6) a set of recurrence relations is obtained characterized by the integer parameters  $N \ge 1$  and  $n \ge 1$ 

$$2(N+1)\sum_{l=0}^{n} E_{n-l}A_{N,l} = \sum_{l=0}^{n} (2N+4+n-l) \times D_{n-l}A_{N+n+2-l,l} - N(N^2-1)A_{N-2,n}/2.$$
(B13)

These relations are not sufficient to determine the unknowns. A suplementary condition is obtained by analysing the effect of a small variation  $\delta\lambda$  of the coupling constant, namely

$$\delta E = \delta \lambda \sum_{n} n E_n \lambda^{n-1} = \delta \lambda \langle \partial V / \partial \lambda \rangle \tag{B14}$$

which is translated into

$$(n+1)E_{N+1} = \sum_{l=0}^{n} (n-l+1)D_{n-l+1}A_{n-l+3,l}.$$
 (B15)

For the practical use of these recurrence relations one must jump alternatively from equation (B13) to equation (B15) and back again to equation (B13), in a manner analogous to the one described in [16].

In the long formulae following this paragraph we include the explicit solution of these equations. Note that all corrections  $E_n$  with odd sub-index are null, because of parity considerations. Our strong coupling expansion is obtained by substituting in this equation the actual values of the constants  $D_n$ .

$$\begin{split} E_2 &= (12D_2 - 11D_1^2)/16\\ E_4 &= (480D_4 - 1040D_3D_1 - 336D_2^2 + 1368D_2D_1^2 - 465D_1^4)/256\\ E_6 &= (26\,880D_6 - 67\,200D_5D_1 - 46\,080D_4D_2 + 103\,360D_4D_1^2 - 28\,736D_3^2\\ &\quad + 182\,016D_3D_2D_1 - 144\,544D_3D_1^3 + 21\,312D_2^3 - 189\,232D_2^2D_1^2\\ &\quad + 182\,028D_2D_1^4 - 39\,709D_1^6)/4096 \end{split}$$

$$\begin{split} E_8 &= (7\,741\,440\,D_8-21\,934\,080\,D_7\,D_1-15\,482\,880\,D_6\,D_2+37\,990\,400\,D_6\,D_1^2\\ &\quad -17\,117\,184\,D_8\,D_3+62\,963\,712\,D_8\,D_2\,D_1-56\,168\,448\,D_5\,D_1^3\\ &\quad -7\,157\,760\,D_4^2+61\,659\,136\,D_4\,D_3\,D_1+22\,978\,560\,D_4\,D_2^2\\ &\quad -142\,829\,568\,D_4\,D_2\,D_1^2+74\,813\,952\,D_4\,D_1^4+26\,984\,448\,D_3^2\,D_2\\ &\quad -73\,326\,080\,D_3^2\,D_1^2-126\,423\,040\,D_3\,D_2^2\,D_1+270\,965\,760\,D_3\,D_2\,D_1^3\\ &\quad -96\,779\,520\,D_3\,D_1^5-7\,906\,560\,D_2^4+119\,097\,600\,D_2^3\,D_1^2\\ &\quad -220\,481\,760\,D_2^2\,D_1^4+119\,670\,288\,D_2\,D_1^6-19\,250\,805\,D_8^8)/262\,144\\ E_{10} &= (681\,246\,720\,D_{10}-2\,157\,281\,280\,D_9\,D_1-1\,548\,288\,000\,D_8\,D_2\\ &\quad +4\,128\,768\,000\,D_8\,D_1^2-1\,587\,511\,296\,D_7\,D_3+6\,620\,479\,488\,D_7\,D_2\,D_1\\ &\quad -6\,496\,387\,072\,D_7\,D_1^3-1\,348\,730\,880\,D_6\,D_4+6\,306\,922\,496\,D_6\,D_3\,D_1\\ &\quad +2\,453\,176\,320\,D_6\,D_2^2-16\,087\,400\,448\,D_6\,D_2\,D_1^2\\ &\quad +9\,096\,865\,792\,D_6\,D_1^4-727105536\,D_5^2+5\,944\,147\,968\,D_5\,D_4\,D_1\\ &\quad +5\,195\,464\,704\,D_5\,D_3\,D_2-15\,591\,161\,856\,D_5\,D_3\,D_1^2\\ &\quad -13\,450\,395\,648\,D_5\,D_2^2\,D_1+31\,289\,384\,960\,D_5\,D_2\,D_1^3\\ &\quad -120\,057\,477\,12\,D_5\,D_1^5+2\,264\,186\,880\,D_4^2\,D_2-7\,389\,556\,736\,D_4^2\,D_1^2\\ &\quad +2\,546\,483\,200\,D_4\,D_3^2-26\,226\,966\,528\,D_4\,D_3\,D_2\,D_1\\ &\quad +30\,198\,779\,904\,D_4\,D_3\,D_1^3-3\,435\,356\,160\,D_4\,D_3^3\\ &\quad +40\,827\,789\,312\,D_3^2\,D_2\,D_1^2-52\,613\,804\,544\,D_4\,D_2\,D_1^4\\ &\quad +15\,147\,285\,888\,D_4\,D_1^6-4\,502\,528\,000\,D_3^3\,D_1-5\,777\,956\,864\,D_3^2\,D_2^2\\ &\quad +40\,827\,789\,312\,D_3^2\,D_2\,D_1^2-26\,299\,471\,360\,D_3^2\,D_1^4\\ &\quad +23\,751\,905\,280\,D_3\,D_3^2\,D_1-95\,328\,762\,880\,D_3\,D_2^2\,D_1^3\\ &\quad +83\,114\,469\,120\,D_3\,D_2\,D_1^5-18\,922\,442\,560\,D_3\,D_1^7+938\,732\,544\,D_2^5\\ &\quad -21\,126\,632\,192\,D_2^4\,D_1^6+23\,131\,433\,052\,D_2\,D_1^8\\ &\quad -61\,365\,048\,672\,D_2^2\,D_1^6+23\,131\,433\,052\,D_2\,D_1^8\\ &\quad -2\,94\,4\,91\,879\,D_1^{0})/4\,194\,304 \end{split}$$

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