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Spherical anharmonic oscillator in self-similar approximation

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Abstract. The method of self-similar approximations is applied here for calculating the eigenvalues of the three-dimensional spherical anharmonic oscillator. The advantage of this method is in its simplicity and high accuracy. For the case considered we show that based only on two terms of perturbation theory we find the spectrum with an error not worse than of the order 10^{-3} for the whole range of anharmonicity parameters, from zero up to infinity, and for any energy levels. The comparison with other known analytical methods proves that our method is more simple and accurate.

1. Introduction

Realistic physical problems are almost always so complicated that it is a very rare occasion when they can be solved exactly. The standard way of tackling them is to invoke perturbation theory. The standard situation is that the use of the latter yields a divergent series. When a number of terms in a series are known (about ten of them) then one may find an effective sum of the asymptotic series by means of some resummation technique. However, in the majority of realistic, that is complicated, cases one is able to extract only the first few terms of perturbation theory, generally not more than two of them. In a situation like that the usual resummation techniques are not applicable. A thorough discussion of these difficulties can be found in Stevenson [1].

A method to find an effective sum of a divergent series, or an effective limit of a divergent sequence, with only a few terms has been recently suggested [2]. The latter was called the method of self-similar approximations since it was based on self-similar relations for subsequent terms, which forces a divergent sequence to become convergent. This method [2] was shown [2–5] to be quite successful for various problems in statistical physics and quantum mechanics, where the ground-state energy is the main interest.

Here we shall demonstrate that the method of self-similar approximations [2] works well for calculating not solely the ground-state energy but also the whole spectrum. To this end, we consider the problem whose mathematical structure is typical of many problems of statistical mechanics and field theory. This is the three-dimensional anharmonic oscillator. The divergences arising in applying perturbation theory to it are of the same nature as those appearing in the perturbation-theory

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calculations for the majority of statistical models with Hamiltonians containing four-operator interactions and also for quantum field theories having the φ^4 structure. A review of these questions has been given by Simon [6].

In section 2 we present the scheme of the method of self-similar approximations, all details of which have been expounded in the early papers [2–5]. In section 3 we apply this method to the three-dimensional anharmonic oscillator with spherical symmetry. We show that our method, invoking only two terms of perturbation theory, allows the calculation of the whole spectrum with very good accuracy, within the order of 10^{-3}, for arbitrary anharmonicity constants ranging from zero up to infinity and for all energy levels. In section 4 we analyse the other known analytical methods: the modified perturbation theory, the quasiclassical approximation, the large-dimensional expansion and the shifted large-dimensional expansion. The analysis proves that among these methods ours is the simplest and most accurate, if accuracy is defined by the maximal error for all anharmonicity constants and energy levels, not only for some of them. Section 5 is a conclusion.

2. Scheme of method to be used

We shall not repeat here the foundation and nuances of the method of self-similar approximations which have been explained in detail in [2–5], but we shall formulate its scheme needed for further investigation.

Assume that we are interested in a function $f(n,g)$, in which n is a multiparameter, for instance enumerating the energy levels, and g is a coupling constant. By perturbation theory or an iterative procedure we obtain a sequence of approximations $f_k(n,g)$ with $k = 0,1,2\ldots$. Introduce an additional sequence of functions $z_k(n,g)$ whose role is to govern the convergence of the sequence of complex functions

$$f_k(n,g) = f_k(n,g,z_k(n,g)). \tag{1}$$

The governing functions are to be defined by one of the fixed-point conditions, for example by the equation

$$\frac{\mathrm{d}}{\mathrm{d}z} f_k(n,g,z) = 0 \qquad z = z_k(n,g). \tag{2}$$

Define the coupling function $g(n,f)$ by the equality

$$f_0(n,g,z(n,g)) = f \qquad g = g(n,f) \tag{3}$$

in which

$$z(n,g) \equiv z_0(n,g) \equiv z_1(n,g).$$

Introduce the distribution of approximations

$$y_{ks} = \{f_s(n,g(n,f),z_k(n,g(n,f))) - f_k(n,g(n,f),z_k(n,g(n,f)))\}^{-1} \tag{4}$$

satisfying the normalization

$$\int_{f_k(n,g)}^{f_*(n,g)} y_{ks}(n,f)\,\mathrm{d}f = 1. \tag{5}$$

The function $f_*(n,g)$ in equation (5) is merely the self-similar approximation for the function $f(n,g)$. Function (4) is called the distribution of approximations since it describes, according to (5), their distribution between $f_k(n,g)$ and the self-similar approximation.

3. Spherical anharmonic oscillator

The three-dimensional anharmonic oscillator with spherical symmetry can be reduced, as is known, to the one-variable problem with the radial Hamiltonian

$$H = -\frac{1}{2m}\frac{d^2}{dr^2} + \frac{l(l+1)}{2mr^2} + \frac{m\omega^2}{2}r^2 + \lambda m^2 r^4 \tag{6}$$

in which m, ω, λ are positive parameters; the radial variable $r \in (0, \infty)$; the azimuthal quantum number $l = 0, 1, 2, \ldots$.

As an initial step for perturbation theory it is reasonable to choose the harmonic form

$$H_0 = -\frac{1}{2m}\frac{d^2}{dr^2} + \frac{l(l+1)}{2mr^2} + \frac{m\omega_0^2}{2}r^2 \tag{7}$$

whose energy levels are given by the expression

$$E_{nl}^{(0)} = (2n + l + \tfrac{3}{2})\omega_0 \qquad n, l = 0, 1, 2, \ldots. \tag{8}$$

Here $n = 0, 1, 2, \ldots$ is the radial quantum number and $l = 0, 1, 2, \ldots$ is the azimuthal quantum number. For the principal quantum number we shall use the notation $\nu \equiv 2n + l$ from which the qualification $l \leqslant \nu$ automatically follows. Let us note that different authors use slightly different notation for these quantum numbers. For example, the radial quantum number is often written as n_r. However, the latter will appear in what follows about 100 times, therefore to write n_r in the place of n would make the majority of formulae unreasonably cumbersome. This is why we opt for the simpler notation defined above, which is also often used in the literature for dealing with anharmonic oscillators.

For what follows it is convenient to introduce the dimensionless coupling, g, and trial, z, parameters,

$$g \equiv \lambda/\omega^3 \qquad z \equiv \omega_0/\omega \tag{9}$$

as well as the dimensionless Hamiltonians

$$H(\xi) \equiv H/\omega \qquad H_0(\xi) \equiv H_0/\omega \qquad \xi \equiv (m\omega)^{1/2} r. \tag{10}$$

Then, equations (6) and (7) read

$$H(\xi) = -\frac{1}{2}\frac{d^2}{d\xi^2} + \frac{l(l+1)}{2\xi^2} + \frac{1}{2}\xi^2 + g\xi^4$$

$$H_0(\xi) = -\frac{1}{2}\frac{d^2}{d\xi^2} + \frac{l(l+1)}{2\xi^2} + \frac{1}{2}z^2\xi^2. \tag{11}$$

The eigenfunctions of $H_0(\xi)$ are

$$\chi_{nl}^{(0)} = \left[\frac{2n!\, z^{l+3/2}}{\Gamma(n + l + \frac{3}{2})}\right]^{1/2} \xi^{l+1} \exp\left(-\frac{z}{2}\xi^2\right) L_n^{l+1/2}(z\xi^2) \quad .$$

where $L_n^l(\cdot)$ is an associated Laguerre polynomial.

Using the Rayleigh–Schrödinger perturbation expansion, we can find the approximate expressions

$$e_k(n,l,g,z) \equiv E_{nl}^{(k)}/\omega \qquad k = 0,1,2,\ldots \tag{12}$$

for the eigenvalues of $H(\xi)$, starting from the zero approximation

$$e_0(n,l,g,z) = (\nu + \tfrac{3}{2})z \qquad \nu \equiv 2n + l. \tag{13}$$

For the first approximation we get

$$e_1(n,l,g,z) = e_0(n,l,g,z) - \left(\nu + \frac{3}{2}\right)\frac{z^2-1}{2z} + \left(\nu + \frac{3}{2}\right)\frac{3g}{2z^2}\gamma_{nl} \tag{14}$$

where

$$\gamma_{nl} \equiv \left(\nu + \frac{3}{2}\right)\left[1 - \frac{l^2 + l - \frac{3}{4}}{3(\nu + \frac{3}{2})^2}\right]. \tag{15}$$

Expression (15) has the following limiting properties:

$$\lim_{n,l\to 0}\gamma_{nl} = \tfrac{5}{3}$$

$$\gamma_{nl} \simeq 2n \qquad n \to \infty \ (l < \infty)$$

$$\gamma_{nl} \simeq -\tfrac{2}{3}l \qquad l \to \infty \ (n < \infty).$$

The second approximation of (12) is

$$e_2(n,l,g,z) = e_1(n,l,g,z) - \left(\nu + \frac{3}{2}\right)\frac{(z^2-1)^2}{8z^3} + \left(\nu + \frac{3}{2}\right)\frac{3g(z^2-1)}{2z^4}\gamma_{nl}$$
$$- \left(\nu + \frac{3}{2}\right)\frac{g^2}{4z^5}\left[10 + 27\left(\nu + \frac{3}{2}\right)\gamma_{nl} - 10\left(\nu + \frac{3}{2}\right)^2\right]. \tag{16}$$

The fixed-point condition (2), i.e.

$$\frac{\mathrm{d}}{\mathrm{d}z}e_1(n,l,g,z) = 0 \qquad z = z(n,l,g) \tag{17}$$

yields the equation

$$z^3 - z - 6g\gamma_{nl} = 0. \tag{18}$$

The solution to the latter gives the governing function

$$z(n,l,g) = \begin{cases} \dfrac{2}{\sqrt{3}}\cos(\alpha_{nl}/3) & g \leqslant g_{nl} \\ A_{nl}^{+} + A_{nl}^{-} & g \geqslant g_{nl} \end{cases} \tag{19}$$

in which

$$\alpha_{nl} = \cos^{-1}(g/g_{nl})$$

$$A_{nl}^{\pm} = (3g)^{1/3}\left[1 \pm \sqrt{1 - \left(\frac{g_{nl}}{g}\right)^2}\right]^{1/3}$$

$$g_{nl} = (9\sqrt{3}\gamma_{nl})^{-1} = 0.064150/\gamma_{nl}.$$

Perturbation theory corresponds to the weak coupling limit, that is to $g \ll g_{nl}$. However, as is seen $|\gamma_{nl}| \to \infty$, as $n, l \to \infty$,because of which

$$g_{nl} \to 0 \qquad n, l \to \infty.$$

Therefore, the weak coupling region practically disappears for higher eigenvalues.

Using for brevity the notation

$$e_k(n, l, g) \equiv e_k(n, l, g, z(n, l, g)) \tag{20}$$

we define the coupling function from (2), which is now

$$e_0(n, l, g) = f \qquad g = g(n, l, f). \tag{21}$$

The latter, together with (13), is equivalent to the equation

$$(\nu + \tfrac{3}{2})z(n, l, g) = f. \tag{22}$$

For the distribution of approximations (4), which can be written as

$$y_{12}(n, l, f) = [e_2(n, l, g(n, l, f)) - e_1(n, l, g(n, l, f))]^{-1} \tag{23}$$

we obtain

$$y_{12}(n, l, f) = -\frac{48f^3/(\nu + \frac{3}{2})^4}{a_{nl}[f^2/(\nu + \frac{3}{2})^2 - 1]^2} \tag{24}$$

where

$$a_{nl} \equiv \left(\nu + \frac{3}{2}\right)\frac{9}{\gamma_{nl}} - \left(\nu^2 + 3\nu + \frac{5}{4}\right)\frac{10}{3\gamma_{nl}^2} - 6. \tag{25}$$

The limiting properties of (25) are

$$\lim_{n,l\to 0} a_{nl} = \tfrac{3}{5} \qquad \lim_{n\to\infty} a_{nl} = -\tfrac{1}{3} \qquad \lim_{l\to\infty} a_{nl} = 0.$$

Substituting distribution (24) into normalization (5), we come to the equation

$$\frac{e_*^2(n, l, g)/(\nu + \frac{3}{2})^2 - 1}{e_1^2(n, l, g)/(\nu + \frac{3}{2})^2 - 1} = \exp\left\{\frac{1}{e_*^2(n, l, g)/(\nu + \frac{3}{2})^2 - 1} - \frac{1}{e_1^2(n, l, g)/(\nu + \frac{3}{2})^2 - 1} - \frac{a_{nl}}{24}\right\} \tag{26}$$

for the self-similar approximation $e_*(n,l,g)$ of the anharmonic oscillator spectrum. The function $e_1(n,l,g)$ in (26), according to (14) and (18), can be written as

$$e_1(n,l,g) = \left(\nu + \frac{3}{2}\right)\frac{3z^2+1}{4z} \qquad z = z(n,l,g)$$

where the governing function is given by (19).

The asymptotic forms of the spectrum $e_*(n,l,g)$ can be easily found from (26) yielding in the weak coupling limit

$$e_*(n,l,g) \simeq \left(\nu + \tfrac{3}{2}\right)\left(1 + \tfrac{3}{2}g\gamma_{nl}\right) \qquad g \to 0 \tag{27}$$

and in the strong coupling limit

$$e_*(n,l,g) \simeq \frac{3}{4}\left(\nu + \frac{3}{2}\right)\exp\left(-\frac{a_{nl}}{48}\right)(6g\gamma_{nl})^{1/3} \qquad g \to \infty. \tag{28}$$

The weak coupling limit (27) coincides with the corresponding exact expansion in powers of g, which can be checked by putting $z = 1$ into (14).

For the ground-state energy from (27) and (28) we have

$$e_*(0,0,g) \simeq \tfrac{3}{2} + \tfrac{15}{4}g \qquad g \to 0$$

$$e_*(0,0,g) \simeq \tfrac{9}{8}\exp(-\tfrac{1}{80})(10g)^{1/3} = 2.393\,631 g^{1/3} \qquad g \to \infty. \tag{29}$$

The behaviour of highly excited energy levels in the self-similar approximation depends on the ratio

$$\theta_{nl} \equiv \frac{l}{\nu} = \frac{1}{2n+l} \tag{30}$$

which defines the limits following from (15),

$$\gamma_{nl} \simeq \nu(1 - \tfrac{1}{3}\theta_{nl}^2) \qquad \nu \to \infty \tag{31}$$

and from (25),

$$a_{nl} \simeq \frac{27}{3-\theta_{nl}^2} - \frac{30}{(3-\theta_{nl}^2)^2} - 6 \qquad \nu \to \infty. \tag{32}$$

In the case when $\nu \to \infty$ but $l < \infty$, we have $\theta_{nl} \to 0$; then

$$\gamma_{nl} \simeq \nu \qquad a_{nl} \simeq -\tfrac{1}{3} \qquad \theta_{nl} \to 0. \tag{33}$$

However, it can be that $\nu \to \infty$, $l \to \infty$ and $\theta_{nl} \to \theta$, where the latter is finite $(0 < \theta < 1)$. Then for small θ (31) and (32) give

$$\gamma_{nl} \simeq \nu(1 - \tfrac{1}{3}\theta^2) \qquad a_{nl} \simeq -\tfrac{1}{3} + \tfrac{7}{9}\theta^2. \tag{34}$$

The strong coupling limit (28) together with (33) yields

$$e_*(n,l,g) \simeq \tfrac{3}{4}e^{1/144}\nu^{4/3}(6g)^{1/3} = 1.372\,338\nu^{4/3}g^{1/3}. \tag{35}$$

In the intermediate case, when $0 < \theta_{nl} < 1$, the expression (28) for the excited energy levels does not allow such a simplification as in (35).

The accuracy of the self-similar approximation given by (26) can be evaluated by comparing it with exact numerical calculations. The latter have been done by a direct numerical solution of the corresponding Schrödinger equation written in the matrix form [7,8]. The low-lying levels have been accurately computed using Hill determinants [9] and recurrence relations [10,11].

Comparing the self-similar approximation $e_*(n,l,g)$ defined in (26) with the numerical results [7–11], we find that for any value of the anharmonicity parameter $g \in (0,\infty)$ and for any energy levels $(n, l = 0,1,2,\ldots)$ the maximal error is about 0.3%.

4. Comparison with other methods

It would be worth comparing the results obtained with those given by other analytical methods. In this comparison, it is natural to define the accuracy of a method by the maximal error of its results for all anharmonicity parameters and energy levels. That is, we shall define the accuracy of an approximate method, yielding $e_{app}(n,l,g)$, by the maximal error

$$\epsilon_{app} \equiv \sup_{g\in(0,\infty)} \sup_{n,l=0,1,2,\ldots} \left| \frac{e_{app}(n,l,g)}{e(n,l,g)} - 1 \right|$$

in which $e(n,l,g)$ is an exact numerical result.

Consider first the quasiclassical approximation applied to the three-dimensional anharmonic oscillator [12–14]. The Bohr–Sommerfeld condition for the energy levels leads to a very cumbersome transcendental equation, invoking the complete elliptic integrals of the first, second and third kinds and, in addition, a system of complicated equations for the turning points expressed through the Jacobian elliptic functions. An analysis of these equations shows [15, 16] that the quasiclassical approximation is quite accurate for high energy levels and strong anharmonicity, yielding an exact asymptotic expansion in the limit $g, n \to \infty$. Then

$$e(n,l,g) \simeq 1.376\,507\nu^{4/3}g^{1/3} \qquad \nu, g \to \infty.$$

However its accuracy drastically worsens for the low-lying energy levels, especially for the ground-state level. The maximal error of the latter level found in the quasiclassical approximation is 3% for the isotropic case and reaches 18% for an anisotropic model.

Another known approach for treating systems with strong interaction is the modified, or renormalized, perturbation theory [17–21]. In this approach one renormalizes the sequence of approximations according to (1) and define the governing functions either from the principle of minimal difference [17–19] or from the principle of minimal sensitivity [20, 21]. The latter, as applied to the anharmonic oscillator, gives more accurate results than the former [4, 20]. The accuracy of the modified perturbation theory with the principle of minimal sensitivity of the form (2) has been carefully analysed [15, 16, 20] for the anharmonic oscillator. The first-order modified perturbation theory gives the energy spectrum (14) with the governing function defined by (17). The maximal error of spectrum (14) is 2%. The second-order approximation corresponds to the energy spectrum (16) with the governing function defined by the condition

$$\frac{\mathrm{d}}{\mathrm{d}z} e_2(n,l,g,z) = 0.$$

The latter equation has no positive solutions for $\nu < 2$ and for $\nu \geqslant 2$ its solution being substituted into (16) leads to the maximal error of about 1%.

In recent years it has been shown that even if the results of physical interest are in three dimensions, it is advantageous to work in D dimensions and use $1/D$ as a perturbation expansion parameter. This large-dimension technique has been briefly called the $1/D$ expansion. The latter provided, in particular, a new way of solving the Schrödinger equation for spherically symmetric potentials. The $1/D$ expansion for the anharmonic oscillator was used in [22, 23]. The results for the energy are written

in the form of complicated series, even for low-lying levels. It must be admitted that the accuracy of the $1/D$ expansion is, to put it mildly, not so good. For example, when seven terms of the $1/D$ expansion are taken into account and, in addition, the resulting series are summed by means of the Padé–Borel transformation, even then the accuracy of the ground-state energy with $g \approx 1$ is about 1%, and the error quickly increases as $g \to \infty$. For higher energy levels the $1/D$ expansion also becomes less accurate with an error increasing together with the radial quantum number n since higher-order perturbation contributions to the energy contain powers of n in the numerator.

The accuracy of the large-dimension expansion can be drastically improved invoking the so-called shifted $1/D$ expansion [24, 25]. In the latter, the expansion parameter is modified by the replacing the space dimensionality D by $D - a$, where a is a suitable shift chosen so that the first-order shifted expansion would give the exact result for the energy of the harmonic-oscillator potential. It is necessary to stress that, in order to obtain the shifted $1/D$ expansion, one needs to resort to the Rayleigh–Schrödinger perturbation theory as well. Using the approach of [25] we have calculated the spectrum of the anharmonic oscillator. The first-order shifted expansion needs the second-order perturbation theory; its maximal error is about 10%. For the second-order shifted expansion one needs to invoke the fourth-order of the Rayleigh–Schrödinger perturbation theory, which is quite complicated and even so gives the maximal error about 0.6%. Thus, if we use, as in our method, only the second-order perturbation theory, we have for the shifted large-dimension expansion the maximal error of the order 10^{-1}. It is also worth noting that the $1/D$ expansions, including the shifted one, are only applicable to spherically symmetric potentials, therefore, being useless for one-dimensional problems.

5. Conclusion

The method of self-similar approximations [2] gives an elegant equation for the energy eigenstates of the three-dimensional spherical anharmonic oscillator. It can be applied with equal success to the one-dimensional anharmonic oscillator [16]. In all cases the accuracy of the method is within the maximal error of the order of 10^{-3}. The method of self-similar approximations surpasses other analytical approximation methods in its domain of applicability, the accuracy of its results and its simplicity.

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