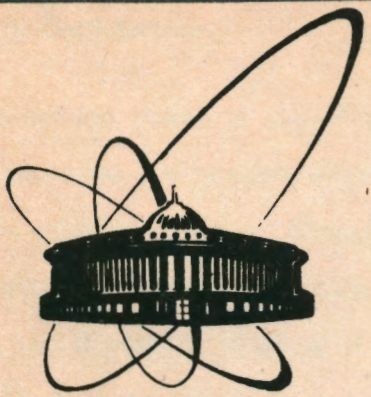

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SELF-SIMILAR APPROXIMATION FOR ANHARMONIC OSCILLATOR OF ARBITRARY DIMENSIONALITY

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1. Introduction

Perturbation theory is one of the principal approximation techniques in theoretical and mathematical physics. Unfortunately, perturbation series expansions diverge strongly for any nonzero coupling constant in the majority of interesting cases. The anharmonic oscillator is, probably, the most illustrative example of this sort [1].

To make perturbation theory a useful computational tool, one has to resort to summation techniques, like the Padé approximation, Borel transformation, Levin and Weniger transformations [2-4]. These techniques, to provide a reasonable accuracy, need to know tens of first terms of perturbation theory. However, in realistic physical problems one usually is able to find only a few first terms therefore the mentioned techniques become inapplicable [5]. How one then could sum a series having at hand a minimal number of perturbation terms?

An answer to this question has been recently given by one of the authors [6] who suggested a new method called the method of self-similar approximations. This method is based on the introduction of a continuous iterative procedure [7,8] and on the consideration of transformations from one approximate term to another as a renormalization group flow [7-9]. An important achievement of the method of self-similar approximations [6] is that the summation of divergent series requires to know only two terms of perturbation theory. By calculating the ground state energy of the one-dimensional anharmonic oscillator it has been demon-

strated[6,10] that the method [6], even with such a minimal information, provides a very good accuracy within an order of 10^{-3}. The aim of the present paper is to generalize the latter result in two aspects. First, we consider the anharmonic oscillator in the space of arbitrary dimensionality, and second, we calculate the whole spectrum of its energy levels. We show that for this general case and for any value of the anharmonicity constant the accuracy of the method [6] is within the same order as for the ground state energy of the one-dimensional oscillator. Comparing this with the results of other known methods using the same number of perturbation terms, we conclude that they are less general and accurate than the method of self-similar approximations [6].

2. Self-similar approximation

The method to be used is expounded in detail in Ref.[6]. This is why we present here only its scheme we shall follow in the subsequent section.

Let us be interested in the calculation of a function $f(n,g)$ in which n is a multiparameter; g, a variable called the coupling constant. Assume that by using perturbation theory, or another iterative procedure, we can obtain a sequence of approximations $f(n,g)$, where $k = 0,1,2,\ldots$ is a number of approximation. To force the sequence to be convergent, we introduce the governing functions $z_k(n,g)$ so that

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

The governing functions are to be found from a fixed point condition, for

instance, from the equation

$$\frac{\partial}{\partial z} f_k(n,g,z) = 0; \qquad z = z_k(n,g), \tag{2}$$

reminding the principle of minimal sensitivity[11].

Then we define the coupling function $g(n,f)$ by the equation

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

in which

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

Introduce the distribution of approximations

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

satisfying the normalization

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

The function $f_*(n,g)$ in (5) is just the sought self-similar approximation.

3. Anharmonic oscillator

Consider the spherical symmetric anharmonic oscillator in D - space of vectors

$$\vec{R}_D = \{r,\vartheta_1,\vartheta_2,\ldots,\vartheta_{D-2},\varphi\}.$$

The radial part of the Hamiltonian has the form

$$H = -\frac{1}{2m}\frac{d^2}{dr^2} + \frac{1}{2mr^2}\left(l+\frac{D-3}{2}\right)\left(l+\frac{D-1}{2}\right) + \frac{m\omega^2}{2}r^2 + \lambda m^2 r^4, \tag{6}$$

in which m and λ are positive constants; $l = 0, 1, 2, \ldots$ is the orbital quantum number. The energy levels E_{nl} of Hamiltonian (6) can be found by the Rayleigh - Schrödinger perturbation theory starting from the harmonic Hamiltonian

$$H_0 = -\frac{1}{2m}\frac{d^2}{dr^2} + \frac{1}{2mr^2}\left(l + \frac{D-3}{2}\right)\left(l + \frac{D-1}{2}\right) + \frac{m\omega_0^2}{2}r^2, \quad (7)$$

containing the trial parameter ω_0. The eigenvalues of (7) are

$$E_{nl}^{(0)} = (2n + l + \frac{D}{2})\omega_0; \qquad n, l = 0, 1, 2, \ldots. \quad (8)$$

It is convenient to introduce the dimensionless operators

$$H(\xi) \equiv \frac{H}{\omega}, \qquad H_0(\xi) \equiv \frac{H_0}{\omega}; \qquad \xi \equiv (m\omega)^{1/2}r, \quad (9)$$

and the dimensionless parameters

$$g \equiv \frac{\lambda}{\omega^3}, \qquad z \equiv \frac{\omega_0}{\omega}. \quad (10)$$

Then, Hamiltinians (6) and (7) transform to

$$H(\xi) = -\frac{1}{2}\frac{d^2}{d\xi^2} + \frac{1}{2\xi^2}\left(l + \frac{D-3}{2}\right)\left(l + \frac{D-1}{2}\right) + \frac{1}{2}\xi^2 + g\xi^4,$$

$$H_0(\xi) = -\frac{1}{2}\frac{d^2}{d\xi^2} + \frac{1}{2\xi^2}\left(l + \frac{D-3}{2}\right)\left(l + \frac{D-1}{2}\right) + \frac{z^2}{2}\xi^2. \quad (11)$$

Let us mention that making the formal substitution $D \to 1, \quad l \to 0$, we return to the one - dimensional case provided the variable ξ is continued from the ray $\xi \geq 0$ to the whole axis $(-\infty, +\infty)$. This will give us the possibility of returning from the spectrum of a spherical D - dimensional oscillator to that of the one - dimensional anharmonic oscillator [12].

The multiparameter n of section 2 becomes now a set of three parameters $\{n, l, D\}$, the radial quantum number, orbital quantum number and dimensionality, respectively. The quantities of interest are, in our case, the dimensionless energy levels

$$e(n, l, D, g) \equiv \frac{E_{nl}}{\omega}$$

of the anharmonic oscillator. The sequence of approximations in eq.(1) consists now of the perturbation terms

$$e_k(n, l, D, g, z) \equiv \frac{E_{nl}^{(k)}}{\omega}, \quad (12)$$

starting from

$$e_0(n, l, D, g, z) = \left(\nu + \frac{D}{2}\right)z; \qquad \nu \equiv 2n + l. \quad (13)$$

These terms are calculated by the Rayleigh - Schrödinger perturbation theory with the basis formed by the eigenvalue of $H_0(\xi)$ which we take in the form

$$\chi_{nl}^{(0)}(\xi) = \left[\frac{2n! z^{l+\frac{D}{2}}}{\Gamma(n + l + D/2)}\right]^{1/2} \xi^{l+\frac{D-1}{2}} \exp(-\frac{z}{2}\xi^2) L_n^{l+\frac{D}{2}-1}(z\xi^2), \quad (14)$$

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

The first approximation gives

$$e_1(n, l, D, g, z) = e_0(n, l, D, g, z) - \left(\nu + \frac{D}{2}\right)\frac{z^2 - 1}{2z} +$$

$$+ \left(\nu + \frac{D}{2}\right)\frac{3g}{2z^2}\gamma_{nl}(D), \quad (15)$$

where

$$\gamma_{nl}(D) \equiv \left(\nu + \frac{D}{2}\right)\left[1 - \frac{(l-2+\frac{D}{2})(l+\frac{D}{2})}{3(\nu+\frac{D}{2})^2}\right]. \qquad (16)$$

For the ground state level eq.(16) yields

$$\lim_{n,l\to 0} \gamma_{nl}(D) = \frac{1}{3}(D+2).$$

Asymptotic properties of (16) corresponding to high energy levels are

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

$$\gamma_{nl}(D) \simeq \frac{2}{3}l; \qquad l \to \infty \qquad (n < \infty).$$

For the high dimensionality limit one has

$$\gamma_{nl}(D) \simeq \frac{D}{3}; \qquad D \to \infty \qquad (n, l < \infty)$$

The second approximation reads

$$e_2(n,l,D,g,z) = e_1(n,l,D,g,z) - \left(\nu+\frac{D}{2}\right)\frac{(z^2-1)^2}{8z^3} +$$

$$+\left(\nu+\frac{D}{2}\right)\frac{3g(z^2-1)}{2z^4}\gamma_{nl}(D) -$$

$$-\left(\nu+\frac{D}{2}\right)\frac{5g^2}{2z^5}\left[1+\frac{27}{10}\left(\nu+\frac{D}{2}\right)\gamma_{nl}(D) - \left(\nu+\frac{D}{2}\right)^2\right]. \qquad (17)$$

Let us emphasize that after the formal substitution $D \to 1, \nu \to n, l \to 0$ expressions (15)and (17) become identical with the corresponding expressions for the one-dimensional anharmonic oscillator [12]. With this substitution in mind, all father results will be valid for an arbitrary space dimensionality $D = 1, 2, \ldots$.

As a fixed point condition (2) we get

$$\frac{\partial}{\partial z} e_1(n,l,D,g,z) = 0; \qquad z = z(n,l,D,g), \qquad (18)$$

which yields the equation

$$z^3 - z - 6g\gamma_{nl}(D) = 0, \qquad (19)$$

for the governing function. Eq.(3), taking account of (1), gives the equation

$$e_0(n,l,D,g) = f; \qquad g = g(n,l,D,f), \qquad (20)$$

defining the coupling function $g(\ldots)$. The latter equation, together with (13), leads to

$$\left(\nu+\frac{D}{2}\right) z(n,l,D,g) = f. \qquad (21)$$

For the distribution of approximations (4) we obtain

$$y_{21}(n,l,D,f) = -\frac{48f^3/\left(\nu+\frac{D}{2}\right)^4}{a_{nl}(D)\left[f^2/(\nu+\frac{D}{2})^2 - 1\right]^2}, \qquad (22)$$

where

$$a_{nl}(D) \equiv \left(\nu+\frac{D}{2}\right)\frac{9}{\gamma_{nl}(D)} + \frac{10}{3\gamma_{nl}^2(D)}\left[1 - \left(\nu+\frac{D}{2}\right)^2\right] - 6. \qquad (23)$$

Expression (23) for the ground state becomes

$$\lim_{n,l\to 0} a_{nl}(D) = \frac{3}{D+2}.$$

Highly excited levels are related to the limiting properties

$$\lim_{n\to\infty} a_{nl} = -\frac{1}{3}, \qquad \lim_{l\to\infty} a_{nl}(D) = 0.$$

The high dimensionality limit is

$$\lim_{D\to\infty} a_{nl}(D) = 0.$$

Taking integral (5) with the distribution of approximations (22), we come to the equation

$$\frac{e_*^2(n,l,D,g)/(\nu+\frac{D}{2})^2-1}{e_1^2(n,l,D,g)/(\nu+\frac{D}{2})^2-1} =$$

$$= \exp\left\{ \frac{1}{e_*^2(n,l,D,g)/(\nu+\frac{D}{2})^2-1} - \frac{1}{e_1^2(n,l,D,g)/(\nu+\frac{D}{2})^2-1} - \right.$$

$$\left. - \frac{a_{nl}(D)}{24} \right\}, \quad (24)$$

for the self-similar approximation $e_*(\ldots)$ ot the spectrum of the D - dimensional anharmonic oscillator. In (24) the notation $e_1(\ldots)$ implies expression

$$e_1(n,l,D,g) = \left(\nu+\frac{D}{2}\right)\frac{3z^2+1}{4z}, \quad (25)$$

obtained from (15) with the governing function given by (19).

Using (24), one can easily derive the asymptotic properties of the self-similar spectrum. Thus, for the weak anharmonicity limit we get

$$e_*(n,l,D,g) \simeq \left(\nu+\frac{D}{2}\right)\left[1+\frac{3}{2}g\gamma_{nl}(D)\right]; \qquad g\to 0. \quad (26)$$

In the strong anharmonicity limit one has

$$e_*(n,l,D,g) \simeq \frac{3}{4}\left(\nu+\frac{D}{2}\right)\exp\left[-\frac{a_{nl}(D)}{48}\right]\gamma_{nl}^{1/3}(D)(6g)^{1/3} \quad (27)$$

where $g\to\infty$. Highly excited levels in the strong anharmonicity case are either

$$e_*(n,l,D,g) \simeq \frac{3}{4}e^{1/144}(2n)^{4/3}(6g)^{1/3} = 3.458074\, n^{4/3}g^{1/3};$$

$$g,n\to\infty, \quad (28)$$

or

$$e_*(n,l,D,g) \simeq \frac{9}{8}\left(\frac{2l}{3}\right)^{4/3}(6g)^{1/3} = 1.190551\, l^{4/3}g^{1/3};$$

$$g,l\to\infty. \quad (29)$$

For a strongly anharmonic oscillator of high dimensionality we find

$$e_*(n,l,D,g) \simeq \frac{9}{8}\left(\frac{D}{3}\right)^{4/3}(6g)^{1/3} = 0.472470\, D^{4/3}g^{1/3};$$

$$g,D\to\infty. \quad (30)$$

The self-similar approximation for the spectrum given by (24) can be compared with direct numerical calculations made for one - , two - and three - dimensional anharmonic oscillators [13-16]. When estimating the accuracy of a method, it is natural to do this by defining the maximal error

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

for the whole range of the anharmonicity constant and of energy levels. The maximal error found in this way is about 0.3% for all $D = 0,1,2,3$.

The accuracy of our method can be compared with that of other analytical approaches. For example, the quasiclassical approximation, as applied to the anharmonic oscillator [12-14] with $D = 1,2,3$, gives quite

good results for highly excited levels in the strong anharmonicity limit. However, its accuracy drastically worsens for low-lying levels, especially, for the ground state energy, the maximal error $\epsilon(D)$ being about 20%. In addition, the Bohr - Sommerfeld condition defining the quasiclassical energy levels leads to a complicated set of transcendental equations [12-14].

The shifted large - dimensional expansion, which is much better than simple $1/D$ expansion, can be applied only to spherically simmetric potentials [17]. For the three - dimensional anharmonic oscillator we have used the shifted $1/D$ expansion and found the maximal accuracy $\epsilon(3)$ to be about 10% when the second order of the Rayleigh - Schrödinger perturbation theory is used, and about 0.6% if the fourth order of the Rayleigh - Schrödinger perturbation theory is invoked. This approach cannot be used for the one - dimensional anharmonic oscillator.

The renormalized perturbation theory [18,19] applied to the anharmonic oscillator [11,12] yields the maximal error of about 2% in the first order and about 1% in the second order.

Thus, the method of self - similar approximations[6] for the anharmonic oscillators of arbitrary dimensionality is more general, simple and accurate than other known analytical methods using about the same number of perturbation terms. Moreover, the method can be extended for solving time - dependent nonlinear Schrödinger equations, starting from a variational approximation (see e.g.[20]) and then following the scheme of section 2.

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Автомодельное приближение для ангармонического осциллятора произвольной размерности

Метод автомодельных приближений применен к ангармоническому осциллятору в пространстве произвольной размерности. Показано, что этот метод, при использовании только двух слагаемых теории возмущений, обеспечивает хорошую точность, порядка 10^{-3} для всех энергетических уровней и всех констант ангармоничности. Сравнение с другими известными аналитическими методами, использующими такое же число слагаемых теории возмущений, показывает, что метод автомодельных приближений, по крайней мере, на порядок точнее.

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Self-Similar Approximation for Anharmonic Oscillator of Arbitrary Dimensionality

The anharmonic oscillator in the space of arbitrary dimensionality is considered by the method of self-similar approximations. This method invoking only two terms of perturbation theory, is shown to be capable of providing quite a good accuracy, within an order of 10^{-3}, for all energy levels and all anharmonicity constants. The comparison with other known analytical methods using the same number of perturbative terms proves that the self-similar approximation is at least by an order more accurate.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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