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# Higher orders and structure of the perturbation-theory series for the anharmonic oscillator

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A simple method of calculating higher orders of perturbation theory (PT) in powers of  $g$  for the  $D$ -dimensional isotropic oscillator with arbitrary anharmonicity  $g v(r)$  is developed. The method is based on transforming from the Schrödinger equation to the Riccati equation (2.3). In the important particular case of power nonlinearity  $v(r) = r^{2N}$ ,  $N = 2, 3, 4, \dots$ , all the terms  $\xi_k(r)$  of the PT series (2.4) become polynomials, and this simplifies considerably the calculation of the higher orders of PT. A new variant of PT is proposed, which converges at all values of the coupling constant  $g$ :  $0 < g < \infty$ . The structure of the PT series for the energy levels is investigated for potentials with a power increase [ $v(r) \sim r^\nu$ ] and exponential increase [ $v(r) \sim \exp(br^{2\nu})$ ] at infinity. It is shown that, in the latter case with  $0 < \nu < 1$ , the PT series is asymptotic for  $g \rightarrow 0$  but is not summable by the Borel method. For  $\nu \geq 1$  a PT series in integer powers of  $g$  does not exist, and the energy difference  $E(g) - E(0)$  vanishes more slowly than  $g$  as  $g \rightarrow 0$ . The energy correction  $E(g) - E(0)$  for small values of  $g$  is calculated. The character of the singular point of  $E(g)$  at  $g = 0$  changes at  $\nu = 1$ .

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## 1. INTRODUCTION

Many papers (see, e.g., Refs. 1-15) have been devoted to the study of the anharmonic oscillator

$$H = \sum_{i=1}^D (p_i^2 + x_i^2) + g \left( \sum_{i=1}^D x_i^2 \right)^N \quad (1.1)$$

( $N = 2, 3, 4, \dots$ ). This is explained by the fact that this problem not only has important applications in solid-state theory and molecular physics but is also of fundamental interest in connection with certain problems in quantum field theory. In a series of papers,<sup>1-5</sup> Bender and Wu investigated the structure of the perturbation-theory (PT) series for the energy levels

$$E(g) = \sum_{k=0}^{\infty} E_k(-g)^k \quad (1.2)$$

and showed that the coefficients of the PT series increase factorially as  $k \rightarrow \infty$ :

$$E_k \approx (k\alpha)! a^k k^k \left( c_0 + \frac{c_1}{k} + \frac{c_2}{k^2} + \dots \right). \quad (1.3)$$

Lipatov<sup>16</sup> established that the coefficients of the PT series for the Gell-Mann-Low function in scalar field theory with the interaction

$$H = \int \frac{d^D x}{n!} g \phi^n, \quad D = \frac{2n}{n-2}$$

behave analogously. In view of this analogy, the an-

harmonic oscillator is a convenient model upon which we can elucidate a number of questions of importance for field theory (e.g., the summability of the PT series by different methods of summation of divergent series, the structure of the expansion (1.3) in powers of  $1/k$ , and so forth).

The present paper is devoted to an investigation of the PT series for the anharmonic oscillator. In Sec. 2 a simple method of systematic calculation of the terms of the PT series, based on transforming from the Schrödinger equation to the nonlinear Riccati equation, is described. The application of this method to the  $D$ -dimensional oscillator with anharmonicity  $g r^{2N}$  enables us to obtain a large number of coefficients of the PT series with ease.

In Sec. 3 a new variant of PT is proposed, in which the expansion is performed not in powers of  $g$  but in the deviation of the wave function from its asymptotic form for  $r \rightarrow \infty$ . This makes it possible, with the aid of a small number of approximations, to obtain the level energies  $\tilde{E}_k(g)$  with good accuracy for all  $0 < g < \infty$ . The analytic properties of the  $\tilde{E}_k(g)$  as functions of  $g$  are close to the properties of the exact solution. In Sec. 4 the energy discontinuity  $\Delta E(g)$  across the cut as  $g \rightarrow -0$  is calculated in the semiclassical approximation for arbitrary anharmonicity  $v(r)$ .

The structure of the PT series for the energy eigen-

values is investigated on the basis of these results in Sec. 5. Besides potentials having a power behavior as  $r \rightarrow \infty$ , potentials growing like  $\exp(br^{2\nu})$  are considered. In the latter case, for  $0 < \nu < 1$  the coefficients of the PT series increase faster than  $(k\alpha)!$  with any finite  $\alpha$ . This leads to examples of asymptotic quantum-mechanics PT series that cannot be summed by the Borel method. If  $\nu \geq 1$ , a PT series in powers of  $g$  does not exist. In Sec. 6 the first correction to the energy for  $g \rightarrow 0$  is calculated for such potentials by the method proposed in Sec. 3. As we should expect, it has a singularity at the point  $g=0$ , and for  $\nu > 1$  (and also for  $\nu = 1$  and  $b > 1$ ) vanishes more slowly than  $g$ .

## 2. MODIFIED PERTURBATION THEORY IN POWERS OF $g$

The Schrödinger equation for the  $D$ -dimensional anharmonic oscillator with anharmonicity  $gv(r)$  has the form

$$R'' + \frac{D-1}{r}R' + \left[ E - r^2 - gv(r) - \frac{l(l+D-2)}{r^2} \right] R = 0, \quad (2.1)$$

where  $R(r)$  is the radial wavefunction,

$$r = \left( \sum_{i=1}^D x_i^2 \right)^{1/2},$$

$l = 0, 1, 2, \dots$ , and  $l(l+D-2)$  is the eigenvalue of the square of the  $D$ -dimensional orbital angular momentum.

Our approach to the PT is based on going over from (2.1) to the nonlinear Riccati equation. Introducing the new function

$$\xi(r) = -\{R'/R + (D-1)/2r\}, \quad (2.2)$$

we obtain, for  $l=0$ ,

$$\xi' - \xi^2 = E - (D-1)(D-3)/4r^2 - r^2 - gv(r) \quad (2.3)$$

(in this section we shall confine ourselves to treating the ground state).

For  $g=0$  the solution of this equation is obvious:

$$\xi = \xi_0 = r - (D-1)/2r, \quad E(0) = D.$$

Let  $\varepsilon(g) = E(g)/E(0)$ , where  $E(g)$  is the energy of the ground level. Expanding  $\varepsilon(g)$  and  $\xi(r, g)$  in PT series:

$$\varepsilon(g) = 1 - \sum_{k=1}^{\infty} \varepsilon_k (-g)^k, \quad \xi(r, g) = \sum_{k=0}^{\infty} \xi_k(r) g^k \quad (2.4)$$

and substituting them into (2.3), we obtain a system of recurrence equations:

$$\xi_1' - 2\xi_0\xi_1 = D\varepsilon_1 - \nu(r), \quad (2.5)$$

$$\xi_n' - 2\xi_0\xi_n = (-1)^{n+1} D\varepsilon_n + \sum_{k=1}^{n-1} \xi_k \xi_{n-k}, \quad n \geq 2, \quad (2.6)$$

with  $\xi_n(0) = 0$ .

The solution of Eq. (2.5) has the form

$$\xi_1(r) = \exp(r^2)r^{1-D} \int_0^r \exp(-x^2)x^{D-1} [D\varepsilon_1 - \nu(x)] dx. \quad (2.7)$$

The constant  $\varepsilon_1$  is determined from the condition that the function  $\xi_1(r)$  not increase like  $\exp(r^2)$  as  $r \rightarrow \infty$ . This gives a result coinciding with that of ordinary perturbation theory:

tion theory:

$$\varepsilon_1 = D^{-1} \langle \nu \rangle, \quad (2.8)$$

where, by definition,

$$\langle \nu \rangle = \frac{2}{\Gamma(D/2)} \int_0^{\infty} \nu(r) \exp(-r^2) r^{D-1} dr.$$

In an analogous way, from (2.6) we find ( $n \geq 2$ )

$$\varepsilon_n = (-1)^n D^{-1} \sum_{k=1}^{n-1} \langle \xi_k \xi_{n-k} \rangle, \quad (2.9)$$

$$\xi_n(r) = \exp(r^2)r^{1-D} \int_0^r \exp(-x^2)x^{D-1} \left[ (-1)^n D\varepsilon_n + \sum_{k=1}^{n-1} \xi_k(x) \xi_{n-k}(x) \right] dx. \quad (2.10)$$

These formulas determine the terms of the PT series (2.4) by successive quadratures. The difference from the ordinary PT is that what is expanded in a series in powers of  $g$  is not the wave function itself ( $R(r, g) = \Sigma R_n(r)g^n$ ) but its logarithmic derivative. We note that the first  $n$  terms of the expansion (2.4) not only completely determine  $R_0, R_1, \dots, R_{n-1}$  but also incorporate part of the higher-order corrections.

We now consider a nonlinearity of the power form

$$\nu(r) = r^\nu, \quad \nu > -D. \quad (2.11)$$

In this case, formula (2.7) gives

$$\xi_1(r) = \frac{1}{2} \exp(r^2)r^{1-D} \left\{ \frac{\Gamma((D+\nu)/2)}{\Gamma(D/2)} \gamma\left(\frac{D}{2}, r^2\right) - \gamma\left(\frac{D+\nu}{2}, r^2\right) \right\},$$

where  $\gamma(p, x)$  is the incomplete gamma function. For the Hamiltonian (1.1),  $\nu = 2N = 4, 6, \dots$ ; in this physical-interesting case  $\xi_1(r)$  becomes a polynomial:

$$\xi_1(r) = \sum_{k=0}^{\alpha} a_k^{(1)} r^{2k+1}, \quad a_k^{(1)} = \frac{\Gamma(\alpha+\delta)}{2\Gamma(k+\delta)}, \quad (2.12)$$

where  $\alpha = N - 1$  and  $\delta = (D+2)/2$  (cf. Appendix A). Using (2.10) we can show that this also happens for the subsequent terms of the PT series. For example,

$$\xi_2(r) = - \sum_{k=0}^{2\alpha} a_k^{(2)} r^{2k+1}, \quad (2.13)$$

$$a_k^{(2)} = \frac{1}{2\Gamma(k+\delta)} \sum_{\substack{i,j=0 \\ i+j=k}}^{\alpha} a_i^{(1)} a_j^{(1)} \Gamma(i+j+\delta).$$

In general,  $\xi_n(r)$  is a polynomial of degree  $2\alpha n + 1$ . The fact that, for even  $\nu$ , the function  $\xi_n(r)$  in any order of PT is a polynomial is an important advantage of this approach (as compared with the ordinary variant of PT) from a calculational point of view.

From (2.9) we obtain the formula

$$\varepsilon_n = \frac{1}{2\Gamma(\delta)} \sum_{k=1}^{n-1} \sum_{i=0}^{k\alpha} \sum_{j=0}^{(n-k)\alpha} a_i^{(k)} a_j^{(n-k)} \Gamma(i+j+\delta), \quad n \geq 2, \quad (2.14)$$

which expresses the  $n$ th order of PT for the energy of the ground level in terms of the coefficients of the polynomials  $\xi_m(r)$  of lower order ( $1 \leq m \leq n-1$ ). Hence,

$$\varepsilon_1 = \frac{\Gamma(\alpha+\delta)}{2\Gamma(\delta)}, \quad \varepsilon_2 = \frac{[\Gamma(\alpha+\delta)]^2}{8\Gamma(\delta)} \sum_{i,j=0}^{\alpha} \frac{\Gamma(i+j+\delta)}{\Gamma(i+\delta)\Gamma(j+\delta)}$$

$$\varepsilon_3 = \frac{[\Gamma(\alpha+\delta)]^3}{16\Gamma(\delta)} \sum_{i,j,k=0}^{\alpha} \sum_{l=0}^{i+j} \frac{\Gamma(i+j+\delta)\Gamma(k+l+\delta)}{\Gamma(i+\delta)\Gamma(j+\delta)\Gamma(k+\delta)\Gamma(l+\delta)} \quad (2.15)$$

[the parameters  $\alpha$  and  $\delta$  are defined after (2.12)]. Expressions for  $\varepsilon_2$  and  $\varepsilon_3$  would be difficult to obtain by the usual PT, and this illustrates the effectiveness of the proposed method.

In the important particular case  $N=2$  (an oscillator with anharmonicity  $gr^4$ ),  $\alpha=1$  and all the formulas are simplified considerably. In this case, the  $\xi_n$  are polynomials of degree  $2n+1$ :

$$\xi_n(r) = (-1)^{n+1} \sum_{k=0}^n a_k^{(n)} r^{2k+1}, \quad (2.16)$$

and the procedure for calculating the coefficients  $a_k^{(n)}$  can be formulated purely algebraically. If the polynomials  $\xi_1, \xi_2, \dots, \xi_n$  are already known we determine the numbers  $b_k$  from the equality

$$\sum_{j=1}^n \xi_j(r) \xi_{n+1-j}(r) = (-1)^{n+1} \sum_{k=1}^{n+2} b_k r^{2k}.$$

By means of (2.6) we can show that the leading coefficient of the polynomial  $\xi_{n+1}(r)$  does not depend on  $D$  and is equal to

$$a_0^{(n+1)} = \frac{\Gamma(n+1/2)}{2^n n!} = \frac{(2n)!}{2^{2n+1} n! (n+1)!} \quad (2.16')$$

and the other coefficients are determined by the recurrence relation

$$a_{k-1}^{(n+1)} = 1/2 [(2k+D)a_k^{(n+1)} + b_k]. \quad (2.16'')$$

Descending successively from  $k=n+1$  to  $k=0$  we determine the correction to the energy:  $a_0^{(n+1)} = \varepsilon_{n+1}$ , after which we move on to the next approximation.

We shall give the first few polynomials  $\xi_n$  and coefficients  $\varepsilon_n$  obtained in this way:

$$\begin{aligned} \xi_1 &= 1/2 r^3 + \varepsilon_1 r, & \xi_2 &= -[1/8 r^5 + 1/16 (3D+8)r^3 + \varepsilon_2 r], \\ \xi_3 &= 1/16 r^7 + 1/32 (5D+16)r^5 + 1/16 (3D^2+17D+25)r^3 + \varepsilon_3 r, \end{aligned} \quad (2.17)$$

$$\begin{aligned} \xi_4 &= -1/128 [5r^9 + 1/2 (35D+128)r^7 + 1/2 (60D^2+399D+700)r^5 + \\ &+ 1/4 (128D^3+1145D^2+3556D+3840)r^3 + 128\varepsilon_4 r], \dots \\ \varepsilon_1 &= 1/4 (D+2), & \varepsilon_2 &= 1/16 (D+2) (2D+5), \\ \varepsilon_3 &= 1/64 (D+2) (8D^2+43D+60), \end{aligned} \quad (2.18)$$

$$\begin{aligned} \varepsilon_4 &= 1/1024 (D+2) (168D^3+1437D^2+4270D+4420), \\ \varepsilon_5 &= 1/16384 (D+2) (1024D^4+12277D^3+57668D^2+126128D+108480), \\ \varepsilon_6 &= 1/32768 (D+2) (13728D^5+215241D^4+1410726D^3 + \\ &+ 4847280D^2+8746112D+6626000). \end{aligned}$$

For  $D=1$  the formulas for  $\varepsilon_k$  agree with the values obtained by Bender and Wu<sup>1</sup> for the coefficients of the PT series for the one-dimensional oscillator with anharmonicity  $gx^4$ . The coefficients  $\varepsilon_k$  increases rapidly with increase of  $k$  (see Fig. 1, from which the influence of the dimensionality  $D$  is clear). As is well known,<sup>3,7</sup> they have a factorial asymptotic form as  $k \rightarrow \infty$ . The corresponding values of the parameters in formula (1.3) are equal to

$$\alpha=1, \quad a = \frac{3}{2}, \quad \beta = \frac{1}{2} (D-2), \quad c_0 = -\frac{4}{\pi \Gamma(D/2)} \left(\frac{3}{2}\right)^{D/2}. \quad (2.19)$$

We note certain properties of the coefficients  $\varepsilon_n$  and  $a_k^{(n)}$ :

1) The coefficient of  $r$  in the polynomial  $\xi_n(r)$  coincides, to within the sign, with  $\varepsilon_n$ :

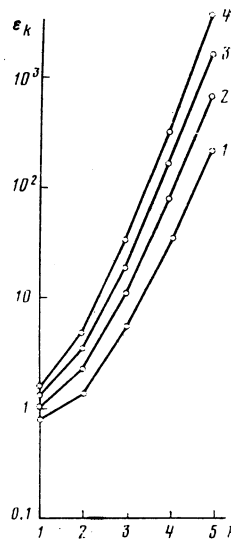


FIG. 1. Coefficients of the PT series for the energy of the ground level of a  $D$ -dimensional oscillator with anharmonicity  $gr^4$ . The values of the dimensionality  $D$  are indicated alongside the curves.

$$a_0^{(n)} = \varepsilon_n, \quad n \geq 1. \quad (2.20)$$

2) The quantity  $\varepsilon_n$  is an  $n$ th degree polynomial in  $D$ , divisible, for  $n \geq 1$ , by  $(D+2)$ .

3) We shall indicate a simple method of calculating the leading coefficients of the polynomials  $\xi_n(r)$ . Making in Eq. (2.3) the replacements  $r \rightarrow t$  and  $\varepsilon \rightarrow \eta$ , where

$$r = g^{-1/2} t, \quad \xi = g^{-1/2} \eta(t, g) - g^{1/2} (D-1)/2t, \quad (2.21)$$

we transform it to the following form:

$$g \left( \frac{d\eta}{dt} + \frac{D-1}{t} \eta \right) - \eta^2 = E g^{-1/2} t^2 - t^4. \quad (2.22)$$

Putting here

$$\eta(t, g) = \sum_{k=0}^{\infty} \eta_k(t) g^k,$$

we obtain for  $k \geq 2$  a recurrence relation for  $\eta_k$ :

$$\eta_k = \frac{1}{2t(1+t^2)^2} \left[ \eta_{k-1}' + \frac{D-1}{t} \eta_{k-1} - \sum_{j=1}^{k-1} \eta_j \eta_{k-j} + (-1)^{k-1} D \varepsilon_{k-1} \right].$$

It is not difficult to show that  $\eta_k(t)$  is a generating function for the coefficients  $a_i^{(n)}$  with a fixed value of the difference  $n-i=k$ . In particular, from the explicit expressions for  $\eta_0$  and  $\eta_1$  we find

$$a_n^{(n)} = \frac{(2n-2)!}{2^{2n-1} n! (n-1)!}, \quad a_{n-1}^{(n)} = \frac{1}{2} \left[ 1 + D \frac{(2n)!}{2^{2n} (n!)^2} \right] \quad (2.23)$$

and the next coefficients  $a_{n-k}^{(n)}$  with  $k=2, 3, \dots$  can be obtained analogously.

To conclude this section we consider a one-dimensional oscillator with cubic nonlinearity:

$$H = p^2 + x^2 + gx^3, \quad -\infty < x < \infty. \quad (2.24)$$

The substitution  $\psi'/\psi = -\xi(x)$  brings the Schrödinger equation to the form

$$\xi' - \xi^2 = \varepsilon(g) - x^2 - gx^3. \quad (2.25)$$

This equation is invariant under the replacement  $x \rightarrow -x, g \rightarrow -g$ ; therefore, the PT series have here the following form:

$$\varepsilon(g) = 1 - \sum_{k=1}^{\infty} \varepsilon_{2k} g^{2k}, \quad (2.26)$$

$$\xi(x, g) = x - \sum_{k=1}^{\infty} \xi_k(x) (-g)^k,$$

with  $\xi_k(-x) = (-1)^{k+1} \xi_k(x)$ . Equations analogous to (2.6) are found for the  $\xi_k(x)$ , and from these we find, successively,<sup>1)</sup>

$$\varepsilon_2 = \frac{11}{16}, \quad \varepsilon_4 = \frac{465}{256}, \quad \varepsilon_6 = \frac{39709}{4096}, \dots \quad (2.27)$$

The energy levels are quasistationary for either sign of the coupling constant  $g$ . The fact that the PT series for  $\varepsilon(g)$  (determining the asymptotic expansion of the real part of the energy of the level for small values of  $|g|$ ) is not alternating, as in the case of the Stark shift of atomic levels in a constant electric field (see example IV in our previous paper<sup>17)</sup>), is connected with this. Analogous results also hold for the Hamiltonian  $H = p^2 + x^2 + gx^{2N+1}$ .

### 3. PERTURBATION THEORY IN THE DEVIATION FROM THE ASYMPTOTIC FORM

An obvious drawback of expanding in powers of  $g$  is the fact that it is applicable only for sufficiently small values of  $|g|$ . In this section a new type of PT, valid for all  $g(0 < g < \infty)$  will be considered. The starting point is the Riccati equation (2.3). Below we shall consider the ground level and first excited level of the one-dimensional  $gx^4$  oscillator. The generalization to other potentials  $v(r)$  is obvious.

For the ground level we choose, as the zeroth approximation, the function

$$\tilde{\xi}_0 = r(1+gr^2)^{1/2}, \quad (3.1)$$

which tends to the exact solution when  $r \rightarrow \infty$  or  $g \rightarrow \infty$ . If we write

$$\varepsilon(g) = \sum_{k=1}^{\infty} \varepsilon_k(g), \quad \xi(r, g) = \sum_{k=0}^{\infty} \tilde{\xi}_k(r, g), \quad (3.2)$$

then  $\tilde{\xi}_k$  satisfies the equation

$$\tilde{\xi}_k' - 2r(1+gr^2)^{-1/2} \tilde{\xi}_k = \varepsilon_k - \varphi_k, \quad k \geq 1, \quad (3.3)$$

where

$$\varphi_1 = (1+2gr^2)(1+gr^2)^{-1/2},$$

$$\varphi_k = - \sum_{j=1}^{k-1} \tilde{\xi}_j \tilde{\xi}_{k-j}.$$

Eq. (3.3) is easily solved:

$$\tilde{\xi}_k(r, g) = e^{f(r)} \int (\varepsilon_k - \varphi_k) e^{-f(r')} dr', \quad (3.4)$$

where

$$f(r) = \frac{2}{3g} [(1+gr^2)^{3/2} - 1].$$

The quantity  $\tilde{\xi}_k$  is determined from the condition  $\tilde{\xi}_k(r=0) = 0$ , which gives

$$\varepsilon_k(g) = \int_0^{\infty} dr e^{-f(r)} \varphi_k(r) - \int_0^{\infty} dr e^{-f(r)}. \quad (3.5)$$

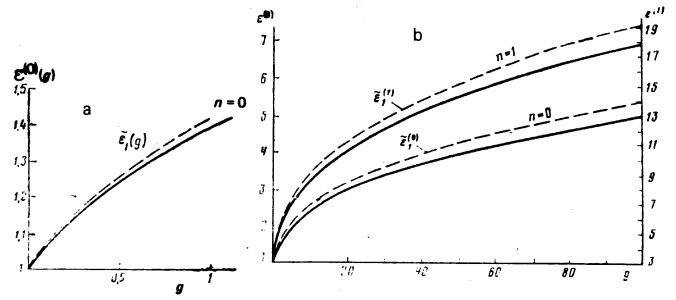


FIG. 2. Energy  $\varepsilon^{(0)}(g)$  of the ground level ( $n=0$ ) and energy  $\varepsilon^{(1)}(g)$  of the first excited level ( $n=1$ ) of a one-dimensional oscillator with anharmonicity  $gx^4$ . The solid curves are the results of the numerical calculation in Ref. 15, and the dashed curves are the results calculated from formula (3.5).

It can be shown that  $\tilde{\varepsilon}_k = O(g^k)$  for  $g \rightarrow 0$  and  $k \geq 2$ . Even the lowest approximation  $\tilde{\varepsilon}_1$  to the energy of the ground level is fairly accurate:

$$\varepsilon_1(g) = \begin{cases} 1 + \frac{3}{4}g - \frac{291}{256}g^2 + \dots, & g \rightarrow 0 \\ \tilde{c}g^{1/3}, & g \rightarrow \infty, \end{cases} \quad (3.6)$$

where  $\tilde{c} = 2^{2/3} \times 3^{1/3} \Gamma(\frac{2}{3}) / \Gamma(\frac{1}{3}) = 1.157$ . At the same time, the exact value<sup>10,11</sup> is  $c = 1.060$ , while the exact coefficient of  $g^2$  is equal to  $-21/16$ , i.e., differs from that in (3.6) by 13%. The results of the calculation of  $\tilde{\varepsilon}_1(g)$  by the formula (3.5) are shown in Figs. 2(a) and 2(b). Even in the worst case  $g \gg 1$  the accuracy of this approximation is ~9%, while, e.g., for  $g=1$  the accuracy is ~2%. The next approximation for  $g \rightarrow \infty$  gives (see Appendix B)  $\tilde{\varepsilon}_2 = -0.109g^{1/3}$ ; then  $\tilde{\varepsilon}_1 + \tilde{\varepsilon}_2 = 1.048g^{1/3}$ , which differs from the exact coefficient  $c$  in the asymptotic form of  $\varepsilon(g)$  by only 1%.

The first excited level can be treated analogously. The only difference is that the zeroth approximation to the function has a pole at  $r=0$ :

$$\tilde{\xi}_0 = r(1+gr^2)^{1/2} - r^{-1}. \quad (3.7)$$

The energy eigenvalues are determined by Eq. (3.5) with the replacement  $dr \rightarrow r^2 dr$ , and  $\varphi_1 = (3+4gr^2) \times (1+gr^2)^{-1/2}$ . The corresponding curve is given in Fig. 2(b).

For  $g \rightarrow \infty$  the lowest approximation to the energy eigenvalue of the first excited level gives  $\tilde{\varepsilon}_1 = 4\Gamma(4/3)(3g/2)^{1/3} = 4.089g^{1/3}$ , whereas the exact result<sup>11</sup> is  $\varepsilon = 3.860g^{1/3}$ . The relative error in this case is somewhat better than for the ground state.

We have proved that the expansion (3.2) under consideration converges at sufficiently small  $|g|$ . However, it seems plausible that it converges in the entire complex  $g$ -plane with the cut  $(-\infty, 0)$ .

We note that the analytic properties of  $\tilde{\varepsilon}_k(g)$  are close to the properties of the exact solution  $\varepsilon(g)$ . The functions  $\tilde{\varepsilon}_k(g)$  have a branch point  $g=0$ , the discontinuity across the cut  $(-\infty, 0)$  at small values of  $g$  being proportional to  $e^{2/3g}$ :

$$\Delta \tilde{\varepsilon}_k^{(0)} = c_0 g^{-1/3} e^{2/3g}, \quad \Delta \tilde{\varepsilon}_k^{(1)} = c_1 g^{-1/3} e^{2/3g} \quad (3.8)$$

(see Appendix B). These expressions differ from the

exact results of Ref. 3 by a factor  $\text{const} \cdot g^{1/3}$ . The question arises as to how summation of the convergent series (3.2) for  $\varepsilon(g)$  can provide a singular ( $\sim g^{-1/3}$ ) factor. The simple example

$$\Delta \varepsilon_k = \text{const} \cdot e^{2/3g} g^{-1/3} (1 - gk^2)^{-1}$$

shows how this might be accomplished.

It is well known that a singularity of the discontinuity of the type  $\Delta \varepsilon(g) \sim g^{-\lambda} e^{2/3g}$  leads to a factorial increase of the coefficients in the expansion of  $\varepsilon(g)$  in powers of  $g$ . Consequently, we see that the convergent expansion considered in this section becomes asymptotic when re-expanded in powers of  $g$ .

The variant of perturbation theory described here is easily generalized to other potentials. In particular, in Sec. 6 we shall apply it to investigate the form of the singularity in the coupling constant  $g$  for exponentially increasing potentials  $v(r) = r^\mu \exp(br^{2\nu})$ , for which an expansion in integer powers of  $g$  does not exist.

#### 4. THE SEMICLASSICAL APPROXIMATION

As is well known,<sup>18,19</sup> to calculate the asymptotic form of the coefficients  $\varepsilon_k$  of the PT series as  $k \rightarrow \infty$  it is sufficient to find the imaginary part  $\gamma$  of the level energy (i.e., the probability of decay of the quasistationary level in unit time) for a coupling constant of the opposite sign:  $g = -\lambda < 0$ . For  $g \rightarrow -0$  this problem is easily solved by the WKB method for a level with arbitrary quantum numbers  $n$  and  $l$ . The semiclassical momentum is equal to

$$|p(r)| = [(2n+D) - \Lambda(\Lambda+1)r^{-2} - r^2 + \lambda v(r)]^{1/2} \quad (4.1)$$

where  $2n+D$  is the energy of a level of the harmonic oscillator (with  $\lambda=0$ ), and  $\Lambda = l + (D-3)/2$ . The centrifugal term in (4.1) is absent in two cases:  $D=1$  (when  $l=0$  automatically) and  $D=3$ ,  $l=0$  (the  $s$ -levels of a three-dimensional oscillator). In the other cases, the Langer correction,<sup>19,20</sup> which improves the accuracy of the WKB approximation for  $r \rightarrow 0$ , must be added to the expression for the momentum. When this correction is taken into account the term  $\Lambda(\Lambda+1)r^{-2}$  in (4.1) is replaced by  $(\Lambda + \frac{1}{2})^2 r^{-2}$ .

The width  $\gamma$  is determined by the penetrability of the barrier in the region  $r_- < r < r_+$ . For  $\lambda \rightarrow +0$  the position of the first turning point  $r_-$  does not depend on  $\lambda$ :

$$r_- = \begin{cases} (2n+D)^{1/2}, & \text{if } \Lambda = -1 \text{ or } 0, \\ n + \frac{1}{2} D + [(n-l+1)(n+l+D-1)]^{1/2}, & \text{if } \Lambda(\Lambda+1) \neq 0, \end{cases}$$

while  $r_+$  is determined from the equation

$$v(r)r^{-2} = \lambda \quad (4.2)$$

and moves away to infinity. Therefore, there exists a region  $r_- \ll r \ll r_+$  in which the semiclassical expression for  $\chi(r) = R_{nl}(r)r^{(D-1)/2}$ , asymptotically exact for  $r \gg r_-$ , matches with the tail of the harmonic-oscillator wavefunction. As a result, we obtain

$$\gamma = A \frac{\omega}{\pi} \exp \left\{ -2 \int_{r_-}^{r_+} |p(r)| dr \right\} \quad (4.3)$$

Here,

$$A = \begin{cases} a \left( \frac{n+D}{2} \right) & \text{for } \Lambda = 0, -1, \\ a \left( \frac{n-l+1}{2} \right) a \left( \frac{n+l+D-1}{2} \right) & \text{otherwise} \end{cases} \quad (4.4)$$

where

$$a(x) = \frac{(2\pi)^{1/2} x^x e^{-x}}{\Gamma(x+1/2)} = \begin{cases} (\pi/e)^{1/2} = 1.07504\dots, & x = 1/2, \\ 2^{1/2} e^{-1} = 1.04052\dots, & x = 1, \\ 1 + 1/24x + \dots, & x \rightarrow \infty. \end{cases}$$

The formula (4.3) has a clear physical meaning. The factor  $\omega/\pi$  is equal to the frequency with which a particle localized in the region  $r < r_-$  strikes the barrier wall (here it is necessary to take into account that for the harmonic oscillator the period of the radial vibrations is half the period  $T = 2\pi/\omega$  of the oscillator in our chosen normalization of the Hamiltonian (1.1),  $\omega = 1$ ). The exponential in (4.3) corresponds to the probability of tunneling on each impact of the particle against the wall at  $r = r_-$ . Finally, the factor  $A$  takes account of the fact that the motion is not semiclassical in the region  $r \lesssim r_-$ . For large quantum numbers (more precisely, for  $n-l \gg 1$ ), the motion in the inner well is semiclassical and  $A$  approximates to unity:  $A \approx 1 + [6n(1 - l^2/n^2)]^{-1}$ .

We note that  $a(x)$  is a sluggish function for  $x > 0.5$ . Therefore, the difference between the exact formula (4.3) and the semiclassical asymptotic form (for which  $A=1$ ) is small for all values of the quantum numbers  $n$  and  $l$  and the dimensionality  $D$ .

The integral in (4.3) is built up in the region of large distances  $r \sim r_+$ , where the principal terms in the momentum  $p(r)$  are  $r^2$  and  $\lambda v(r)$ . Using this, we can transform formula (4.3) to a form more convenient for calculations:

$$\gamma = 2r_+^{2n+D} \exp \left\{ -2 \int_0^{r_+} [r^2 - \lambda v(r)]^{1/2} dr \right\} / \Gamma \left( \frac{n-l}{2} + 1 \right) \Gamma \left( \frac{n+l+D}{2} \right), \quad (4.5)$$

where the integration is carried out up to the point  $r = r_+$  determined from the condition (4.2). The details of the calculations leading to the formulas (4.3) and (4.5) for  $\gamma$  will be described elsewhere. We emphasize that the expressions (4.3) and (4.5) are equivalent to each other only in the limit  $\lambda \rightarrow -0$ .

The formulas (4.3) and (4.5) were obtained using the semiclassical approximation in the region  $r \gg r_-$ . The condition for applicability of the semiclassical approximation is

$$\frac{d}{dr} \left( \frac{1}{p(r)} \right) = \frac{1 - \lambda(u + \rho u')}{\rho(1 - \lambda u)^{3/2}} \ll 1, \quad (4.6)$$

where  $\rho = r^2$ ,  $u(\rho) \equiv v(r)r^{-2}$ , and the prime denotes the derivative with respect to  $\rho$ . For potentials with a power behavior at infinity we have

$$u(\rho) \sim \rho^\nu, \quad u + \rho u' \approx (\nu + 1)u \quad \text{for } \rho \rightarrow \infty.$$

It can be seen from this that the condition (4.6) is fulfilled for  $\rho \gg 1$  everywhere except in a small neighborhood of the turning point  $r = r_+$ . The matching of the solutions on both sides of the turning point  $r_+$ , which is necessary for the calculation of the flux of particles as  $r \rightarrow \infty$  and the level width  $\gamma$ , is carried out in the standard way. Therefore, the formula (4.3) has, in the

given case, an exact pre-exponential factor, if the constant  $\lambda$  is sufficiently small.

For potentials with exponential growth as  $r \rightarrow \infty$

$$v(r) \sim \exp(br^{2\nu}), \quad b, \nu > 0, \quad (4.7)$$

$u'/u \sim b\nu\rho^{\nu-1}$  increases without limit as  $\rho \rightarrow \infty$ , if  $\nu > 1$ ; in this case the condition (4.6) is violated for large  $\rho$ . Thus, the formulas (4.3) and (4.5) are asymptotically exact in the limit  $\lambda \rightarrow +0$ , if the potential  $v(r)$  increases more slowly than  $\exp(br^{2\nu})$  at infinity.

## 5. THE STRUCTURE OF THE PERTURBATION-THEORY SERIES

Using the results of the preceding section we shall determine the rate of increase of the coefficients  $\varepsilon_k$  of the series (2.4) as  $k \rightarrow \infty$ . We shall start from the formula (4.5) and consider anharmonicities  $v(r)$  of different types.

**I. Power anharmonicity:**  $v(r) \propto r^\nu$  as  $r \rightarrow \infty$ ,  $\nu > 2$ . The integral (4.5) determines the energy discontinuity  $\Delta E(g) = \gamma$  across the cut as  $g = -\lambda \rightarrow -0$ :

$$\gamma(\lambda) = \gamma_0 \lambda^{-(2n+D)/(v-2)} \exp(-b_1 \lambda^{-2/(v-2)}), \quad (5.1)$$

where

$$\gamma_0 = 4 \left[ \Gamma\left(\frac{n-l}{2} + 1\right) \Gamma\left(\frac{n+l+D}{2}\right) \right]^{-1},$$

$$b_1 = \pi^{1/2} \Gamma\left(\frac{\nu}{v-2}\right) / 2\Gamma\left(\frac{3\nu-2}{2(v-2)}\right).$$

Using the formulas from Ref. 17 that give the relationship between the discontinuity of a function across the cut and the asymptotic form of the power series corresponding to it, for  $\varepsilon_k$  as  $k \rightarrow \infty$  we obtain the expression (1.3) with the parameters

$$\alpha = 1/2\nu - 1, \quad \beta = n + (D-2)/2, \quad c_0 = -\gamma_0 \pi^{-1} \alpha^{\beta+1} a^{(\beta+1)/\alpha},$$

$$a = \left[ 2\Gamma\left(\frac{3\nu-2}{2(v-2)}\right) / \pi^{1/2} \Gamma\left(\frac{\nu}{v-2}\right) \right]^\alpha. \quad (5.2)$$

For a power potential  $v(r) = r^{2N}$ ,  $0 < r < \infty$ , these results were obtained in Refs. 3 and 7.

**II. We turn to nonpolynomial interactions.** Let, for  $r \rightarrow \infty$ ,

$$v(r) \sim r^\nu \exp(br^{2\nu}), \quad 0 < \nu < 1. \quad (5.3)$$

Then from (4.5) we obtain ( $\lambda \rightarrow +0$ )

$$\gamma(\lambda) \propto \exp\{-b_2(\ln \lambda^{-1})^{1/\nu}\}, \quad b_2 = b^{-1/\nu} \quad (5.4)$$

(here we have omitted the pre-exponential factor). Substituting this expression into the dispersion relation

$$\varepsilon_k = \frac{1}{\pi} \int_{-\infty}^0 \frac{dg}{g^{k+1}} \operatorname{Im} E(g) = \frac{(-1)^{k+1}}{\pi} \int_0^\infty d\lambda \gamma(\lambda) \lambda^{-(k+1)} \quad (5.5)$$

and calculating the integral by the method of steepest descents, we find

$$|\varepsilon_k| \propto \exp(a' k^\sigma), \quad k \rightarrow \infty, \quad (5.6)$$

where  $\sigma = 1/(1-\nu)$ ,  $a' = (\sigma-1)^{\sigma-1} (b/\sigma)^\sigma$ . Thus, the coefficients  $\varepsilon_k$  increase faster than  $(k\alpha)!$  with any finite value of the parameter  $\alpha$ ; therefore, the PT series for potentials (5.3) is not summable by the Borel method. In particular, for  $\nu = \frac{1}{2}$  (i.e., for potentials of the form

$v(r) = \operatorname{sh} 2\nu r/r, \operatorname{ch} 2\nu r - 1$ , etc.), we obtain

$$\gamma(\lambda) \propto \exp\{-1/\lambda \kappa^{-2} (\ln \lambda)^2\}, \quad |\varepsilon_k| \propto \exp(\kappa^2 k^2). \quad (5.7)$$

**III. As  $\nu \rightarrow 1$  the parameter  $\sigma \rightarrow \infty$ , i.e., the growth of  $\varepsilon_k$  becomes arbitrarily rapid.** The reason for this is easily understood by considering successive terms of the PT series for  $v(r) \propto \exp(br^{2\nu})$ . If  $b > 1$ , the first order already leads to a divergent integral  $\int v(r) \psi_0^2 dr$ , in which the integrand increases like  $\exp\{(b-1)r^2\}$  as  $r \rightarrow \infty$ . In the second order of PT the correction to the energy of the ground level is

$$E_0^{(2)} = \sum_n' \frac{|v_{0n}|^2}{E_0 - E_n} = - \sum_{n=1}^{\infty} \frac{1}{n} |v_{0n}|^2.$$

The leading term in this sum behaves like

$$(v^2)_{00} \sim \int_0^\infty \exp\{(2b-1)r^2\} dr,$$

i.e., it diverges as soon as  $b > \frac{1}{2}$ . In an analogous way, the  $k$ th order of PT behaves like  $(v^k)_{00}$  and begins to diverge when  $b > k^{-1}$ .

Thus, for a potential with the behavior (5.3) with  $\nu = 1$ ,  $b > 0$ , the coefficients  $\varepsilon_k$  of the PT series become infinite for all  $k > b^{-1}$ ; therefore, a PT series in integer powers of  $g$  does not exist. This also follows from the formula (5.4), which for  $\nu = 1$  gives

$$\gamma(\lambda) \propto \lambda^{1/\nu}, \quad (5.8)$$

i.e., the singularity of  $E(g)$  at  $g=0$  changes its character, being transformed into a branch point of the power type. In the next section it will be shown that for  $\nu \geq 1$  the ratio  $[E(g) - E(0)]/g \rightarrow \infty$  as  $g \rightarrow \infty$ .

**IV. For potentials of the form**

$$v(r) \sim r^{2\mu} (\ln r)^\mu, \quad \mu > 0 \quad (r \rightarrow \infty), \quad (5.9)$$

analogous calculations give

$$\gamma(\lambda) \propto \exp\{-b_3 \lambda^{1-2\mu} \exp(2\lambda^{-1\mu})\}, \quad (5.10)$$

$$|\varepsilon_k| \propto \exp(\mu k \ln \ln k), \quad (5.11)$$

i.e., the coefficients of the PT series increase more slowly than  $(k\alpha)!$  for any, arbitrarily small,  $\alpha > 0$ .

The examples considered show that the stronger is the growth of the anharmonicity  $v(r)$  at large distances the faster the coefficients of the PT series increase as  $k \rightarrow \infty$ . For potentials (5.3) with exponential growth the PT series in integer powers of  $g$  ceases to exist if  $\nu \geq 1$ .

**V. Up to now we have considered potentials with spherical symmetry, which, in the one-dimensional case, correspond to even potentials:  $v(-x) = v(x)$ .** We now discuss an oscillator with odd anharmonicity:

$$H = p^2 + x^2 + g x^{2N+1}, \quad -\infty < x < \infty, \quad (5.12)$$

where  $D=1$  and  $N=1, 2, 3, \dots$ . The width  $\gamma$  is calculated in the same way as in Sec. 4 (the only difference is that the flux of particles flying away to infinity is now in one direction, and this gives an extra factor  $\frac{1}{2}$ ).

In place of (4.3) we obtain

$$\gamma = \frac{A}{2\pi} \exp\left\{-2 \int_{x_-}^{x_+} |p(x)| dx\right\}, \quad (5.13)$$

where  $A = a(n + \frac{1}{2})$  for the  $n$ th level of the oscillator. Hence, for  $g \rightarrow 0$ ,

$$\gamma(g) = \frac{2^n}{n! \pi^n} |g|^{-(2n+1)/(2N-1)} \exp(-b_i |g|^{-2/(2N-1)}), \quad (5.14)$$

where

$$b_i = \pi^{1/2} \Gamma\left(\frac{2N+1}{2N-1}\right) / 2\Gamma\left(\frac{6N+1}{2(2N-1)}\right).$$

We now take into account an essential difference between the Hamiltonian (5.12) and the previous examples. In the potential  $v(x) = |x|^{2N+1}$  all levels for  $g > 0$  are stable, and when  $g$  changes sign decay occurs. Because of this the energy  $E(g)$  has a cut along  $-\infty < g < 0$ , and the discontinuity  $\Delta E(g)$  across this cut coincides with the level width  $\gamma$ . At the same time, for  $v(x) = x^{2N+1}$  decay is possible for either sign of  $g$ , and all the levels are quasi-stationary. Therefore, a suitable variable is  $z = -g^2$  (compare with the treatment of the Stark effect in Ref. 17). Rewriting the formula (5.14) in terms of the variable  $\xi = -z = g^2$  [ $\xi > 0$  on the cut for the function  $E(z)$ ], we determine the asymptotic form of the coefficients of the PT series. For the energy of the  $n$ th level we obtain

$$\varepsilon^{(n)}(g) = \sum_{k=0}^{\infty} a_k (-z)^k = \sum_{k=0}^{\infty} a_k g^{2k}, \quad (5.15)$$

in which  $a_k$  as  $k \rightarrow \infty$  has the form (1.3), with

$$\alpha = 2N-1, \quad \beta = n^{-1/2}, \quad (5.16)$$

$$a = \left[ 2\Gamma\left(\frac{6N+1}{2(2N-1)}\right) / \pi^{1/2} \Gamma\left(\frac{2N+1}{2N-1}\right) \right]^{2N-1}.$$

The coefficients  $a_k$  for  $k \gg 1$  are negative (according to (2.27), the same is also true for small  $k$ ); i.e., the PT series, unlike the cases considered earlier, is not alternating in sign.

## 6. CORRECTION TO THE ENERGY AS $g \rightarrow 0$ FOR EXPONENTIALLY INCREASING POTENTIALS

We shall calculate the leading (for  $g \rightarrow 0$ ) correction  $\delta E = E(g) - E(0)$  to the energy of the ground level for potentials of the form (5.3) with  $\nu \geq 1$ . We shall make use of the method described in Sec. 3. The first approximation  $\tilde{E}_1(g)$  for arbitrary anharmonicity  $v(r^2)$  has the form

$$E_1 = \int_0^{\infty} d\rho e^{-f(\rho)} \frac{1 + gv'(\rho)}{[\rho + gv(\rho)]^{1/2}} / \int_0^{\infty} d\rho e^{-f(\rho)} \rho^{-1/2}, \quad (6.1)$$

where

$$\rho = r^2, \quad f(\rho) = \int_0^{\rho} [1 + gv(x)/x]^{1/2} dx$$

[for  $v(\rho) = \rho^2$  and  $k = 1$  this formula coincides with (3.5)].

It can be shown that for small  $g$  the next-order correction  $\tilde{E}_2 \propto [\tilde{E}_1(g) - E(0)]^2$ , and therefore the leading (for  $g \rightarrow 0$ ) term in  $\delta E$  is determined by the expression (6.1). For  $g \rightarrow 0$  the singularity in  $\tilde{E}_1(g)$  is determined by the region of large  $\rho$ , and therefore for  $v(\rho)$  we can use the asymptotic form (5.3). After rather cumbersome calculations we obtain<sup>2)</sup>:

$$a) \nu > 1 \quad \delta E = K_1 \exp\{-(-b^{-1} \ln g)^{1/\nu}\} (-\ln g)^{(2\nu-1)/2\nu} \quad (6.2)$$

$$b) \nu = 1, b > 1 \quad \delta E = K_2 g^{1/b} (-\ln g)^{1/2 + (\mu-2)/b}, \quad (6.3)$$

$$c) \nu = b = 1 \quad \delta E = K_3 g (-\ln g)^{(\mu+1)/2} \quad \text{for } \mu > -1, \quad (6.4)$$

$$d) \nu = 1, b < 1 \quad \delta E = K_4 g. \quad (6.5)$$

From this it can be seen that in those cases in which the anharmonicity  $v(r)$  increases faster than  $\exp(r^2)$  as  $r \rightarrow \infty$  the first correction to the energy already decreases more slowly than  $g$ , so that  $[E(g) - E(0)]/g \rightarrow \infty$  as  $g \rightarrow 0$ . In this case the dependence of  $\delta E$  on  $g$  is non-trivial. It is clear from the expressions (6.2)–(6.4) that  $E(g)$  cannot be expanded in a series in integer powers of  $g$ .

To conclude we indicate a nonrigorous but intuitive derivation of the dependence of  $\delta E$  on  $g$ , which permits us to obtain the principal (exponential) factor in formula (6.2). For  $g \rightarrow 0$  the anharmonic term  $gv(r)$  is comparable with the oscillator term  $r^2$  only in the region of very large  $r$ . Defining  $r_0$  from the condition  $r^2 = gv(r)$ , taking (5.3) into account we find

$$r_0 \sim \left(-\frac{1}{b} \ln g\right)^{1/2\nu}. \quad (6.6)$$

Near  $r = r_0$  we have

$$r^2 + gv(r) \approx \exp\{bv r_0^{\nu-1} (r - r_0)\}, \quad \nu \geq 1,$$

whence it can be seen that the interval  $\Delta r_{\text{eff}}$  over which the anharmonicity  $gv(r)$  becomes substantially larger than  $r^2$  tends to zero:

$$\Delta r_{\text{eff}} \propto (-\ln g)^{(1-2\nu)/2\nu}.$$

Therefore, in the limit  $g \rightarrow 0$  we arrive at the problem of an oscillator with a wall:

$$v(x) = \begin{cases} x^2, & -x_0 < x < x_0, \\ \infty, & |x| > x_0. \end{cases}$$

As shown in the book by Heading,<sup>20</sup> for such a potential the corrections to the energies of the levels for  $x_0 \gg 1$  are equal to

$$\delta E_n = C_n x_0^{2n+1} e^{-x_0^2}. \quad (6.7)$$

Substituting the value of  $x_0$  from (6.6) into this, we obtain the exact form of the exponential factor in formula (6.2). Unfortunately, this simple method does not give the correct pre-exponential factor in  $\delta E$  that was obtained above.

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## APPENDIX A

We shall consider in more detail the properties of the expansion (2.4) for the case of the power nonlinearity (2.11). In the expression for the first-order correction  $\xi_1(r)$  it is convenient to transform from  $\gamma(\alpha, x)$  to the modified function

$$\tilde{\gamma}(\alpha, x) = \frac{x^{-\alpha}}{\Gamma(\alpha)} \gamma(\alpha, x) = \frac{1}{\Gamma(\alpha)} \int_0^1 e^{-xt} t^{\alpha-1} dt, \quad (A.1)$$

which is an entire function of  $x$  and has the representation<sup>21</sup>

$$\tilde{\gamma}(\alpha, x) = e^{-x} \sum_{k=0}^{\infty} \frac{x^k}{\Gamma(k+1+\alpha)}. \quad (A.2)$$

The correction  $\xi_1(r)$  takes the form

$$\xi_1(r) = \frac{1}{2} \Gamma\left(\frac{D+\nu}{2}\right) e^{r^2} \left[ \gamma\left(\frac{D}{2}, r^2\right) - r^\nu \gamma\left(\frac{D+\nu}{2}, r^2\right) \right]. \quad (\text{A.3})$$

If  $\nu$  is not an integer,  $\xi_1(r)$  has a branch point  $r=0$  and a cut  $(-\infty, 0)$ . For integer  $\nu$  the cut disappears and  $\xi_1(r)$  becomes a single-valued analytic function of  $r$ . From (A.2) and (A.3) we find

$$\xi_1(r) = \frac{1}{2} \Gamma\left(\frac{D+\nu}{2}\right) \left\{ \sum_{k=0}^{\infty} r^{2k+1} / \Gamma\left(k + \frac{D+2}{2}\right) - \sum_{k=0}^{\infty} r^{2k+1+\nu} / \Gamma\left(k + \frac{D+2+\nu}{2}\right) \right\}. \quad (\text{A.4})$$

For even  $\nu=4, 6, 8, \dots$  the infinite sums cancel each other and  $\xi_1(r)$  reduces to a polynomial—cf. formula (2.12). But if  $\nu=3, 5, 7, \dots$ , then  $\xi_1(r)$  is an entire function of  $r$  and not a polynomial. In this case there are directions in the  $r$ -plane along which  $\xi_1(r)$  increases exponentially. For example, for  $D=1, \nu=3$  (a one-dimensional oscillator with Hamiltonian  $H = p^2 + x^2 + g|x|^3$ ), we obtain

$$\xi_1(r) = \frac{1}{2} \{ r^2 + 1 - \exp(r^2) \text{Erfc}(r) \}, \quad r = |x|. \quad (\text{A.5})$$

As  $r \rightarrow \infty$  in the sector  $|\arg r| < 3\pi/4$  the asymptotic expansions

$$e^{r^2} \text{Erfc}(r) = \frac{1}{x^{3/2}} \left( 1 - \frac{1}{2r^2} + \dots \right), \quad \xi_1(r) \approx \frac{1}{2} r^2 + \dots$$

are valid, but in the sector  $3\pi/4 < |\arg r| \leq \pi$  the function  $\xi_1(r)$  increases exponentially. For example when  $r \rightarrow -\infty$  along the negative real semi-axis,  $\text{Erfc}(r) \rightarrow 2$  and  $\xi_1(r) \approx -\exp(r^2)$ .

Thus, the anharmonicity  $v(r) = r^\nu$  with even  $\nu$  is distinct in the respect that the function  $\xi_1(r)$  is transformed into a polynomial. This is also true for the next terms  $\xi_n(r)$  of the expansion (2.4) (cf. Sec. 2). In this case, the advantages over the ordinary PT of the PT variant based on the use of the Riccati equation are obvious.

For  $D > 1$  the analyticity of the potential  $v(r) = r^\nu$  is destroyed at the point  $r=0$ , except for  $\nu=4, 6, 8, \dots$ . But if  $D=1$ , then  $v(x) = x^\nu$  is an analytic function of  $x$  for integer  $\nu$ . The analyticity of the potential leads to a substantial simplification of the terms  $\xi_n(r)$  of the PT series. Thus, for  $v(x) = x^3$  we have

$$\xi_1(x) = \frac{1}{2} (x^2 + 1), \quad (\text{A.6})$$

which can be compared with the formula (A.5) for the potential  $v(x) = |x|^3$ , which is not regular at zero.

## APPENDIX B

In this Appendix an account is given of the derivation of some of the formulas from Sec. 3.

For large  $g$  the function  $f(r) \rightarrow 2g^{-1/2} r^3/3$ , so that it is convenient to make a change of variable in the integral (3.5):

$$r = \left(\frac{3}{2}\right)^{1/2} g^{-1/2} t^{3/2}.$$

Substituting  $\varphi_2(r) = -\bar{\xi}_1^2(r)$  into the expression (3.5), where  $\bar{\xi}_1(r)$  is determined by the equality (3.4) and  $\bar{\xi}_1$  by the equality (3.6), for  $g \rightarrow \infty$  we easily obtain

$$\bar{\xi}_2 = - \left(\frac{2}{3}\right)^{3/2} g^{3/2} \frac{\Gamma^2(2/3)}{\Gamma(1/3)} \int_0^\infty \frac{dz e^z}{z^{3/2}} \left[ \frac{\Gamma(2/3, z)}{\Gamma(2/3)} - \frac{\Gamma(1/3, z)}{\Gamma(1/3)} \right]^2, \quad (\text{B.1})$$

where

$$\Gamma(\alpha, z) = e^{-z} \int_0^\infty dt e^{-tz} (1+t)^{\alpha-1} = \Gamma(\alpha) - \gamma(\alpha, z).$$

Using the latter expression for  $\Gamma(\alpha, z)$  and integrating first over  $z$  in (B.1), we find

$$\bar{\xi}_2 = - \left(\frac{2}{3}\right)^{3/2} g^{3/2} \frac{\Gamma^2(2/3)}{\Gamma(1/3)} (I_1 + I_2), \quad (\text{B.2})$$

where

$$I_1 = \frac{2}{3\Gamma(2/3)} \int_0^1 \int_0^1 du dv [(u+v-uv)^{-1/2} - v^{1/2} (u+v-uv)^{-3/2}],$$

$$I_2 = \frac{1}{\Gamma^2(1/3)} \int_0^1 \int_0^1 du dv (u+v-uv)^{-1} (uv)^{-3/2}$$

(the substitution  $t = u^{-1} - 1$  has been made). The first integral is easily calculated:

$$I_1 = \frac{3}{2\Gamma(2/3)} (\ln 3 - 3^{1/2} \arctg 3^{1/2}). \quad (\text{B.3})$$

As regards the second, we proceed as follows:

$$I_2 \Gamma^2(1/3) = 2 \int_0^1 \frac{du}{u^{3/2}} \int_0^1 \frac{dv}{v^{1/2} (u+v-uv)} = 2 \int_0^1 \frac{du}{u^{3/2}} \int_0^1 \frac{dw}{w^{1/2} [1+w(1-u)]}, \quad (\text{B.4})$$

and, expanding the integrand in a series in powers of  $w(1-u)$ , we finally obtain

$$\bar{\xi}_2 = - \frac{2}{3} \left(\frac{3g}{2}\right)^{3/2} \frac{\Gamma^2(2/3)}{\Gamma(1/3)} \left[ \frac{3}{2} (\ln 3 - 3^{1/2} \arctg 3^{1/2}) + \frac{2\Gamma(2/3)}{\Gamma(1/3)} \sum_{k=0}^{\infty} \frac{(-1)^k \Gamma(k+1)}{(k+2/3)\Gamma(k+1/3)} \right]. \quad (\text{B.5})$$

Numerical summation gives  $\bar{\xi}_2 = -0.109g^{1/3}$ .

We now discuss the derivation of the first of the formulas (3.6) and the formula (3.8). Putting  $t = (1+g r^2)^{3/2}$  and  $\mu = 2/3g$  in (3.5), we have

$$\bar{\xi}_1 = J_1/J_2; \quad J_i = \int_1^\infty e^{-\mu f_i(t)} dt, \quad (\text{B.6})$$

$$f_1(t) = \frac{2-t^{-3/2}}{[t^{3/2}-1]^{3/2}}, \quad f_2(t) = t^{-3/2} (t^3-1)^{-3/2}.$$

Expressions for  $J_1$  and  $J_2$  for small  $g$  are obtained by expanding the integrand functions  $f_i(t)$  about the point  $t=1$ :

$$J_1 = e^{-\mu} \left(\frac{3\pi}{2\mu}\right)^{1/2} \left[ 1 + \frac{3}{8\mu} - \frac{455}{1152\mu^2} + \dots \right],$$

$$J_2 = e^{-\mu} \left(\frac{3\pi}{2\mu}\right)^{1/2} \left[ 1 - \frac{1}{8\mu} + \frac{145}{1152\mu^2} + \dots \right],$$

whence follows the first formula (3.6) for  $\bar{\xi}_1$ .

To calculate the discontinuity of  $\bar{\xi}_1(g)$  as  $g \rightarrow -0$  we make in (B.6) the replacement  $t = 1 + y/\mu$ ,  $\mu = |\mu| e^{\pm i\pi}$ . The imaginary part of the integral  $J_1$  and  $J_2$  is connected with the appearance of the imaginary part of the functions  $f_i(1+y/\mu)$  when  $y > |\mu|$ . As a result, we obtain formula (3.8), in which the constant  $c_0 = -\left(\frac{2}{3}\right)^{2/3} \pi^{1/2} / \Gamma\left(\frac{2}{3}\right)$ .



<sup>1)</sup>In the present case the polynomials  $\xi_k(x)$  have degree  $k+1$  and a definite parity, equal to  $(-1)^{k+1}$ :

$$\begin{aligned} \xi_1 &= \frac{1}{2}(x^2+1), & \xi_2 &= -\frac{1}{16}(2x^3+7x), \\ \xi_3 &= \frac{1}{32}(2x^4+13x^2+20), & \xi_4 &= -\frac{1}{256}(10x^5+98x^3+305x), \\ \xi_5 &= \frac{1}{512}(14x^6+191x^4+917x^2+1362), \text{ etc.} \end{aligned}$$

<sup>2)</sup>Here, the  $K_i$  are certain coefficients, depending on the parameters  $\nu$ ,  $b$ , and  $\mu$ . We shall give details of the calculations, and also the explicit form of the coefficients  $K_i$ , in another publication.

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## Resonance broadening of two-photon S-S transitions

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A theoretical investigation is made of the influence of resonance excitation-exchange collisions on the line profile of a two-photon S-S transition. It is shown that the profile differs from the form predicted by the adiabatic collision theory of the broadening. In particular, the ratio of the line width  $\Gamma$  to the shift  $\Delta\omega_m$  does not obey the relationship  $\Gamma/|\Delta\omega_m| = 1.4$ . The characteristics of the broadening in the presence of hyperfine splitting of the levels are considered.

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### §1. INTRODUCTION

The theoretically predicted<sup>1</sup> advantages of two-photon absorption as the most accurate method for investigating atomic and molecular transitions have recently been confirmed convincingly by several experimental investigations.<sup>2-5</sup> One of the most attractive features of this method is that it can be used to eliminate in principle and reduce considerably in practice the influence of the Doppler effect on the line width. Therefore, beginning from relatively low pressures of ~1 Torr, when the collisional line width becomes comparable with the radiative width, collisions play the dominant role in the formation of a line profile.

We shall consider the characteristics of the broadening of two-photon transitions in atoms. In a typical experimental situation the line profile of such a transition is formed as a result of collisions with neutral particles, which are atoms and molecules of the same substance in the form of a gas or of an impurity. The van der

Waals interaction plays the main role in such collisions and its influence on the broadening of one-photon transition lines has been investigated quite thoroughly.

We shall also assume that the density of the perturbing particles is sufficiently low so that the collision (impact) theory of the broadening can be applied. The broadening of the two-photon transition lines by a foreign gas does not require any special treatment. We can use the standard formulas of the collision theory for the broadening of one-photon absorption spectra.<sup>6</sup>

The situation is different in the case of the broadening of two-photon transition lines by the gas of the same substance. In this case the broadening may be greatly affected by the resonance exchange of excitations in collisions between identical atoms, whose role is not taken into account in the standard adiabatic collision theory of the broadening. The analogous question of the influence of the resonance transfer of excitation on the profile of a one-photon line has been considered on many occa-