New approach to perturbation theory for a discrete spectrum (anharmonic oscillator)

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An effective method is developed for calculating the higher orders of perturbation theory for the states of a discrete spectrum; it is based on a transition from the Schrödinger equation to a Riccati equation for the logarithmic derivative of the wave function. For potentials of polynomial type (in particular, in the case of an anharmonic oscillator with nonlinearity gr^{2N}, $N=2, 3, 4,...$) the calculation of the higher orders of perturbation theory reduces to simple recursion relations, by means of which the coefficients in the perturbation series for the energy levels can be found exactly for $k \lesssim 10$ and numerically up to $k \approx 200$ (k is the order of the perturbation theory). The Riccati equation is used to construct a rapidly converging perturbation theory in which allowance is made for the behavior of the potential at singular points.

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§1. INTRODUCTION

The calculation of higher orders of perturbation theory is of interest for field theory and quantum mechanics. Significant progress has been achieved in this direction in recent years. In quantum field theory, this has been associated with the application of the method of steepest descent (in the neighborhood of classical solutions) to the calculation of functional integrals for the Green's functions.[1-3] Many studies have been devoted to the development of perturbation-theory methods in quantum mechanics, especially for the anharmonic oscillator (see, for example, Refs. 4 and 5 and the review in Ref. 6). This problem is interesting because it has many physical applications (in the theory of molecules, solid-state physics, etc.) and also in account of the analogy with scalar field theory with the interaction $g\varphi^{2N}$.

In Refs. 7 and 8, we proposed (for the example of a gr^4 oscillator) a variant of perturbation theory based on a transition from the Schrödinger equation to the Riccati equation. A feature of the method is that to calculate the corrections to the energy level and wave function in any order of the perturbation theory it is not necessary to know the complete spectrum of the unperturbed Hamiltonian.[1)] We considered applications to concrete problems in our papers Refs. 7 8, 14, and 15. An approach to the construction of a perturbation theory close to ours developed in Refs. 7 and 8 was also proposed by Aharonov and Au.[16] It was recently shown[17,18] that this method admits a natural generalization to the multidimensional case.

In the present paper, we consider our study of this group of questions. In §2, we consider an oscillator with anharmonicity gr^{2N} in D-dimensional space, i.e., a system with the Hamiltonian

$$H=\sum_{i=1}^{D}(p_i^2+x_i^2)+g\left(\sum_{i=1}^{D}x_i^2\right)^{N/2}, \quad N=2,3,4,\ldots. \tag{1.1}$$

Perfecting the method of our previous paper Ref. 7, we reduce the calculation of the higher orders of perturbation theory in powers of the coupling constant g to the solution of a system of recursion relations with integral numbers. This system [see (2.8) below] is very convenient for computer calculations and, in particular, makes it possible to express the first ($k \lesssim 10$) perturbation orders in an exact form, and for large k, up to several hundred, to find the coefficients of the perturbation series numerically. We investigate in detail the dependence of the coefficients of the perturbation series on the dimension D of space.

The asymptotic behavior of the coefficients ε_k of the perturbation series as $k \to \infty$ is determined[1-4] by the probability of tunneling of a particle in the potential r^2+gr^{2N} when the sign of the coupling constant is reversed ($g<0$). The calculation of the higher orders of the perturbation theory makes it possible to determine the rate at which ε_k approaches the asymptotic $\tilde{\varepsilon}_k$ and estimate the magnitude of the power corrections in the expansion (3.6). It is shown that the power corrections increase rapidly with increasing dimension D.

In §4, to calculate the energy levels, we use the special form of perturbation theory proposed earlier in Ref. 7. It is based on the separation of the most singular terms in the logarithmic derivative of the wave function as $r \to 0$ and $r \to \infty$. The perturbation theory is constructed, not in powers of g^k, but in terms of more complicated functions of the coupling constant g, which are determined with allowance for the behavor of the potential $V(r)$ at the singular points ($r=0, \infty$). In contrast to ordinary perturbation theory, which, as a rule, is divergent,[2)] this variant of perturbation theory ensures rapid convergence of the successive approximations. In §4, this is demonstrated for examples, and a general proof of convergence is outlined briefly in Appendix B.

§2. PERTURBATION THEORY ON THE BASIS OF THE RICCATI EQUATION

The calculation of the higher orders of perturbation theory is simplified by going over from the radial Schrödinger equation

$$R''+\frac{D-1}{r}R'+(E-r^2-gr^{2N})R=0$$

to a Riccati equation for the logarithmic derivative of the wave function:

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$$\xi_0(r)=-\left(\frac{R'}{R}+\frac{D-1}{2r}\right), \tag{2.1}$$

$$\xi_0'-\xi_0^2=E-r^2-gr^{2N}-\frac{(D-1)(D-3)}{4r^2}. \tag{2.2}$$

We shall restrict ourselves here, for simplicity, to the case of the ground state, whose wave function has no nodes[3]; we denote its energy by $E_0=E_0(g,D)$. To the Hamiltonian (1.1) there corresponds $E_0=(0,D)=D$. Setting $\varepsilon(g,D)=E_0(g,D)/E_0(0,D)$, we expand ε and ξ in series in powers of g:

$$\varepsilon(g)=1-\sum_{k=1}^{\infty}\varepsilon_k(-g)^k, \quad \xi(r,g)=\sum_{k=0}^{\infty}\xi_k(r)g^k. \tag{2.3}$$

Substituting these expansions in (2.2), we find that $\xi_0(r)=r-(D-1)/2r$, and for $k\geq 1$ the functions $\xi_k(r)$ are polynomials:

$$\xi_k(r)=\sum_{m=0}^{M}a_m^{(k)}r^{2m+1}, \quad M=(N-1)k. \tag{2.4}$$

This can be seen by calculating ξ_1 explicitly:

$$\xi_1(r)=\frac{1}{2}\sum_{m=0}^{N-1}\frac{\Gamma(N+D/2)}{\Gamma(m+1+D/2)}r^{2m+1}$$

and then using induction.[4]

Substituting (2.4) in Eq. (2.6) of our previous paper Ref. 7, we arrive at recursion relations for the coefficients of the polynomial $\xi_k(r)$:

$$2a_{m-1}^{(k)}=(D+2m)a_m^{(k)}+\sum_{i=1}^{k-1}\sum_{p+q=m-1}a_p^{(i)}a_q^{(k-i)}. \tag{2.5}$$

Here $1\leq m\leq M$, and the leading coefficients ($m=M$, $M-1,\ldots$) can be found explicitly:

$$a_M^{(k)}=(-1)^{k+1}2^{-[(N+3)k-1]}C_k$$
$$a_{M-1}^{(k)}=(-1)^{k+1}2^{-(N+3)k}[(2k-1)C_kD+(N-1)2^{2k-1}],\ldots \tag{2.6}$$

where C_k are Catalan numbers known in combinatorial analysis[5]:

$$C_k=(2k-2)!/k!(k-1) \quad \text{for } k\geq 1.$$

Redefining the coefficients

$$A_m^{(k)}=(-1)^{k+1}2^{(N+1)k-m-1}a_m^{(k)}, \tag{2.7}$$

we go over from (2.5) to the simpler recursion relations

$$A_{m-1}^{(k)}=(D+2m)A_m^{(k)}+\sum_{i=1}^{k-1}\sum_{p+q=m-1}A_p^{(i)}A_q^{(k-i)}, \tag{2.8}$$

the leading coefficient being $A_M^{(k)}=C_k$.

It follows that $A_m^{(k)}$ for all values of k and m are positive integers. Because of this property, the exact values of $A^{(k)}$ (and, thus, the coefficients ε_k for the energy levels) can be found in accordance with Eqs. (2.8) by means of numerical calculations on a computer. Note that these equations do not contain (explicitly) the degree of anharmonicity $2N$. Only the total number of recursion relations in a given perturbation order depends on N.

Equations (2.5) or (2.8) give a procedure for successive "descent with respect to m" in a given perturbation order. Using them to descend to $m=0$, we find the correction to the energy:

$$\varepsilon_k=(-1)^{k+1}a_0^{(k)}=2^{1-(N+1)k}A_0^{(k)}, \tag{2.9}$$

which completes the calculation of the k-th order of the perturbation theory. Since

$$R(r)=\exp\left\{-\left[\frac{r^2}{2}+\sum_{k=1}^{\infty}g^k\int_0^r\xi_k(r')\,dr'\right]\right\}$$
$$=\exp\left\{-\frac{r^2}{2}\left[1+\sum_{k=1}^{\infty}g^k\sum_{m=0}^{M}\frac{a_m^{(k)}}{m+1}r^{2m}\right]\right\}, \tag{2.10}$$

this means that the correction $\sim g^k$ to the wave function is also determined. However, the perturbation series for the wave function has a more complicated construction than for $\xi(r)$.

Using Eqs. (2.8), we calculated some of the first orders of the perturbation theory exactly, i.e., in the form of rational fractions, for oscillators with anharmonicity gr^4 and gr^6 (see the tables in our papers Ref. 8). Note that in the case $D=1, N=2$ (one-dimensional gx^4 oscillator) these results agree with the calculations of Bender and Wu[4] made by a different method.[6] Using the relations (2.8) and (2.9), we can readily make similar calculations for other degrees of anharmonicity $2N$ and different dimensions D of space. The method of calculating the higher orders of perturbation theory proposed above is more convenient than the method of Bender and Wu,[4] and it enables one, by means of the recursion relations (2.8), to calculate the coefficients of the perturbation series for the energy of the ground state up to very high orders k.

§3. DEPENDENCE OF THE COEFFICIENTS ε_k ON D

We now consider how the structure of the perturbation series for an anharmonic oscillator changes with the dimension D. The parameter D occurs explicitly in Eqs. (2.5) and (2.8). Calculations in the lowest orders give

$$\varepsilon_1=2^{-N}(D+2)(D+4)\ldots(D+2N-2),$$
$$\varepsilon_2=\frac{1}{2^{N+2}}(D+2)(D+4)\ldots(D+2N-2)\sum_{i,j=1}^{N}\frac{\Gamma\left(i+j+\frac{D-2}{2}\right)\Gamma\left(N+\frac{D}{2}\right)}{\Gamma\left(i+\frac{D}{2}\right)\Gamma\left(j+\frac{D}{2}\right)}. \tag{3.1}$$

The following factorization holds:

$$\varepsilon_k(D)=(D+2)(D+4)\ldots(D+2N-2)P_k(D), \tag{3.2}$$

where $P_k(D)$ is a polynomial in D of degree $(N-1)(k-1)$. For $k=1$ and 2 this can be seen from Eqs. (3.1). For arbitrary k, the factorization (3.2) can be proved by induction if it is noted that $A_m^{(k)}$ is a polynomial in D of degree $M-m=Nk-(k+m)$ and the equations with $m=1,2,\ldots N-1$ in (2.8) are considered.

It follows from these equations that all the coefficients of the polynomial $P_k(D)$ are rational numbers whose denominators are powers of 2:

$$P_k(D)=2^{-\nu_k}\sum_{m=0}^{(N-1)(k-1)}p_m^{(k)}D^m, \tag{3.3}$$

where ν_k and $p_m^{(k)}$ are positive integers. For the case $N=2$, detailed tables, which determine $\varepsilon_k(D)$ for all $k\leq 14$ and arbitrary dimension D, are contained in the previous paper Ref. 19.

As $k\to\infty$, the coefficients of the perturbation-theory

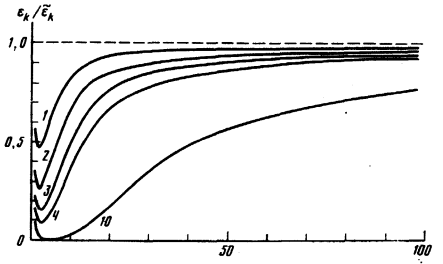

FIG. 1. The ratio $\varepsilon_k/\tilde{\varepsilon}_k$ for a gr^4 oscillator as a function of the order k of perturbation theory. The numbers next to the curve give the dimension D of space.

series increase factorially. Their asymptotic behavior (which we denote by $\tilde{\varepsilon}_k$) is determined by the barrier penetrability in the potential r^2+gr^{2N} for $g<0$ and can be found by the WKB method (see Refs. 2, 4, and 7):

$$\tilde{\varepsilon}_k = C_0(k\alpha)!a^k k^\beta, \quad \alpha = N-1, \quad \beta = (D-2)/2, \tag{3.4}$$

$$a = \frac{1}{4}\left[\Gamma\left(\frac{2N}{N-1}\right)\Big/\Gamma^2\left(\frac{N}{N-1}\right)\right]^{N-1},$$

$$C_0 = \left[\Gamma\left(\frac{2N}{N-1}\right)\Big/\Gamma^2\left(\frac{N}{N-1}\right)\right]^{D/2}(N-1)^{D/2}/\pi\Gamma\left(\frac{D+2}{2}\right). \tag{3.5}$$

On the other hand, Eqs. (2.8) enable one to find ε_k numerically on a computer with a high accuracy for k right up to several hundred. We made such calculations for $N=2$ and 3. The rate at which ε_k approaches the asymptotic $\tilde{\varepsilon}_k$ for these cases is shown in Figs. 1 and 2. These calculations show that the asymptotic expansion of ε_k has the form

$$\varepsilon_k = \tilde{\varepsilon}_k\left(1+\frac{c_1}{k}+\frac{c_2}{k^2}+\ldots\right), \quad k\to\infty \tag{3.6}$$

and they enable one to determine the magnitude of the power corrections to the principal term in the asymptotic $\tilde{\varepsilon}_k$. It can be seen from comparison of Figs. 1 and 2 that for $N=3$ the coefficients ε_k tend to the asymptotic behavior more rapidly, and the maximal deviation of $\varepsilon_k/\tilde{\varepsilon}_k$ from unity is much less than for $N=2$. Accordingly the power corrections in the expansion (3.6) are less important in the case of the gr^6 oscillator than for the quadratic (gr^4) oscillator. On the other hand, when the dimension D is increased, ε_k does not tend to the asymptotic behavior so rapidly, and the power corrections in (3.6) increase rapidly (see Fig. 3).

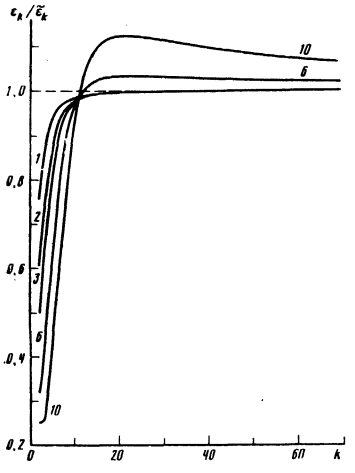

FIG. 2. The same as in Fig. 1 for a gr^6 oscillator.

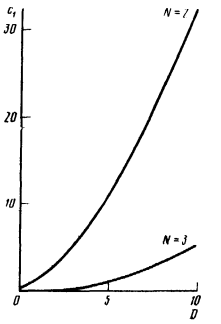

FIG. 3. The coefficient c_1 in the expansion (3.6) for a gr^{2N} oscillator as a function of D.

The determination of the power corrections [i.e., the coefficients $c_1, c_2, \ldots$ in the expansion (3.6)] enables one by means of Borel's summation method to establish the energy $E(g)$ of the level in a fairly wide range of values of the coupling constant g.

§4. RAPIDLY CONVERGING PERTURBATION THEORY

Since the coefficients ε_k for the anharmonic oscillator increase factorially with increasing order k of the perturbation theory, the radius of convergence of the series (2.3) is zero and the series is only asymptotic. Because of this, the calculation of the energy $\varepsilon(g)$ with allowance for the higher orders of perturbation theory requires the use of methods of generalized summation of divergent series (see, for example, Refs. 20 and 21).

The variant of perturbation theory discussed below is free of these shortcomings and leads to a rapidly converging series. This method was proposed in Ref. 7, in which the examples $v(r)=r^4$ and $v(r)=r^\mu\exp(br^{2\nu})$ were considered for $D=1$. Below, we consider the case of arbitrary dimension D and an anharmonicity of power form: $v(r)=r^{2N}$. The generalization to an arbitrary potential $v(r)$ is obvious.

The perturbation theory is constructed on the basis of the Riccati equation (2.2), the choice of the zeroth approximation y_0 for the logarithmic derivative ξ taking into account[7,8] the behavior of the wave function at the singular points ($r=0, \infty$). The asymptotic behavior of the exact solutions of the Schrödinger equation as $r\to 0$, can be readily found, and we have[7)]

$$y_0(r,g) = [r^2+gv(r^2)]^{1/2} - (D-1)/2r, \tag{4.1}$$

$$\xi(r,g) = \sum_{k=0}^{\infty} y_k(r,g), \quad E = \sum_{k=0}^{\infty} E_k(g). \tag{4.2}$$

Thus, the "small parameter" of the perturbation theory is associated with the difference $\xi - y_0$ and it is not obvious in advance that it is literally small (in the previous Ref. 7, this variant of perturbation theory was called "perturbation theory in the departure from the asymptotic behavior"). Moreover, in contrast to the series (2.3), the expansion of $\xi(r,g)$ is in terms of more complicated functions of the coupling constant g than the powers g^k. The standard perturbation theory

in powers of g corresponds to the choice

$$\xi_0(r)=r-(D-1)/2r$$

of the zeroth potential (see §2). The difference between ξ_0 and y_0 is that the ansatz (4.1) completely includes the singularity of the exact Hamiltonian as $r\to\infty$, and therefore the potential V_1 of the perturbation is now less singular than the unperturbed potential V_0.

Indeed, suppose $V=\rho+gv(\rho)$, $\rho=r^2$; then

$$V_1=g\left[v'(\rho)-\frac{v(\rho)}{\rho}\right]\left[1+g\frac{v(\rho)}{\rho}\right]^{-1/2}+D\left\{\left[1+g\frac{v(\rho)}{\rho}\right]^{1/2}-1\right\} \quad (4.3)$$

[see Eq. (4.5) below]. As $g\to 0$, the perturbation V_1 becomes small:

$$V_1=g\left\{v'(\rho)+\frac{D-2}{2\rho}v(\rho)\right\}+O(g^2).$$

In addition, $V_1/V_0\to 0$ as $r\to\infty$ (and this ratio is smaller, the larger is the coupling constant g). Thus, for potentials of power-law growth $v(\rho)=\rho^\nu$ we have

$$\frac{V_1}{V_0}\approx\begin{cases}(D/2+\nu-1)gr^{2(\nu-2)}, & r\to 0,\\ (D+\nu-1)g^{-1/2}r^{-(\nu+1)}, & r\to\infty.\end{cases}$$

This also explains why the use of this variant of perturbation theory makes it possible to go beyond the framework of weak coupling, i.e., to reach values $g\sim 1$ and even (as will be shown below) $g\to\infty$ (see also Ref. 22).

Substituting (4.1) and (4.2) in Eq. (2.2), we arrive at the system of equations for $k\geq 1$:

$$y_k'-2\left(V^{1/2}-\frac{D-1}{2r}\right)y_k=E_k-V_k, \quad (4.4)$$

where

$$V=r^2+gv(r^2)\equiv V_0+V_1,$$

$$V_1=\frac{1}{2}V^{-1/2}\frac{dV}{dr}+\frac{D-1}{r}V^{1/2}-D, \quad (4.5)$$

and for $k\geq 2$

$$V_k(r,g)=-\sum_{j=1}^{k-1}y_jy_{k-j}. \quad (4.6)$$

The unperturbed potential V_0 is completely determined by the choice of the zeroth approximation $y_0(r,g)$. The explicit expression for V_0 follows from (2.2) if we replace ξ there by y_0 and the energy E by $E_0=D$. Since y_0 is chosen such that $y_0\to\xi$ as $r\to 0$ and $r\to\infty$, it can be seen that $y_k(r,g)\to 0$ for $k\geq 1$ at both ends of the interval $(0,\infty)$. These boundary conditions uniquely determine $y_k(r,g)$ and $E_k(g)$.

The solution of Eq. (4.4) that decreases at infinity has the form

$$y_k(r,g)=\frac{1}{\chi_0^2(r)}\int_0^r(E_k-V_k)\chi_0^2(r')dr'=-\frac{1}{\chi_0^2(r)}\int_r^\infty(E_k-V_k)\chi_0^2(r')dr', \quad (4.7)$$

$$\chi_0(r)=r^{(D-1)/2}\exp\left\{\int^r[V(r')]^{1/2}dr'\right\}.$$

From the condition $y_k(0)=0$, we find the correction of k-th order to the energy level:

$$E_k=\langle V_k\rangle=\int_0^\infty V_k\chi_0^2dr\Big/\int_0^\infty\chi_0^2dr. \quad (4.8)$$

Note that $E_k(g)$ are nontrivial functions of the coupling constant g, namely, they have a cut in the complex plane of g for $g<0$, which agrees with the behavior of the exact solution.

The analysis made in Ref. 7 (for $N=2, D=1$ and 3) shows that even the lowest approximations for the energy of the ground state,

$$E^{(k)}=\sum_{j=1}^k E_j(g), \quad (4.9)$$

agree well with the numerical solution of the Schrödinger equation,[23] and the accuracy of $E^{(k)}(g)$ is better, the smaller is g (see Fig. 2 in Ref. 7). Suppose

$$E^{(1)}(g)=D(1+\tilde{\varepsilon}_1g-\tilde{\varepsilon}_2g^2+\ldots).$$

Then $\tilde{\varepsilon}_1$ is equal to the exact coefficient (3.1), and the following coefficients are numerically close to the exact coefficients. This explains the proximity of $E^{(1)}(g)$ to the exact solution in the region of small g. One can show that $E_k(g)\sim g^k$ for $g\to 0$, so that the k-th approximation (4.9) exactly reproduces the first k terms of the perturbation series.

We consider in more detail the least favorable (from the point of view of numerical agreement with the exact solution) case of strong coupling, $g\to\infty$, when

$$V\approx gv(r),\quad V_1=g^{1/2}\left(\frac{1}{2v}\frac{dv}{dr}+\frac{D-1}{r}v^{1/2}\right).$$

For $v(r)=r^{2N}$, Eqs. (4.6)–(4.8) give

$$\varepsilon^{(k)}=\frac{E^{(k)}(g,D)}{D}\approx C_kg^\nu,\quad \nu=\frac{1}{N+1}. \quad (4.10)$$

The degree of the coupling constant g is equal to the corresponding degree in the asymptotic behavior of the exact solution of the Schrödinger equation:

$$\varepsilon(g,D)\approx C_\infty g^\nu,\quad g\to\infty, \quad (4.11)$$

so that the entire difference between the k-th approximation $\varepsilon^{(k)}$ and the exact eigenvalue $\varepsilon(g,D)$ reduces here to the difference between the constants C_k and C_∞.

It is readily seen that to calculate C_k we must assume

TABLE I. Ground-state energy of a gr^4 oscillator in the limit of strong coupling.

D	C_1	C_2	C_3	C_∞
1	1.157233 (9.1%)	1.047692 (1.2%)	1.061284 (0.09%)	1.060362
2	1.268037 (8.2%)	1.163717 (0.73%)	1.172131 (0.03%)	1.1724
3	1.362942 (7.6%)	1.259885 (0.53%)	1.265830 (0.06%)	1.266558
4	1.446541 (7.3%)	1.343073 (0.37%)	1.347628	1.348
6	1.590099 (6.9%)	1.483825 (0.28%)	–	1.488
9	1.766776	1.654860	–	–
12	1.914008	1.796311	–	1.80

Note. The coefficients C_k of the asymptotic behavior (4.10) are given here for the first three approximations. The error (the deviation of C_k from C_∞) is given in the brackets. The exact values C_∞ of the coefficient are taken from Ref. 6. We have here used the fact that the lowest level of a two-dimensional oscillator with angular momentum l corresponds to the ground-state level for dimension $D=2l+2$.

in Eqs (4.4)–(4.8) that $V(r)=r^{2N}$ and take the perturbation $V_1(r)=(N+D-1)r^{N-1}$. Then $y_0=r^N-(D-1)/2r$, and the zeroth approximation for the normalized wave function has the form

$$\chi_0(r)=\left[\frac{2^{D\nu}\nu^{D\nu-1}}{\Gamma(D\nu)}\right]^{1/2} r^{(D-1)/2}\exp(-\nu r^{1/\nu}),\quad \nu=\frac{1}{N+1}. \tag{4.12}$$

i.e., it has the same asymptotic behavior as $r\to 0$ and $r\to\infty$ as the exact solution of the Schrödinger equation. The expressions for χ_0 and V_1 are so simple that the first two approximations (C_1 and C_2) can be found analytically for arbitrary N and D (see Appendix A). The results of the calculations are given in Table I and compared there with the exact values for the coefficient $C_\infty=C_\infty(N,D)$. It can be seen from Table I that: 1) the approximations (4.9) converge rapidly to the exact solution; 2) the accuracy of the approximation $\varepsilon^{(k)}$ improves with increasing dimension D.

For the rapid convergence of the approximations $E^{(k)}$, a felicitous choice of the zeroth approximation $y_0(r,g)$ is important. This is analogous to the situation with regard to the choice of trial functions in the variational method.[18] It is natural to attempt other ansatzes for y_0 in addition to (4.1). Turbiner[22] suggested that the zeroth approximation for the wave function should be taken in the form

$$\chi_0=r^{(D-1)/2}\exp\left\{-\left[\frac{r^2}{2}+\int_0^r [V(r')]^{1/2}dr'\right]\right\}, \tag{4.13}$$

which corresponds to

$$y_0=r+\int_0^r V^{1/2}dr-\frac{D-1}{2r}.$$

For the gr^4 oscillator, the accuracy of this approximation is somewhat worse than when y_0 is chosen in the form (4.1). However, the ansatz (4.13) has an advantage at large N. A further increase in the accuracy could be achieved[18] by varying the coefficient of r^2 in the exponential in (4.13). It should however be noted that the volume of computational work then increases. Whereas the first two approximations ε_1 and ε_2 can be calculated analytically in the case (4.1), numerical calculations are already needed for the first approximation when the transition to the ansatz (4.13) is made.

§5. CONCLUSIONS

The quantum D-dimensional oscillator with anharmonicity gr^{2N} is the simplest example of a system with nonquadratic Hamiltonian. We should like to point out that the transition from the Schrödinger equation to the Riccati equation (i.e., delinearization of the problem) is an effective device for calculating the higher orders of perturbation theory in a number of other problems of quantum mechanics as well.

The Stark effect in the hydrogen atom was considered earlier in Ref. 14. Separating the variables in the parabolic coordinates ξ, η, φ and making the substitution

$$\psi(\mathbf{r})=\exp\left\{-\frac{1}{2}\left[\int_0^\xi x(\xi')d\xi'+\int_0^\eta y(\eta')d\eta'\right]+im\varphi\right\}. \tag{5.1}$$

one can obtain for $x(\xi,\mathscr{E})$ and $y(\eta,\mathscr{E})$ a system of Riccati equations. The energy E and the functions x and y are expanded in powers of the electric field $\mathscr{E}$ as in (2.3). It can be shown that $x_k(\xi)$ and $y_k(\eta)$ are polynomials of degree k, and recursion relations of the type (2.5) with $N=D=2$ are obtained for the determination of their coefficients. In this manner, the hyperpolarizabilities α_k were calculated[14] up to the 160-th order of perturbation theory:

$$E(\mathscr{E})=-\frac{1}{2}\left(1+\sum_{k=1}^{\infty}\alpha_{2k}\mathscr{E}^{2k}\right)$$

(for the ground state). It was also shown how this method can be generalized to the case of excited states whose wave functions have nodes.[24]

The method of §2 also works effectively in the problem of a screened Coulomb potential,[8]

$$V(r)=-r^{-1}f(\mu r), \tag{5.3}$$

where $f(x)\to 1$ as $x\to 0$, and $f(x)\to 0$ as $x\to\infty$. Assuming that the screening function $f(x)$ can be expanded in a Taylor series at the point $x=0$, one can show that $\xi_k(r)$ for $k\geq 2$ is a polynomial of degree $k-1$, and recursion relations can be obtained for the coefficients. The perturbation-theory series in powers of μ makes it possible to calculate the level energy and, in particular, to determine the value of μ at which a bound state arises. These questions will be considered in more detail later.

With regard to the variant of perturbation theory presented in §4, this method requires numerical calculations on a computer, and the calculation of higher orders by means of it is hardly possible. However, this is not required because of the rapid convergence of the successive approximations. The numerical effectiveness of the method follows from the data in Table I and the analogous results of Turbiner and one of the authors.[15;18] We have succeeded in proving the convergence of the method for sufficiently small g for perturbations $gv(r)$ of general form by constructing a majorant for the series (4.2) (this proof is given in Appendix B). The good agreement between the approximations $E^{(k)}(g)$ and the exact eigenvalues $E(g)$ even in the limit $g\to\infty$ suggests that this method may also converge at large values of $|g|$. It would be interesting to apply it to the calculation of the polarizations of atoms and molecules in the ground state.

We note finally that in Refs. 17 and 18 the case of multidimensional potentials that do not possess spherical symmetry was considered. On the transition from the wave function $\psi(\mathbf{r})$ to $\xi(\mathbf{r})=-\nabla\psi/\psi$, which is analogous to the logarithmic derivative (2.1), a system of recursion relations of the same type as (4.4) arises, but these are now differential equations. In contrast to the one-dimensional case, their solution does not reduce to quadrature. The development of effective numerical methods of solution of such equations would make it possible to consider a large class of problems.

We are grateful to V. M. Vaĭnberg and and A.V. Turbiner for discussing the results of the work.

APPENDIX A

As we have already noted in §4, the first two orders of the perturbation theory can be calculated analytically for the anharmonic gr^{2N} oscillator with the initial ansatz (4.1). We give here the necessary formulas. In what follows, we shall use the fact that the coefficient C_∞ in the asymptotic behavior (4.11) is equal to the energy eigenvalue for the Hamiltonian

$$H=p^2+v(r)=-\Delta+r^{2N}.$$

In the first order of perturbation theory, we readily obtain

$$E^{(1)}=E_0+E_1=\langle V_1\rangle$$
$$=(N+D-1)\left(\frac{N+1}{2}\right)^{(N-1)/(N+1)}\Gamma\left(\frac{N+D-1}{N+1}\right)\Big/\Gamma\left(\frac{D}{N+1}\right), \quad (A.1)$$

$$y_1(r)=\frac{N+D-1}{N+1}\left(\frac{N+1}{2}\right)^{(N+D-1)/(N+1)}\frac{1}{\Gamma(D/(N+1))}$$
$$\times\left\{\Gamma\left(\frac{D}{N+1}\right)\Gamma\left(\frac{N+D-1}{N+1},z\right)-\Gamma\left(\frac{N+D-1}{N+1}\right)\Gamma\left(\frac{D}{N+1},z\right)\right\}e^{z}r^{1-D}, \quad (A.2)$$

where $z=2r^{N+1}/(N+1)$, and $\Gamma(\alpha,z)$ is the incomplete gamma function.[24] It can be seen from this that $y_1\sim r$ as $r\to 0$, and $y_1\sim r^{-1}$ as $r\to\infty$ so that $y_1(r)$ is bounded for all $0<r<\infty$.

The second-order correction E_2 is obtained by averaging $y_1^2(r)$ with weight $\chi_0^2(r)$. Using (A.2), we find

$$E_2=-J\left(\frac{N+1}{2}\right)^{2N/(N+1)}\left[\Gamma\left(\frac{D+2N}{N+1}\right)\right]^2\Big/\Gamma\left(\frac{D}{N+1}\right), \quad (A.3)$$

$$J=\int_0^\infty\left\{\frac{\Gamma(\alpha,x)}{\Gamma(\alpha)}-\frac{\Gamma(\beta,x)}{\Gamma(\beta)}\right\}^2e^xx^{\lambda-1}dx=J(\alpha,\alpha,\lambda)+J(\beta,\beta,\lambda)-2J(\alpha,\beta,\lambda), \quad (A.4)$$

$$\alpha=\frac{D}{N+1},\quad \beta=\frac{N+D-1}{N+1},\quad \lambda=\frac{2-D}{N+1},$$
$$J(\alpha,\beta,\lambda)=\frac{1}{\Gamma(\alpha)\Gamma(\beta)}\int_0^\infty\Gamma(\alpha,x)\Gamma(\beta,x)e^xx^{\lambda-1}dx.$$

Replacing here the incomplete gamma functions by the integral representation

$$\Gamma(\alpha,x)=x^\alpha\int_0^1e^{-x/u}u^{-(\alpha+1)}du$$

and calculating the integral over x, we obtain

$$J(\alpha,\beta,\lambda)=\frac{\Gamma(\alpha+\beta+\lambda)}{\Gamma(\alpha)\Gamma(\beta)}\int_0^1du\,dv\frac{u^{\alpha+\lambda-1}v^{\beta+\lambda-1}}{(u+v-uv)^{\alpha+\beta+\lambda}}. \quad (A.5)$$

For the above values of the parameters α, β, and λ the relation $\beta+\lambda=1$ holds, by virtue of which the two integrals in (A.4)can be readily calculated:

$$J(\beta,\beta,\lambda)=-\left[C+\psi\left(\frac{2-D}{N+1}\right)\right]\Big/\Gamma\left(\frac{N+D-1}{N+1}\right), \quad (A.6)$$

$$J(\alpha,\beta,\lambda)=\left[\psi\left(\frac{2}{N+1}\right)-\psi\left(\frac{2-D}{N+1}\right)\right]\Big/\Gamma\left(\frac{N+D-1}{N+1}\right), \quad (A.7)$$

where $\psi(z)$ is the logarithmic derivative of the gamma function, and $C=-\psi(1)$ is Euler's constant. The remaining integral can be reduced by means of formula (7.512.12) in the handbook Ref. 25 to the generalized hypergeometric series:

$$J(\alpha,\alpha,\lambda)=\frac{\Gamma[(D+2)\nu]}{(2-D)[\nu\Gamma(D\nu)]^2}\,{}_3F_2\left[\begin{matrix}1,2\nu,(D+2)\nu;-1\\2\nu+1,(2-D)\nu+1\end{matrix}\right],$$

where $\nu=1/(N+1)$. Further, using Whipple's identity (see Ref. 26, p. 33), which for $a=1$ takes the form

$${}_3F_2\left[\begin{matrix}1,b,c;-1\\k-b,k-c\end{matrix}\right]=\frac{\Gamma(k-b)\Gamma(k-c)}{\Gamma(k)\Gamma(k-b-c)}\,{}_3F_2\left[\begin{matrix}b,c,(k-1)/2;\ 1\\k-1,(k+1)/2\end{matrix}\right],$$

and the formula given on p. 14 in Ref. 26, we transform the hypergeometric function to an argument equal to unity:

$$J(\alpha,\alpha,\lambda)=\frac{D^2\Gamma((D+2)\nu)}{2(2-D)[\Gamma(1+D\nu)]^2}\,{}_3F_2\left[\begin{matrix}1,2\nu,1-D\nu;1\\2\nu+1,(2-D)\nu+1\end{matrix}\right]$$
$$=\frac{\Gamma((2-D)\nu)\Gamma((D+2)\nu)}{\Gamma(1-D\nu)[\Gamma(D\nu)]^2}\sum_{n=0}^\infty\frac{\Gamma(n+1-D\nu)}{(n+2\nu)\Gamma(n+1+(2-D)\nu)}. \quad (A.8)$$

This series converges for all values of N and D (the n-th term of the series decreases as $\sim n^{-(2\nu+1)}$) and is convenient for numerical calculations. Finally, the second order of the perturbation theory for the energy of the ground state is determined by Eqs. (A.3–A.8), and these were the ones used in calculating Table I.

In a number of cases, the above formulas admit a further simplification. For example, for the three-dimensional gr^4 oscillator $D\nu=1$, and the hypergeometric function in (A.8) becomes unity. At the same time

$$\varepsilon_1=(2/3)^{5/3}\Gamma(1/3),\quad \varepsilon_2=-(2/3)^{4/3}\Gamma(1/3)[3-C-2\pi/\sqrt{3}-\psi(2/3)]. \quad (A.9)$$

Note that for $D=2$ the expressions (A.6)–(A.8) contain pole singularities that cancel each other (so that E_2 remains finite).

APPENDIX B

Proof of the convergence of the iteration procedure of §4

We construct a convergent sequence that majorizes the series

$$\sum_k y_k(r,g).$$

We assume that for all $k<l$ the functions y_k are bounded: $|y_k(r)|<C_k$. Then

$$V_l=-\sum_{k=1}^{l-1}y_ky_{l-k}$$

is also bounded:

$$|V_l(r)|<\sum_{k=1}^{l-1}C_kC_{l-k}. \quad (B.1)$$

In accordance with (4.6) and (4.7) we now obtain

$$\max_{0\le r<\infty}|y_l(r)|\le C_l=2\left(\sum_{k=1}^{l-1}C_kC_{l-k}\right)\max I(r),$$

$$I(r)=\int_0^r dx\left(\frac{x}{r}\right)^{D-1}\exp[f(r)-f(x)],\quad r<r_0,$$

$$I(r)=\int_r^\infty dx\left(\frac{x}{r}\right)^{D-1}\exp[f(r)-f(x)],\quad r>r_0,$$

$$f(r)=\int^r dr'V^{1/2}(r'),$$

and r_0 will be fixed below. Denoting

$$\max_{0<r<\infty}I(r)=A/2,$$

we see that the majorizing series

$$S=\sum_{k=1}^{\infty} C_k$$

converges if $AC_1<\frac{1}{4}$. Indeed, since by construction

$$C_l = A\sum_{k=1}^{l-1} C_k C_{l-k},$$

it follows that $S=AS^2+C_1$, whence

$$S=\frac{1}{2A}[1-(1-4AC_1)^{1/2}]. \qquad \text{(B.2)}$$

Since S has a singularity at $4AC_1=1$, it is clear that the series ΣC_k converges if $AC_1<\frac{1}{4}$.

We shall show that thus condition is indeed satisfied as $g\to 0$. For small g, $f(r)\approx r^2$ and the integral $I(r)$ does not depend on g (we set $r_0\approx 1$). Further, we use the circumstance that

$$V_1\sim gr^{2N-2},\quad E^{(1)}=D+g\Gamma(N+D/2)/\Gamma(D/2)+O(g^2).$$

Sunstituting this in (4.7), we find that $y_1(r,g)=O(g)$ and accordingly $C_1=O(g)$ as $g\to 0$. Therefore, we definitely have $AC_1<\frac{1}{4}$.

Although the attempt to make a similar estimate for $g\gg 1$ was not crowned with success, we believe that a detailed study will lead to proof of the convergence of the series (4.2) at large $|g|$ as well. An indication of this is the rapid convergence of the approximations $E^{(k)}(g)$ to the exact energy eigenvalue even in the limit $g\to\infty$ (see Table I).

[1)]That in fact the entire perturbation theory can be constructed using the wave function of only the level to which the corrections are sought was established by Zel'dovich (see Ref. 9 and also the book Ref. 10, p. 143). Concretely, in Ref. 9, using Lagrange's method, Zel'dovich obtained an expression for the corrections of second order to the energy of the level in the form of a multiple integral containing the unperturbed wave function of the given level. One can show that this expression is equivalent to (4.8) for $k=2$. The same formula was obtained by Kirzhnits.[11] Polikanov[12] considered in detail the calculation of the higher orders of perturbation theory on the basis of Riccati's equation. He noted particularly that any order of perturbation theory can in principle be calculated by means of the wave function of the zeroth approximation. However, the scheme he develops for calculating the k-th order of perturbation theory for $k>2$ differs from the one presented below and is more cumbersome. The construction of perturbation theory on the basis of Riccati's equation was also discussed by Pekar.[13] We are grateful to V. A. Kolkunov and A. V. Turbiner for acquainting us with these studies.

[2)]Suppose, for example, $V(r)=r^2+gv(r)$, where $v(r)$ is regular at all finite r and increases faster than r^2 as $r\to\infty$. Then the coefficients ε_k increase factorially as $k\to\infty$, and the perturbation series has zero radius of convergence.

[3)]For the generalization of the method to excited states, see Refs. 14 and 16.

[4)]See the equations for ξ_k given in §2 of the previous paper Ref. 7 (in which it is necessary to set $v(r)=r^{2N}$). Note that the anharmonicity $v(r)$ occurs only in the equation for the first correction ξ_1. The equations for ξ_k when $k\geq 2$ have standard form and do not contain the anharmonicity $v(r)$ (see Eq. (2.6) in Ref. 7). This leads to important simplifications compared with ordinary perturbation theory.

[5)]For all k, C_k are integers, and C_k is odd if and only if $k=2^n$. The generating function for the Catalan numbers has the form

$$\sum_{k=1}^{\infty} C_k z^k = \frac{1}{2}[1-(1-4z)^{1/2}].$$

[6)]If A_k are the coefficients of Bender and Wu, the $\varepsilon_k=(-\frac{1}{2})^{k-1}A_k$. The difference between our ε_k and their A_k arises because their Hamiltonian in Ref. 4 has a different normalization from our (1.1). In Ref. 4, the coefficients A_k are calculated exactly for $k\leq 9$ and numerically (to 12 decimal figures) up to $k=75$ [see Eqs. (2.12) and Table 1 in Ref. 4].

[7)]The terms of the perturbation-theory series for the logarithmic derivative $\xi(r,g)$ are denoted here by y_k (and not ξ_k), since $\xi_k(r)$ has already been used earlier (§2) in the construction of the perturbation theory in powers of g. As can be seen from Eqs. (4.1) and (4.7), the dependence of $y_k(r,g)$ on g does not have a simple power form [in §2, the k-th order of perturbation theory had the form $g^k\xi_k(r)$].

[8)]This problem was also considered by Polikanov,[12] who calculated seven orders of perturbation theory in powers of the screening parameter μ.

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Perturbation theory and variation principle in quantum mechanics

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A nonstandard perturbation theory (PT) is developed in many-dimensional quantum mechanics; in this theory knowledge of the entire spectrum of the unperturbed problem is not required, and only the characteristics of the level for which corrections are to be determined must be known. In the one-dimensional case this theory reduces to the PT proposed by Zel'dovich. It is shown that the problem of constructing the PT in the k-dimensional case is equivalent to that of k-dimensional electrostatics with a variable dielectric constant. The relation between the variational principle and PT is found, and it is shown that the PT developed here makes it possible to estimate the accuracy of variational calculations and to improve this accuracy by using an iteration method. A recipe is formulated for constructing an unperturbed problem so as to get converging PT series. A theorem on the uniqueness of PT series is proved. Examples considered are the ground states in the potentials x^{2n} $(n = 2, 3, 4)$ and $m^2x^2 + gx^4$; it is shown that the first two or three approximations are enough to calculate the energy to an accuracy of 10^{-3}–10^{-5} (for arbitrary g). For the two-dimensional anharmonic oscillator calculations are made of the first several coefficients of the PT series in powers of the coupling constant.

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1. INTRODUCTION

One of the problems most frequently encountered in quantum mechanics is that of finding the energies of bound states. It is analyzed in detail in practically all books on quantum mechanics (cf., e.g., Ref. 1). Its importance is due to the fact that many phenomena in various fields of physics can be described by means of potentials, so that frequently an investigation reduces to the solution of the Schrödinger equation with some particular potential. The main difficulty in almost all cases is that the Schrödinger equation with a potential that describes an actual physical phenomenon is almost always incapable of exact integration. This makes necessary the use of various approximate methods. Here it must be stressed that the present possibilities for numerical integration of the Schrödinger equation are rather limited: It can be used successfully only for one-dimensional problems, and is practically helpless even in two-dimensional quantum-mechanical problems (see the discussion in Ref. 2). For this reason, in dealing with many-dimensional problems or studying the analytic properties of solutions of the Schrödinger equation one has to use approximate methods.

The most frequently used approximate methods are the Rayleigh-Schrödinger perturbation theory and the Rayleigh-Ritz variation principle. Let us examine each of them in more detail. To construct the Rayleigh-Schrödinger perturbation theory (PT) it is necessary to know the entire spectrum of the unperturbed problem or, equivalently, its Green's function, since the corrections to the wave function and the energy are expressed as sums over intermediate states or integrals containing the Green's function. This means that the unperturbed problem must be exactly soluble. Up to now the number of exactly solved problems is rather limited. A typical situation is that of a perturbation potential that is more singular than that of the unperturbed problem, or, in other words, is large compared with it. This is the main cause of the divergence of PT series in physically interesting cases. Consequences are the difficulties with coupling constants of the order of unity and with strong-coupling cases (see the discussion in an earlier paper[3]). Besides this, the use of the Schrödinger-Rayleigh PT gives rise to technical difficulties with calculating matrix elements and finding multiple sums over intermediate states. These difficulties are especially marked in attempts to deal with many-dimensional problems.

The Rayleigh-Ritz variation method and other variational methods of the Hartree-Fock type are practically the only tool for investigating the spectra of many-dimensional problems. However, when this tool is used it is a very complicated problem to estimate the accuracy of the results (see, e.g., Ref. 4). There are other difficulties with variational calculations; in particular it is rather complicated to construct a one-parameter family of test functions. All of these difficulties of the two approaches, those of principle and

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