Logarithmic perturbation theory and its application to the Stark effect in the hydrogen atom

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The method considered by Dolgov and the authors [Phys. Lett **79B**, 403 (1978), **86B**, 185, (1979); Sov. Phys. JETP **48**, 1012 (1979); Phys. Lett. **94B**, 65 (1980), **73A**, 103 (1979), **78A**, 43 (1980); Sov. Phys. Dokl. **25**, 851 (1980)] for the calculation of higher orders of perturbation theory (PT) in quantum mechanics is generalized to include excited states whose wave functions have nodes. The calculation of the coefficients E_k of the PT series for a level energy is reduced to recurrence relations that are convenient for numerical calculation. By way of example, the Stark effect in the hydrogen atom is considered for levels with $n = 1$ and 2, as well as for states with $n_1 = n_2 = 0$. The asymptotic form of E_k as $k \to \infty$ is obtained and is determined by the level width in weak fields. The use of the methods for summation of diverging PT series makes it possible to determine the Stark shift and level width in a strong electric field. The asymptotic value of the energy $E(\mathscr{E})$ in extremely strong fields is obtained for an exactly solvable model (Stark effect for a one-dimensional δ-potential).

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Considerable progress was made in the last few years in calculations of higher perturbation-theory (PT) orders in quantum field theory (see, e.g., Refs. 1–3) and in quantum mechanics.[4–13] In particular, a "logarithmic PT" was developed[6–13] for discrete-spectrum states. This theory uses a transition from the Schrödinger equation to the Riccati equation for the logarithmic derivative of the wave function (this artifice was used in a somewhat different form earlier by Polikanov[14] to construct a PT). For perturbations of the type

$$V_1(x) = \sum_{-2 \leqslant k \leqslant N} c_k x^k$$

(in particular, for polynomial potentials), the calculation of the coefficients of the PT series reduces in this case to recurrence relations,[6–9] which are convenient for computer calculations. Thus, the ground state was considered for an oscillator[6,7] with anharmonicity gr^{2N} and for the Stark effect in the hydrogen atom.[8–10] We continue the study of these questions and generalize the method of the earlier papers[6–9] to include the case of excited states whose wave functions have nodes.

The presence of a node in a wave function raises a definite difficulty in this method,[2)] since a node of $\psi(x)$ corresponds to a pole of the function $y(x) = -\psi'/\psi$ and generates a singularity in the Riccati equation. The main idea of the proposed approach will be described below with the Stark effect in a hydrogen atom as the example. The application of this method to other problems of quantum mechanics will be made clear subsequently.

1. It is known that the variables in the Schrödinger equation with Hamiltonian

$$H = -{}^1/_2\Delta - r^{-1} + \mathscr{E}z$$

separate if the parabolic coordinates $\xi = r + z$ and $\eta = r - z$ are used,

$$\psi(\mathbf{r}) = f_1(\xi) f_2(\eta) e^{im\varphi},$$

and this leads to standard equations (see, e.g., Ref. 15, p. 322 of Russian original)

$$\frac{d}{d\xi}\left(\xi \frac{df_1}{d\xi}\right) + \left[\frac{1}{2}E\xi - \frac{1}{4}\mathscr{E}\xi^2 - \frac{m^2}{4\xi} + \beta^{(1)}\right] f_1 = 0,$$
$$\frac{d}{d\eta}\left(\eta \frac{df_2}{d\eta}\right) + \left[\frac{1}{2}E\eta + \frac{1}{4}\mathscr{E}\eta^2 - \frac{m^2}{4\eta} + \beta^{(2)}\right] f_2 = 0, \quad \beta^{(1)} + \beta^{(2)} = 1. \tag{1.1}$$

Here $\hbar = e = m = 1$, E is the energy, $\mathscr{E}$ is the field intensity (in atomic units $\mathscr{E}_{at} = m^2e^5/\hbar^4 = 5.142 \cdot 10^9$ V/cm), $\beta^{(i)}$ are the separation constants, n_1, n_2, and m are the parabolic quantum numbers, and $n = n_1 + n_2 + |m| + 1$ is the principal quantum number of the level. The PT series for the level energy is of the form

$$E^{(n_1 n_2 m)}(\mathscr{E}) = -\frac{1}{2n^2} + \sum_{k=1}^{\infty} E_k^{(n_1 n_2 m)} \mathscr{E}^k. \tag{1.2}$$

We are interested in the coefficients E_k for high orders k and in the summation of the asymptotic series (1.2).

The calculation of the coefficients E_k is considered in Sec. 2 for the states $(0, 0, n-1)$ and in Sec. 3 for all states with $n = 2$. A system of recurrence relations was obtained for the determination of E_k [see Eq. (2.7) and Appendix A], and made it possible to reach $k = 160$ in the case of the ground state and $k = 100$ for excited levels. The calculation of such high PT orders makes it possible to study the approach of E_k to the asymptotic value $\tilde{E}_k$ as $k \to \infty$, connected with the probability of ionizing an atomic level in electric field $\mathscr{E}$ (Sec. 4). We determine the power-law corrections to E_k, i.e., the coefficients c_j in the expansion (4.4). It is shown in Sec. 5 how to use this information to calculate the widths and the Stark shifts of the levels in strong fields. The behavior of the energy $E(\mathscr{E})$ in extremely strong fields $\mathscr{E} \gg \mathscr{E}_{at}$ is considered in Sec. 6 with the one-dimensional model as the example.

The literature on the Stark effect in the hydrogen atom is immense. We have confined ourselves to a minimum number of references,[16–28] mainly to recent papers. A more complete bibliography can be found in Refs. 10 and 18.

2. Logarithmic PT for states without nodes[3)]. The wave functions of the states with $n_1 = n_2 = 0$ and $|m| = n - 1$

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have no nodes. In this case the Riccati-equation method is simplest. At $n_1=n_2$ the following symmetry relations hold

$$E(\mathscr{E})=E(-\mathscr{E}),\quad f_1(\xi,\mathscr{E})=f_2(\xi,-\mathscr{E}),\quad \beta^{(1)}(\mathscr{E})=\beta^{(2)}(-\mathscr{E}), \tag{2.1}$$

and it suffices therefore to consider only one of the equations in (1.1). The substitution

$$f_1(\xi,\mathscr{E})=\rho^{|m|/2}\exp\left\{-\frac{1}{2}\int_0^\rho x(\rho',F)\,d\rho'\right\},$$
$$\rho=\xi/n,\quad F=n^3\mathscr{E},\quad E=-\varepsilon/2n^2 \tag{2.2}$$

transforms (1.1) into the Riccati equation

$$\rho\frac{dx}{d\rho}+nx-\frac{1}{2}\rho x^2=2n\beta^{(1)}-\frac{1}{2}\varepsilon\rho-\frac{1}{2}F\rho^2. \tag{2.3}$$

Expanding ε, $\beta^{(1)}$, and $x(\rho,F)$ in the formal PT series:

$$\varepsilon=\sum_{k=0}^{\infty}\varepsilon_kF^k,\quad \beta^{(1)}=\sum_{k=0}^{\infty}\beta_kF^k,\quad x=\sum_{k=0}^{\infty}x_k(\rho)F^k. \tag{2.4}$$

We obtain in the lowest orders

$$\varepsilon_0=1,\quad \beta_0=1/2,\quad x_0(\rho)=1,$$
$$\varepsilon_1=0,\quad \beta_1=(n+1)/4,\quad x_1(\rho)=1/2(\rho+n+1)$$

and at $k\geqslant 2$

$$2\left(\frac{dx_k}{d\rho}+\frac{n}{\rho}x_k\right)-\sum_{j=0}^{k}x_jx_{k-j}-\frac{4n}{\rho}\beta_k+\varepsilon_k=0. \tag{2.5}$$

It follows therefore that $x_k(\rho)$ is a polynomial of degree k:

$$x_k(\rho)=(-1)^{k+1}\sum_{j=0}^{k}a_j^{(k)}\rho^j. \tag{2.6}$$

Substituting (2.6) in (2.5), we arrive at the sought recurrence relations ($0\leqslant j\leqslant k$):

$$a_j^{(k)}=(j+n+1)a_{j+1}^{(k)}+\frac{1}{2}\sum_{l=1}^{k-1}\sum_{p+q=j}a_p^{(l)}a_q^{(k-l)}+\frac{1}{2}(-1)^{k+1}\varepsilon_k\delta_{j0}, \tag{2.7}$$

$$a_0^{(k)}+2(-1)^k\beta_k=0. \tag{2.8}$$

The higher-order coefficients can be obtained in explicit form[10]:

$$a_k^{(k)}=2^{1-2k}C_k,\quad C_k=(2k-2)!/[k!(k-1)!], \tag{2.9}$$

where C_k are the Catalan numbers known from combinatorics. By the same token, a procedure is given for a successive lowering of the index j, starting with $j=k$. If k is odd, by descending to $j=0$ we determine $\beta_k=\frac{1}{2}a_0^k$. In the case of even k we have $a_0^{(k)}=\beta_k=0$, and the last equation of (2.7) determines the correction to the Stark shift of the level:

$$E_k=-n^{3k-2}\left[(n+1)a_1^{(k)}+\frac{1}{2}\sum_{j=1}^{k-1}a_0^{(j)}a_0^{(k-j)}\right]. \tag{2.10}$$

This completes the calculations in the k-th order of PT. We note the following.

1) For states with $n_1=n_2$ there is no linear Stark effect. By virtue of (2.1), the PT series for the energy contains only even powers of the field . This agrees with the result $\varepsilon_{2k+1}=\beta_{2k}=0$ obtained above from the recurrence relations.

2) It can be shown that

$$a_j^{(k)}=2^{1-2k}A_j^{(k)},$$

where $A_j^{(k)}$ are positive integers for all j and k. This makes it possible to determine with a computer the coefficients E_k exactly, i.e., in the form of rational fractions. The hydrogen-atom hyperpolarizabilities obtained in this manner for levels with $n=1$ and 2 for states of the type $(0,0,n-1)$ are given in our preceding paper.[9]

3) For the ground state, we have previously[8] calculated 160 PT orders:

$$E^{(000)}(\mathscr{E})=-\frac{1}{2}-\frac{9}{4}\mathscr{E}^2-\frac{3555}{64}\mathscr{E}^4-\frac{2\,512\,779}{512}\mathscr{E}^6$$
$$-\frac{13\,012\,777\,803}{16\,384}\mathscr{E}^8-\frac{25\,497\,693\,122\,265}{131\,072}\mathscr{E}^{10}-\ldots \tag{2.11}$$

and, e.g., $E_{100}=-6.823\,749\cdot 10^{175}$ and $E_{150}=-2.717\,978\cdot 10^{289}$. The coefficients E_k were calculated in exact form, and for $k>15$, approximately (to 22 decimal places). The computer time $\tau\sim k^4$ and, e.g., amounted to 40 minutes for $k=100$ (with the BÉSM-6 computer).

4) Starting with (2.7), the first few orders were calculated analytically (for arbitrary n):

$$E^{(0,0,n-1)}(\mathscr{E})=-\left\{\frac{1}{2n^2}+\frac{n+1}{8}\left[n^4(4n+5)\mathscr{E}^2\right.\right.$$
$$+\frac{n^{10}}{16}(192n^3+933n^2+1550n+880)\mathscr{E}^4$$
$$+\frac{n^{16}}{128}(11\,776n^5+109\,013n^4+415\,522n^3+814\,928n^2$$
$$\left.\left.+821\,540n+340\,000)\mathscr{E}^6+\ldots\right]\right\}. \tag{2.12}$$

For comparison with results by others, we note that E_2 and E_4 for the ground state of the hydrogen atom were known long ago, but the correct value of the next coefficient E_6 was obtained (exactly, i.e., in the form of a rational fraction) only most recently.[8,19] The values of E_6 and E_8 given in Ref. 16 are in error. Numerical values of E_k with $k\leqslant 10$ were obtained earlier by Mendelsohn,[17] who used a rather cumbersome calculation method. For a state with arbitrary quantum numbers (n_1,n_2,m), a correct expression for E_4 was first obtained by Alliluev and Malkin (see Ref. 18, where earlier references can be found), and seven PT orders are given in a paper by Silverstone.[19] It is very difficult to proceed to higher values of k, since the coefficients $E_k^{(n_1n_2m)}$ become extremely cumbersome.

It is clear from the foregoing that the method developed here for the construction of the PT offers in certain cases significant advantages over other methods. We proceed now to generalize it to the case of excited states.

3. States with nodes. We consider the first excited level (100), for which the function $f_1(\xi,\mathscr{E})$ has one node.[4)] We seek the solution of the perturbed problem in the form

$$f_1=[\xi-\xi_0(\mathscr{E})]\exp\left\{-\frac{1}{2}\int_0^\xi x(\xi')\,d\xi'\right\},$$
$$f_2=\exp\left\{-\frac{1}{2}\int_0^\eta y(\eta')\,d\eta'\right\}, \tag{3.1}$$

where account was taken of the possibility of a shift of the node with change in the field $\mathscr{E}$. Substituting (3.1) in (1.1), we obtain a system of Riccati equations

$$(\xi-\xi_0)\left[-\frac{1}{2}\frac{d}{d\xi}(\xi x)+\frac{1}{4}\xi x^2+\frac{1}{2}E\xi-\frac{1}{4}\mathscr{E}\xi^2+\beta^{(1)}\right]-\xi x+1=0,$$
$$-\frac{1}{2}\frac{d}{d\eta}(\eta y)+\frac{1}{4}\eta y^2+\frac{1}{2}E\eta+\frac{1}{4}\mathscr{E}\eta^2+\beta^{(2)}=0. \tag{3.2}$$

Expanding all the quantities in powers of $\mathscr{E}$, we arrive at a system of recurrence relations similar to (2.7), albeit much more cumbersome (see Appendix A). The results of the calculations for the levels (010) and (100) were given earlier.[9,10] The following relations hold

$$E_k^{(n_1n_2m)}=(-1)^kE_k^{(n_2n_1m)}, \tag{3.3}$$

and follow from the symmetry of the initial equations with respect to the substitutions

$$\mathscr{E}\to-\mathscr{E},\quad f_1\to f_2,\quad f_2\to f_1,\quad \beta^{(1)}\to\beta^{(2)},\quad \beta^{(2)}\to\beta^{(1)}. \tag{3.4}$$

We note that for all the Stark sublevels with $n=2$, the coefficients $E_k^{(n_1n_2m)}$ are integers (at $k\geq 1$). For the states (010) and (001) all the E_k are negative, i.e., these level are shifted downward. At the same time, for the state (100) the PT series is of alternating sign: $E_k>0$ for odd k and $E_k<0$ for even k.

We can proceed in similar fashion when considering the Stark effect for an arbitrary level (n_1, n_2, m), as well as in other quantum-mechanical problems with polynomial Hamiltonians. It is necessary to separate explicitly the factors corresponding to the nodes of the wave function:

$$f_1(\xi,\mathscr{E})=P_{n_1}(\xi)\exp\left\{-\frac{1}{2}\int_0^\xi x(\xi')d\xi'\right\},$$
$$P_{n_1}(\xi)=\prod_{j=1}^{n_1}(\xi-\xi_j)\equiv\xi^{n_1}+a_1\xi^{n_1-1}+\ldots+a_{n_1}. \tag{3.5}$$

We expand[5)] each of the nodes ξ_j in powers of the external field $\mathscr{E}$. Substitution of the corresponding expansions in (1.1) leads to a system of recurrence relations for the coefficients of the polynomials $x_k(\xi)$ and $P_{n_1}(\xi)$. Although the system becomes more complicated with increasing n_1, this is not very important from the point of view of computer calculation.

Another approach to the construction of a PT for states with nodes was proposed by Aharonov and Au[11] and by Turbiner.[12] The PT coefficients for the zeros of the wave function are expressed in this case in the form of successive quadratures. Although this approach is quite general, it entails more cumbersome numerical calculations. In those cases when the calculation of the higher PT orders can be reduced to recurrence relations, our method makes it possible to proceed to much higher orders k.

4. We consider now the asymptotic forms of the higher order of the PT and its connection with the quasiclassical approach.

As already noted, for states with $n_1=n_2$ there are left in the expansion (1.2) only even powers of $\mathscr{E}$, i.e., $E=E(\mathscr{E}^2)$. In the absence of an external field we have for such states $\beta^{(1)}=\beta^{(2)}$, and $f_1(\xi)=f_2(\xi)$. It is convenient to start with the case of a pure imaginary field. $\mathscr{E}=i|\mathscr{E}|$. In this case Eqs. (1.1) are satisfied if we put $\beta^{(2)}=\beta^{(1)}*$, $f_2(\xi)=f_1(\xi)*$ and $E=E*$; the natural variable is $z=-\mathscr{E}^2>0$. The PT series in powers of z is of alternating sign and can be summed by the Borel method to an exact solution.[20]

In the case of an arbitrarily weak external field ($z<0$) the level becomes quasistationary and the energy E acquires an imaginary part. The asymptotics of the coefficients E_k as $k\to\infty$ are determined by the behavior of the discontinuity of E on the cut $z<0$:

$$\Delta E=\frac{1}{2i}[E(z+i0)-E(z-i0)]=\frac{1}{2}\gamma(\mathscr{E}),$$

where $z=-\mathscr{E}^2$. As $\mathscr{E}\to 0$ the potential has a broad barrier and the quasiclassical approximation can be used. We write down the width γ for the level (n_1, n_2, m) in the form

$$\gamma_{n_1n_2m}=\gamma^{cl}_{n_1n_2m}(\mathscr{E})\,\Phi_{n_1n_2m}(\mathscr{E}), \tag{4.1}$$
$$\Phi_{n_1n_2m}(\mathscr{E})=1+h_1\mathscr{E}+h_2\mathscr{E}^2+h_3\mathscr{E}^3+\ldots,\quad \mathscr{E}\to 0, \tag{4.2}$$

where $\gamma^{cl}(\mathscr{E})$ corresponds to the quasiclassical approach,[21] and the function $\Phi(\mathscr{E})$ yields the correction to it. In the case $n_1=n_2=(n-|m|-1)/2$ we have

$$\gamma^{cl}_{n_1n_2m}=A(-z)^{-n/2}\exp[-1/a(-z)^{1/2}],\quad a=\frac{3n^2}{2},$$
$$A=\frac{2^{2n}}{n^{3(n+1)}}\left[\left(\frac{n+m-1}{2}\right)!\left(\frac{n-m-1}{2}\right)!\right]^{-1}. \tag{4.3}$$

From this we obtain the sought asymptotic form[6)]:

$$E_k=\frac{1+(-1)^k}{2}\bar{E}_k\left(1+\frac{c_1}{k}+\frac{c_2}{k^2}+\ldots\right),\quad \bar{E}_k=c_0k!\,a^kk^\beta, \tag{4.4}$$

$$\beta=n-1,\qquad c_0=-6^n\Big/\pi n^3\left(\frac{n+m-1}{2}\right)!\left(\frac{n-m-1}{2}\right)!. \tag{4.5}$$

In the general case ($n_1\neq n_2$) the expansion (1.2) contains all the powers of the field $\mathscr{E}$. The dispersion relations are sought for the combinations $E^{(n_1n_2m)}(\mathscr{E})+E^{(n_1n_2m)}(\mathscr{E})$ and $\mathscr{E}^{-1}[E^{(n_1n_2m)}(\mathscr{E})-E^{(n_2n_1m)}(\mathscr{E})]$; this yields[23]

$$E_k^{(n_1n_2m)}=-\frac{1}{2\pi}\int_0^\infty\frac{d\mathscr{E}}{\mathscr{E}^{k+1}}[\gamma_{n_1n_2m}(\mathscr{E})+(-1)^k\gamma_{n_2n_1m}(\mathscr{E})]. \tag{4.6}$$

A quasiclassical formula for $\gamma(\mathscr{E})$ at arbitrary n_1, n_2, and m was obtained by Slavyanov.[24] The widths of the levels (n_1n_2m) and (n_2n_1m) differ because the pre-exponential factor

$$\gamma_{n_2n_1m}/\gamma_{n_1n_2m}\sim\mathscr{E}^{2(n_2-n_1)}$$

as $\mathscr{E}\to 0$. In the case $n<n_2$ the level width $\gamma_{n_1n_2m}$ greatly exceeds $\gamma_{n_1n_2m}$ and it is seen from (4.6) that the $E_k^{(n_1n_2m)}$ are negative. At $n_1=n_2$ the coefficient $E_{2k}<0$ and $E_{2k+1}=0$. Finally, in the case $n_1>n_2$ the term $(-1)^k\gamma_{n_1n_2m}$ in (4.6) predominates and the PT series is of alternating sign. Substituting γ^{cl} in the dispersion integral (4.6) and calculating its value as $k\to\infty$, we can obtain the asymptotic $\bar{E}_k^{(n_1n_2m)}$ for an arbitrary level. The corresponding equations are rather cumbersome and are given in our earlier paper.[10] In the case $n_1=n_2$ they go over into (4.4).

We consider now the manner in which the exact coefficients of the PT series approach the asymptotic form (4.4). Figure 1 shows the ratio $E_k/\bar{E}_k$ for all levels with $n=1, 2$, as well as for the first five states of the type $(0, 0, n-1)$. It is seen that the power-law corrections to $\bar{E}_k$ (i.e., the terms c_1/k, c_2/k^2) are large, and their role increases with increasing principal quantum num-

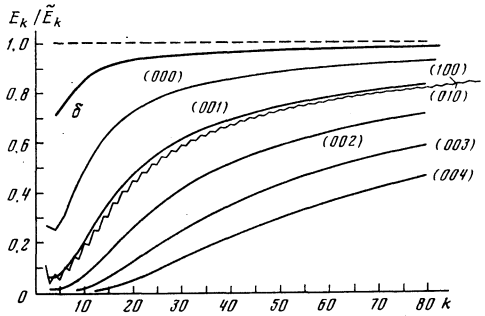

FIG. 1. Approach of the coefficients E_k of the PT series to the asymptotic value $\tilde{E}_k$. The numbers in the parentheses denote the parabolic quantum numbers (n_1, n_2, m). The curve δ pertains to the case of the on-dimensional δ-potential (see Sec. 6).

ber n. For states with $n_1=n_2$ the PT coefficients E_k approach monotonically the asymptotic value $\tilde{E}_k$, whereas for the levels (100) and (010) the curve has a sawtooth shape. This is due to the presence of a term with a factor $(-1)^2$ in the dispersion integral (4.6). The amplitude of these oscillations is proportional to $k^{-2|n_1-n_2|}$, i.e., it decreases rapidly with increasing $|n_1-n_2|$ and fades away as $k\to\infty$.

To calculate the coefficient c_j in the expansion (4.4) we used a numerical fit of the ratio $E_k/\tilde{E}_k$ in the interval $k=50-150$. This enabled us to obtain the first five coefficients (see Table 3 of Ref. 9, and also Ref. 23). We note that ananlytic calculation of the power-law calculations calls for the determination of the corrections to the quasiclassical approximation for the wave function and the level width γ, and this leads to very cumbersome calculations. It was possible to determine in this manner only two coefficients, c_1 and c_2, for the anharmonic gx^4 oscillator[4] and for the Stark effect.[25]

5. What is the physical information obtained by calculating the higher PT orders and the power-law corrections to E_k? We shall show that this makes it possible to calculate with good accuracy the Stark shift of the level and its width in the region of strong fields comparable with $\mathscr{E}_{at}$.

We note first that the power-law corrections (c_j) are connected in simple fashion with the coefficients h_k of the expansion (4.2):

$$h_k=a^k\sum_{j=0}^{k}q_{k-j}(\beta-j)c_j. \tag{5.1}$$

Here $q_n(x)$ are the polynomials of degree $2n$ introduced in Ref. 22:

$$q_0=1,\quad q_1=-{}^1/_2x(x+1),\quad q_2={}^1/_8x(x-{}^2/_3)(x^2-1),$$

etc. Since the parameters a and β are known, we can calculate h_j from the already known coefficient c_j (Ref. 9). We note that the coefficients c_j and h_j increase rapidly together with j. Thus, for the ground level

$$c_1=-5.944,\quad c_5\approx-1.1\cdot10^3,\quad h_1=-8.917,\quad h_5\approx-1.0\cdot10^4.$$

This indicates that the series (4.3) and (4.4) diverge in all probability and are only asymptotic. On going over to excited states, the coefficients c_j and h_j increase.

To calculate the width γ it is desirable to decrease the coefficients of the Taylor series (4.2); this is done with the aid of the transformation

$$\mathscr{E}\to w=A\mathscr{E}(1+B\mathscr{E})^{-1}.$$

It is natural to choose the parameters A and B such that the power-law series for $\Phi(\mathscr{E})$ in terms of the new variable w have the simplest form:

$$\Phi=1+w+b_3w^3+b_4w^4+\ldots \tag{5.2}$$

(i.e., $b_1=1$ and $b_2=0$). This yields $A=h_1$, $B=-h_2/h_1$, and next $(k\geqslant3)$

$$b_k=\frac{1}{A}\sum_{j=1}^{k}(-1)^{k-j}\frac{(k-1)!}{(k-j)!(j-1)!}B^{1-j}h_j.$$

Calculation by this formula shows that the coefficients b_k, unlike h_k, are indeed numerically small.[9]

We summed the series (5.2) by using the Padé approximants $[N,0](w)$ (the notation is standard, see Ref. 26). The results for the levels with $n=1$ and 2 are shown in Fig. 2. The curves are marked with the values of N; the points correspond to the results of Refs. 25 and 27 (numerical solution of the Schrödinger equation). The indicated summation procedure makes it possible to find the level width $\gamma(\mathscr{E})$ for fields several times larger than the region of applicability of the ordinary PT. The advantage of the change from the polynomials

$$P_N(\mathscr{E})=1+\sum_{j=1}^{N}h_j\mathscr{E}^j$$

to the Padé approximants $[N,0](w)$ for the serise (5.2) are clearly seen from Fig. 3. The difference between $\gamma(\mathscr{E})$ and the quasi-classical asymptotic form (4.3) is quite appreciable, i.e., the procedure for summing the divergent series (4.2) does not reduce here to small corrections.

Similar results are obtained[8-10] when summing the PT series for $\mathrm{Re}E(\mathscr{E})$, i.e., for the Stark shift of the level (a detailed exposition can be found in Ref. 10).

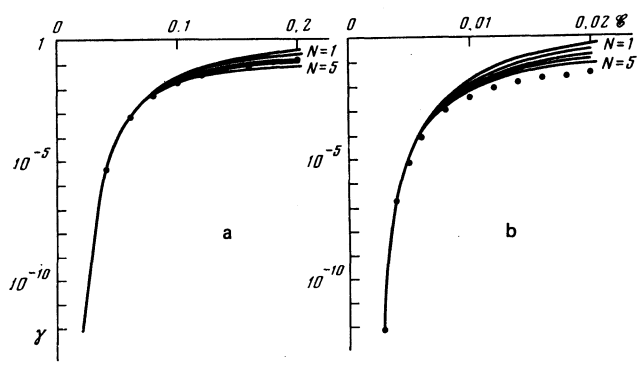

FIG. 2. Width $\gamma(\mathscr{E})$ of the ground level (000) (a) and of the (100) level (b). Points—result of numerical solution of the Schrödinger equation[25,27]; the curves are obtained with the aid of the Pade aproximants $[N,0](w)$. The field $\mathscr{E}$ is measured in atomic units.

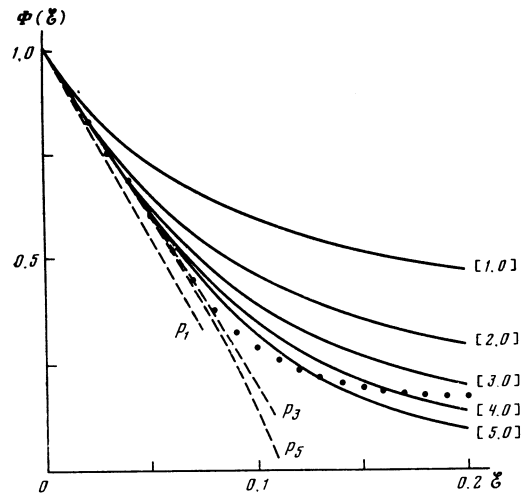

FIG. 3. The function $\Phi(\xi)$ from (4.1) in the case of the ground level of the hydrogen atom. In this case $\gamma^{cl} = 4\mathscr{E}^{-1}\exp(-2/3\mathscr{E})$, see Ref. 15. The points show the values of $\Phi = /\gamma(\mathscr{E})/\gamma^{cl}(\mathscr{E})$, recalculated in accord with the results of Ref. 25 and 27. The solid curves are the Padé approximants $[N, 0]$ (w) for the series (5.2); the dashed curves p_N are the sums of the $N+1$ first terms of the expansion (4.2).

The general conclusion is that allowance for the asymptotic form of the coefficients of the PT as $k \to \infty$, together with a sufficiently large number of exactly calculated coefficients E_k, makes it possible to determine the level energy and the width far beyond the framework of applicability of ordinary PT. This conclusion is of interest for quantum field theory[3] and is corroborated by other examples. We note that the situation with the Stark effect is quite unfavorable from the point of view of summing the PT series: this series is of constant sign for the ground state. In those cases when the PT series are of alternating sign, the use of the methods of summing diverging series is much more effective (see, e.g., Ref. 22).

6. The one-dimensional model. A number of workers have recently considered the asymptotic form of $E(\mathscr{E})$ in the limit as $\mathscr{E} \to \infty$. For the ground state of the hydrogen atom we have according to Ref. 28

$$E_0(\mathscr{E}) = 2^{-5/3}e^{-i\pi/3}(\mathscr{E}\ln\mathscr{E})^{2/3} \times\left[1+\alpha_1\frac{\ln\ln\mathscr{E}}{\mathscr{E}\ln\mathscr{E}}+\ldots\right], \qquad (6.1)$$

where $\alpha_1 = 8/3$. What remains unclear here, however, is the question whether this asymptotic form can be matched to the PT expansion in the weak-field region. We consider in this connection a model problem that admits of an exact solution, namely the Stark effect for a one-dimensional δ-potential,[7)]

$$H = p^2/2 - \varkappa\delta(x) - \mathscr{E}x.$$

In the dimensionless variables $u = \varkappa x$, $E = -\varkappa^2\varepsilon/2$, and $\mathscr{E} = \varkappa^3 F$ the problem takes the form

$$\frac{d^2\psi}{du^2} + (2Fu - \varepsilon)\psi = 0, \quad \frac{d\psi}{du}(0+) - \frac{d\psi}{du}(0-) = -2\psi(0). \qquad (6.2)$$

Using the condition for matching at zero and a boundary condition of the "diverging wave" type as $x \to \infty$, we arrive at the transcendental equation

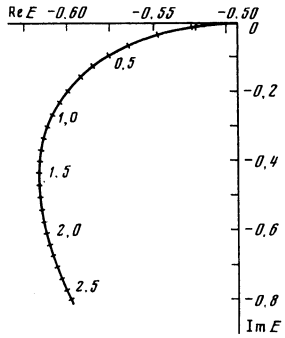

FIG. 4. Trajectory of quasistationary level on the complex E plane at $\varkappa = 1$. The values of the field F are marked on the curve.

$$z^{1/3}K_{1/3}(z)\left[I_{1/3}(z) + I_{-1/3}(z) + \frac{i}{\pi}K_{1/3}(z)\right] = (3F)^{1/3}, \qquad (6.3)$$

which determines the energy of the quasistationary levels as a function of the field F. Here $z = \varepsilon^{3/2}/3F$.

At $F \ll 1$ the level energy is expanded in a PT series:

$$\varepsilon = \sum \varepsilon_{2k}F^{2k}.$$

The coefficients ε_k can be obtained from (6.3), but it is more convenient to reduce the problem to recurrence relations (see Appendix D), the approach of ε_k to the asymptotic value

$$\bar{\varepsilon}_k = \frac{2}{\pi}k!\left(\frac{3}{2}\right)^k k^{-1}$$

is faster than in the three-dimensional problem (the ground level of the hydrogen atom), cf. the corresponding curves in Fig. 1.

Let now $\mathscr{E} \to \infty$. As shown in Appendix B, the solution of Eq. (6.2) takes here the form (6.2), differing only in the value $\alpha_1 = \frac{2}{3}$. This indicates that the behavior of the energy $F(\mathscr{E})$ in the limit $\mathscr{E} \gg \mathscr{E}_{at}$ depends weakly on the concrete form of the bare potential V_0 that produces the bound state.

Numerical solution of Eq. (6.3) yields the curve shown in Fig. 4. In weak fields the Stark shift is negative in accordance with the PT. At $F \sim 1$ the curve becomes gently sloping; $\mathrm{Re}E(F)$ begins next to increase, in qualitative agreement with the asymptotic relation (6.1).

APPENDIX A

We present recurrence relations for the coefficients of the PT in the case of the excited level (100).

Expanding all the quantities that enter in (3.2) in powers of the field

$$x(\xi,\mathscr{E}) = \sum_{k=0}^{\infty} 2^{2k}x_k(\xi)\mathscr{E}^k, \quad y(\xi,\mathscr{E}) = \sum_{k=0}^{\infty} 2^{2k}y_k(\xi)\mathscr{E}^k$$

$$E(\mathscr{E}) = -\sum_{k=0}^{\infty} 2^{2k-3}\varepsilon_k\mathscr{E}^k, \quad \xi_0(\mathscr{E}) = \sum_{k=0}^{\infty} 2^{2k+1}d_k\mathscr{E}^k, \qquad (A.1)$$

$$\beta^{(1)} = 1 - \beta^{(2)} = \frac{3}{4} + \sum_{k=1}^{\infty} 2^{2k}\beta_k\mathscr{E}^k$$

and retaining in (3.2) terms of order $\mathscr{E}^k$, we obtain

$$-\xi^2\frac{dx_k}{d\xi}-3\xi x_k+\frac{1}{2}\xi^2\sum_{l=0}^{k}x_lx_{k-l}+2\beta_k\xi+\frac{1}{8}\xi^2(2d_{k-1}-\varepsilon_k)-\frac{1}{8}\xi^3\delta_{k1}$$
$$+\sum_{m=0}^{k}d_{k-m}\left[2\frac{d}{d\xi}(\xi x_m)-\xi\sum_{l=0}^{m}x_lx_{m-l}+\frac{1}{4}\xi\varepsilon_m-4\beta_m\right]=0, \qquad (A.2)$$

$$-\frac{d}{d\eta}(\eta y_k)+\frac{1}{2}\eta\sum_{l=0}^{k}y_ly_{k-l}-\frac{1}{8}\eta\varepsilon_k-2\beta_k+\frac{1}{8}\eta^2\delta_{k1}=0 \quad (k\geqslant 1).$$

From this we see (by induction with respect to k) that x_k and y_k are polynomials of degree k:

$$x_k(\xi)=\sum_{j=0}^{k}2^{-(j+1)}a_j^{(k)}\xi^j, \quad y_k(\eta)=\sum_{j=0}^{k}2^{-(j+1)}b_j^{(k)}\eta^j. \qquad (A.3)$$

Substituting these expressions in (A.2), we obtain $2k+5$ eauations for $a_j^{(k)}$, $b_j^{(k)}$, β_k, d_k, and ε_k. In analogy with (2.9), the senior coefficients of the polynomials x_k and y_k are expressed in terms of the Catalan numbers:

$$b_k^{(k)}=(-1)^ka_k^{(k)}=-2^{1-k}C_k, \quad k\geqslant 1. \qquad (A.4)$$

This is followed by "successive lowering of the index j":

$$a_j^{(k)}=(j+4)a_{j+1}^{(k)}-\frac{1}{2}\sum_{l=1}^{k-1}\sum_{p+q=j}a_p^{(l)}a_q^{(k-l)}$$
$$-\sum_{l=1}^{k}d_{k-l}\left[(j+3)a_{j+2}^{(l)}-\frac{1}{2}\sum_{m=0}^{l}\sum_{p+q=j+1}a_p^{(m)}a_q^{(l-m)}\right], \qquad (A.5)$$

$$b_j^{(k)}=(j+2)b_{j+1}^{(k)}-\frac{1}{2}\sum_{l=1}^{k-1}\sum_{p+q=j}b_p^{(l)}b_q^{(k-l)}, \quad 1\leqslant j\leqslant k. \qquad (A.6)$$

This enables us, after calculating the coefficients with $j=1$, to obtain the k-th order correction to the level energy.

$$E_k=-2^{2k-3}\varepsilon_k, \qquad (A.7)$$

$$\varepsilon_k=-9a_1^{(k)}-b_1^{(k)}+2d_{k-1}+\frac{1}{4}\sum_{l=1}^{k-1}[3a_0^{(l)}a_0^{(k-l)}-8a_0^{(l)}a_1^{(k-l)}+b_0^{(l)}b_0^{(k-l)}]$$
$$+\frac{1}{4}\sum_{l=1}^{k-1}d_{k-l}\left[\varepsilon_l-4a_1^{(l)}-2a_0^{(l)}-\sum_{m=1}^{l-1}a_0^{(m)}(a_0^{(l-m)}+8a_1^{(l-m)})\right]+6\sum_{l=2}^{k}d_{k-l}a_2^{(l)}. \qquad (A.8)$$

Thus, E_k is expressed in terms of $a_1^{(k)}$, $a_2^{(k)}$, $b_1^{(k)}$, and the coefficients $a_p^{(l)}$, $b_q^{(l)}$, d_l, and ε_l of the preceding orders. After this we determine $a_0^{(k)}$, $b_0^{(k)}$, and the k-th order of PT for the node of the wave function (i.e., d_k):

$$a_0^{(k)}=\frac{1}{2}\varepsilon_k-d_{k-1}+4a_1^{(k)}-\frac{1}{2}\sum_{l=1}^{k-1}a_0^{(l)}a_0^{(k-l)}-\sum_{l=1}^{k}d_{k-l}\left[3a_2^{(l)}-\sum_{m=0}^{l-1}a_0^{(m)}a_1^{(l-m)}\right],$$

$$b_0^{(k)}=-4\beta_k=\frac{1}{2}\varepsilon_k+2b_1^{(k)}-\frac{1}{2}\sum_{l=1}^{k-1}b_0^{(l)}b_0^{(k-l)}, \qquad (A.9)$$

$$d_k=\frac{1}{2}\sum_{l=1}^{k}d_{k-l}(a_0^{(l)}+b_0^{(l)}).$$

In the foregoing equations we must assume that $k\geqslant 2$. For the first two orders, the recurrence relations have a somewhat different form. The reason is that (3.2) contains terms $\sim\mathscr{E}$, and this leads to terms of the type δ_{kl} in (A.2). Inasmuch as in the calculation of k-th PT order one used all the coefficients $a_j^{(l)}$ with $l\leqslant k$, we present their explicit forms for $k=0$ and 1:

$$a_0^{(0)}=b_0^{(0)}=d_0=\varepsilon_0=1, \quad a_1^{(1)}=a_0^{(1)}=-b_1^{(1)}=1,$$
$$b_0^{(1)}=-5, \quad d_1=-2, \quad \varepsilon_1=-6. \qquad (A.10)$$

The algorithm for the calculation of any order of perturbation theory is thus fully described. There is no need for additional calculations for the level (010), in view of (3.3).

APPENDIX B

We present several formulas for the one-dimensional model considered in Sec. 6. Changing over from the wave function ψ to the logarithmic derivative $y=-d\ln\psi/du$, we replace (6.2) by the Riccati equation

$$\frac{dy}{du}-y^2=2Fu-\varepsilon.$$

Putting next

$$y=1+\sum_{k=1}^{\infty}y_k(u)F^k, \quad \varepsilon=1+\sum_{k=1}^{\infty}\varepsilon_{2k}F^{2k}, \qquad (B.1)$$

$$y_k(u)=-\sum_{j=0}^{k}2^{1+j-2k}A_j^{(k)}u^j, \qquad (B.2)$$

we arrive at the recurrence relations

$$A_j^{(k)}=(j+1)A_{j+1}^{(k)}+\sum_{l=1}^{k-1}\sum_{p+q=j}A_p^{(l)}A_q^{(k-l)}, \qquad (B.3)$$

which are similar to (2.7) at $n=0$; here $A_k^{(k)}=C_k$. At even k, the descent from $j=k$ to $j=0$ with the aid of (B.3) yields $A_0^{(k)}$

$$\varepsilon_k=2^{2-2k}\left[A_1^{(k)}+\sum_{l=1}^{k-1}A_0^{(l)}A_0^{(k-l)}\right]. \qquad (B.4)$$

If on the other hand k is odd, then $A_0^{(k)}=A_1^{(k)}$ and $\varepsilon_k=0$. The PT coefficient up to $k=100$ were calculated in this manner.[8)]

We shall show now how to obtain from the exact equation (6.3) the limiting cases of weak and strong fields. The left-hand side of (6.3) has singularities only up to points $z=0$ and ∞. With the aid of power-law expansions of the Bessel functions we can verify that no self-consistent solution is obtained as $z\to 0$. The only remaining possibility is therefore $|z|\to\infty$. Using the asymptotic forms of $K_\nu(z)$ and $I_\nu(z)$, we transform (6.3) into

$$z^{-1/2}(1+ie^{-2z})+O(z^{-1/2})=(3F)^{1/2}, \quad -\pi/2<\arg z<3\pi/2. \qquad (B.5)$$

In the right-hand half-plane ($|\arg z|<\pi/2$) e^{-2z} is exponentially small compared with unity. Iterating (B.5) we obtain

$$z=\frac{1}{3F}\left[1+\frac{15}{8}F^2+\ldots+i\exp\left(-\frac{2}{3}F^{-1}\right)\right], \qquad (B.6)$$

i.e., as $F\to 0$ the curve $z=z(F)$ goes off to infinity, hugging the real axis. For $\varepsilon=(3Fz)^{2/3}$ we obtain from this $\varepsilon_0=1$, and $\varepsilon_1=\frac{5}{4}$; in principle, this method can be used to obtain also the succeeding ε_k, but it is simpler to use Eq. (B.3) for this purpose.

In the left-hand half-plane, on the contrary, $|e^{-2z}|\gg 1$. From (B.5) we obtain the solution

$$z=-\frac{1}{6}\left\{\ln F+\ln\ln F+i\frac{3\pi}{2}+\ldots\right\}, \qquad (B.7)$$

which corresponds to the case of a strong field. From this follows Eq. (6.1) with $\alpha_1=\frac{2}{3}$.

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Note: (12 October 1981). A recent article[29] contains an expression for the fifth-order correction $E^{(n_1 n_2 m)}$ [see Eq. (28) in Ref. 29, which was obtained by the method of hypervirial relations]. This equation, however, is incorrect, since it does not lead to the correct answer[9] $E_5^{(100)} = 14214816$ for the state (100). The correct expression is

$$E_5^{(n_1 n_2 m)} = \frac{3n^{13}q}{1024}\,[10563n^4 - 21q^4 + 725m^4 + 98n^2q^2 + 772n^2m^2 + 220m^2q^2 + 90708n^2 + 780q^2 + 830m^2 + 59293],$$

where $q = n_1 - n_2$ is the electric quantum number. We recall that the four preceding PT orders at arbitrary n_1, n_2, and m were given earlier.[18] It is easy to verify that the foregoing expression agrees both with our calculation[9] for concrete levels, and with Silverstone's result.[19]

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[2)] We have in mind a moving node whose position depends on the parameters of the problem, namely the coupling constant g in the case of an anharmonic oscillator, the electric field $\mathscr{E}$ in the Stark effect, etc. The "kinematic" nodes ψ, located at fixed points, (e.g., at $r = 0$ because of the centrifugal barrier) raise no difficulties[8,9] [see, e.g., the separation of the factor $\xi^{|m|/2}$ in Eq. (2.2)].

[3)] A brief exposition of the results of this section was published earlier.[8]

[4)] Thus, in the absence of an electric field we have $f_1 = (\xi - 2)e^{-\xi/4}$, $f_2 = e^{-\eta/4}$. The number of nodes is an adiabatic invariant and does not change when the field $\mathscr{E}$ is turned on (at least in the region of weak field and at distances $r \ll 1/\mathscr{E}$).

[5)] At $\mathscr{E} = 0$ the polynomial $P_{ni}(\xi)$ reduces to a Laguerre polynomial (Ref. 15, § 37), whose coefficients are simple in form. At the same time the zeros of $\xi_j = \xi_j(\mathscr{E})$ can be determined only numerically even at $\mathscr{E} = 0$. It is therefore more convenient to expand in powers of $\mathscr{E}$ not the nodes ξ_j themselves, but the coefficients a_j of the polynomial $P_{ni}(\xi)$.

[6)] To obtain this formula it suffices ot substitute (4.3) in (4.6) and calculate the dispersion integral as $k \to \infty$, or to use the equations already obtained in Ref. 22.

[7)] We note that a one-dimensional δ-potential is similar in certain respects to the three-dimensional Coulomb problem. For example, in both cases the potential energy is a homogeneous function of the degree -1 and the virial theorem $E = -\overline{T} = \overline{V}/2$ is satisfied.

[8)] See Table II of Ref. 10. Just as for the ground state of the hydrogen atom, the coefficients of the PT series increase factorially. Thus, $E_2 = 5/8$; $E_4 = 55/8$, $E_6 = -10625/32$, and $E_{100} = -1.194\,136 \cdot 10^{173}$. Here $E_k = -\varepsilon_k/2$.

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