The $1/n$ expansion for a hydrogen atom in an external field

V. M. Vaĭnberg, V. S. Popov, and A. V. Sergeev

Institute of Theoretical and Experimental Physics
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We construct a $1/n$ expansion for a hydrogen atom in constant electric and magnetic fields. The summation of the $1/n$ expansion enables us with a large degree of accuracy to find the position and the width of atomic levels in a strong field. The method is generalized to resonances in a repulsive Coulomb center and to two-electron atoms.

1. The study of the Rydberg states of atoms and molecules, including in external fields, is a vital problem in atomic physics and recently has attracted considerable interest (see the review papers 1 and 2 and the references cited there). For instance, Refs. 3–8 were devoted to the calculation of the energy levels of the hydrogen atom in constant electric and magnetic fields. The main method of calculation has up to the present been perturbation theory. Meanwhile, thanks to the development of laser technology and atomic spectroscopy it has become possible to reach a range of strong fields comparable with the field at the atomic orbit of the electron (especially for Rydberg states where $n \gg 1$). In that case it is natural to use a $1/n$ expansion since there is the small parameter $1/n$ in the problem.

In the present paper, which is a continuation of Ref. 9, the semiclassical $1/n$ expansion is applied to the problem of a hydrogen atom in electric ($\vec{\mathscr{E}}$) and magnetic ($\vec{\mathscr{H}}$) fields. We restrict ourselves to the case of parallel fields and, basically, to states with $|m| = n - 1$ (m is the magnetic and n the principal quantum number). Such states minimize in the limit as $n \to \infty$ the $\Delta p_r \Delta r$ and $\Delta p_z \Delta z$ uncertainty relations (i.e., for the radial component and the component transverse to the plane of the orbit of p and r) so that they are the closest to classical mechanics.[9,10] This considerably simplifies the calculations, especially to the lowest orders in $1/n$.

2. Basic equations. We give a very intuitive derivation of the equations of the $1/n$ expansion (compare a similar approach[11] for the Stark effect). We use the fact that in the case of large quantum numbers the Bohr atom model is applicable where the nodeless ($|m| = n - 1$) state corresponds to a circular orbit of the electron perpendicular to the z axis, which is the direction of the $\vec{\mathscr{E}}$ and $\vec{\mathscr{H}}$ fields. It is clear from Fig. 1 that when the external fields are switched on the classical orbit is shifted and changes its radius, remaining circular as before (i.e., it is stable). The parameters of the orbit are determined from the equilibrium condition for the forces in the rest frame of the electron and the quantization condition for the component of the momentum:[1)]

$$\frac{1}{2\pi\hbar}\oint (p_\varphi - A_\varphi)\rho\, d\varphi = m, \qquad \mathbf{p} = \mathbf{v} + {}^1/_2[\vec{\mathscr{H}}\mathbf{r}],$$

where $\rho = (r^2 - z^2)^{1/2}$ and $\mathbf{v}$ is the electron velocity. Carrying out a scale transformation

$$\mathbf{r} = n^2\tilde{\mathbf{r}}, \quad \mathbf{v} = \tilde{\mathbf{v}}/n, \quad F = n^4\mathscr{E}, \; B = n^3\mathscr{H}, \quad \varepsilon = 2n^2E = \varepsilon' - i\varepsilon'', \tag{1}$$

we change to reduced variables ε, F, and so on, which remain finite as $n \to \infty$ ("Rydberg limit"). Here $m/n = \pm(1 + n^{-1}) \to \pm 1$. Using Fig. 1 we see that (for simplicity we drop henceforth the tilde on $\tilde{r}$ and $\tilde{v}$):

$$\rho r^{-3} - Bv = v^2\rho^{-1}, \quad F = -zr^{-3}, \quad \rho(v + {}^1/_2 B\rho) = 1, \tag{2}$$

where $\rho = (r^2 - z^2)^{1/2} = r(1 - F^2r^4)^{1/2}$. Eliminating the velocity v we find the equation which determines the distance $r = r_0(F,B)$ from the nucleus to the equilibrium electron orbit:

$$r(1 - F^2r^4)^2(1 + {}^1/_4 B^2r^3) = 1. \tag{3}$$

In the weak field region

$$\begin{aligned} r_0 &= 1 + 2F^2 - {}^1/_4 B^2 + 19F^4 + {}^1/_4 B^4 - 4F^2B^2 + \ldots, \\ \rho_0 &= 1 + {}^3/_2 F^2 - {}^1/_4 B^2 + {}^{111}/_8 F^4 + {}^1/_4 B^4 - {}^{27}/_8 F^2B^2 + \ldots, \\ \alpha_0 &= F(1 + {}^{25}/_6 F^2 - {}^1/_2 B^2 + \ldots) \end{aligned} \tag{4}$$

(for the notation see Fig. 1). The electric field thus increases the radius of the orbit and shifts it, and the magnetic field compresses the orbit; see also Eq. (A12) in Appendix A. We note that when there is no electric field Eq. (3) changes to the equation obtained in Ref. 12 and in the case $B = 0$ to Eq. (4) of Ref. 11. In both these cases we can evaluate all coefficients of the expansion of r_0 and of the reduced energy ε in powers of F and B (see Appendix A).

The first term in the $1/n$ expansion

$$\varepsilon = \varepsilon^{(0)} + \frac{\varepsilon^{(1)}}{n} + \frac{\varepsilon^{(2)}}{n^2} + \ldots \tag{5}$$

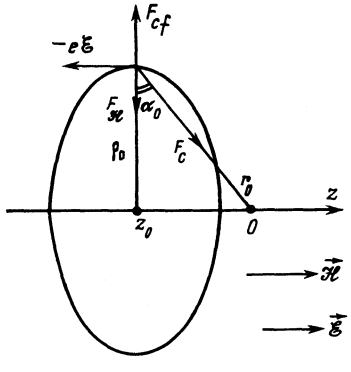

FIG. 1. Classical orbit of an electron corresponding to states with $m = n - 1 \gg 1$ (the nucleus is situated at the origin). We have indicated the forces acting upon the electron in the rest frame: $F_c = e^2/r_0^2$, $F_{cf} = v^2/\rho_0$, $F_{\mathscr{H}} = (e/c)v\mathscr{H}$.

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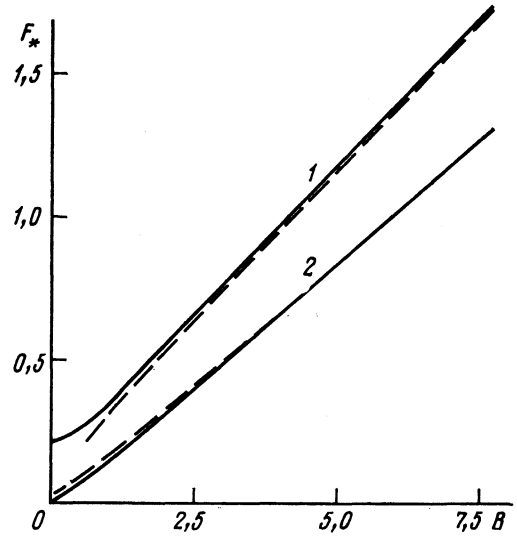

FIG. 2. Classical ionization threshold $F_*(B)$ in the presence of a magnetic field: 1: hydrogen atom, 2: resonance in a repulsive center. The asymptotic behavior as $B\to\infty$ is indicated by the dashed curves; see Eqs. (9′) and (12′).

is equal to the energy of the electron in the equilibrium orbit, the second one ($\varepsilon^{(1)}$) is determined by the small oscillations around it:

$$\varepsilon^{(0)}=2U(\mathbf{r}_0)=\frac{2}{\rho_0^2}+\frac{\rho_0^2}{r_0^3}-\frac{4}{r_0},$$

$$\varepsilon^{(1)}=(2n_1+1)\omega_1+(2n_2+1)\omega_2-\frac{2(n_1+n_2+1)}{\rho_0^2}, \qquad (6)$$

where $n_1+n_2+1=n-|m|=1,2,3,\ldots$; $n_i\geqslant 0$ are the oscillatory quantum numbers and the frequencies ω_i equal:

$$\omega_{1,2}=\{r_0^{-3}+{}^1/_2B^2\pm[9F^2r_0^{-2}+3F^2B^2r_0+{}^1/_4B^4]^{1/2}\}^{1/2} \qquad (7)$$

(for details see Appendix B). Higher orders of the $1/n$ expansion ($\varepsilon^{(k)}$, $k\geqslant 2$) take into account the anharmonicity in the effective potential $U(\mathbf{r})$ and can be calculated using the Rayleigh-Schrödinger perturbation theory recurrence relations for an anharmonic oscillator (compare Refs. 12–14).

As in the Stark effect case, the effective potential $U(\mathbf{r})$ given by Eq. (B3) has a minimum only for a sufficiently weak electric field, when $F<F_*(B)$. When $F=F_*$ the frequency ω_2 vanishes, which corresponds to the intersection of the two classical solutions; the equilibrium orbit considered by us then loses it stability.[2)] Hence we get the equation

$$1+B^2r^3-9F^2r^4-3F^2B^2r^7=0, \qquad (8)$$

which together with (3) determines $F_*(B)$. We note that Eq. (8) also follows from the condition $(\partial\varphi/\partial r)|_{r=r_0}=0$ corresponding to the merging of the two roots of Eq. (3) with their subsequent departure into the complex plane [here $\varphi=\varphi(r;F,B)$ is the polynomial in the left-hand side of Eq. (3)]. Hence

$$F_*(B)=\begin{cases} F_*(0)[1+aB^2+O(B^4)], & B\to 0, \qquad (9)\\ c_1B+c_2B^{1/2}+c_3+O(B^{-1/2}), & B\to\infty, \qquad (9')\end{cases}$$

where $F_*(0)=2^{12}\cdot 3^{-9}=0.2081$, $a=3^{12}\cdot 2^{-19}\approx 1.1014$, $c_1=3^{-3/2}$, $c_2=\frac{2}{27}$, and $c_3=3^{-9/2}\cdot 2^{-1}$ [see (A13) in Appendix A].

Following Ref. 3 we may call F_* the classical ionization threshold. We show in Fig. 2 how F_* depends on B. We note that when $F_*\gtrsim 0.5$ the dependence is close to linear. We have drawn additionally in Fig. 2 the function $F_*(B)$ for a repulsive Coulomb center (curve 2; for details see § 5 below).

Using Eqs. (6) and (A10) we get the expansion of the reduced energy ε for any n:

$$\begin{aligned}\varepsilon_n=\sum_{k=0}^{\infty}\varepsilon^{(k)}n^{-k}=&-1+\frac{1}{4}(1+n^{-1})\Big[-(4+5n^{-1})F^2+B\\&-\frac{1}{16}(192+933n^{-1}+1550n^{-2}+880n^{-3})F^4\\&-\frac{1}{48}(12+27n^{-1}+14n^{-2})B^4\\&+\frac{1}{8}(24+75n^{-1}+60n^{-2})F^2B^2-\frac{1}{128}(11\,776+109\,013n^{-1}\\&+415\,522n^{-2}+814\,928n^{-3}+821\,540n^{-4}+340\,000n^{-5})F^6\\&+\frac{1}{1\,152}(216+1\,089n^{-1}+2\,048n^{-2}+1\,700n^{-3}+528n^{-4})B^6\\&-\frac{1}{384}(1\,440+8\,361n^{-1}+17\,918n^{-2}\\&+16\,380n^{-3}+5\,096n^{-4})F^2B^4\\&+\frac{1}{128}(3\,840+27\,735n^{-1}+77\,220n^{-2}\\&+98\,160n^{-3}+48\,000n^{-4})F^4B^2+\ldots\Big].\end{aligned} \qquad (10)$$

The coefficients of B^4 and B^6 differ from the corresponding coefficients in the expansion (22) in Ref. 16. For $n=1$ we have

$$\begin{aligned}\varepsilon_1=&-1-\frac{9}{2}F^2+\frac{1}{2}B^2-\frac{3\,555}{32}F^4-\frac{53}{96}B^4\\&+\frac{159}{16}F^2B^2-\frac{2\,512\,779}{256}F^6\\&+\frac{5\,581}{2\,304}B^6+\frac{254\,955}{256}F^4B^2-\frac{49\,195}{768}F^2B^4+\ldots,\end{aligned} \qquad (10')$$

which agrees with the expansion of the ground state energy in the case $\vec{\mathscr{E}}\parallel\vec{\mathscr{H}}$ obtained by other means.[3)]

We note that for the nonphysical values $n=m+1=-1,-2,-3,\ldots$ the Schrödinger equation admits the solution:

$$\psi(\mathbf{r})=\Big\{(\xi\eta)^{m/2}\sum_{i,j\geqslant 0}c_{ij}\xi^i\eta^j+(\xi\eta)^{-m/2}\sum_{i,j\geqslant 0}c_{ij}'\xi^i\eta^j\Big\}e^{im\varphi},$$

where $\xi=r+z$, $\eta=r-z$, and φ are parabolic coordinates. One easily finds for the coefficients c_{ij} recurrence relations which in the simplest case $n=-1$ have the following form:

$$\begin{aligned}&(i^2-1)c_{i+1,j}+(j^2-1)c_{i,j+1}+c_{ij}+{}^1/_4\mathscr{E}(c_{i-2,j}-c_{i,j-2})\\&-{}^1/_{16}\mathscr{H}^2(c_{i-2,j-1}+c_{i-1,j-2})+{}^1/_2E(c_{i-1,j}+c_{i,j-1})=0.\end{aligned}$$

TABLE I. Coefficients $\varepsilon^{(k)}$ of the $1/n$ expansion.

k	$F=0{,}1,\ B=1$	$F=0{,}2,\ B=1$	$F=B=1$	$F=1,\ B=0{,}1$
0	−0,7951	−0,81559	−1,16248−0,49863i	−1,286−0,601i
1	0,1461	0,10452	0,06450−0,67977i	0,0211−0,7219i
2	−0,04680	−0,07538	0,00041+0,03463i	0,0585+0,4003i
3	0,01052	−0,01070	0,04153−0,00902i	0,03590−0,00523i
4	−0,003872	−0,03119	−0,04913−0,03432i	−0,03705−0,02935i
5	0,001246	−0,05083	−0,02663+0,09148i	−0,02441+0,05817i
6	−0,001145	−0,12158	0,23497−0,00099i	0,1434+0,0233i
7	0,001337	−0,34250	−0,21248−0,64715i	−0,0475−0,3733i
8	−0,002298	−1,12927	−1,94255+1,36108i	−1,110+0,443i
9	0,003656	−4,24186	7,56330+5,78870i	2,665+3,437i
10	−0,025965	−17,8976	14,7197−40,5717i	10,646−14,320i

Note. The $\varepsilon^{(k)}$ coefficients are complex for $F>F_*(B)$ where $F_*(0.1)=0.2102$ and $F_*(1.0)=0.345$.

They determine the singular part of the wave function

$$\psi_{\text{sing}}=(\xi\eta)^{-1}(1+{}^1/_2\xi)\,(1+{}^1/_2\eta)\,e^{-2i\varphi},$$

where $E=-\frac{1}{2}$ for all $\vec{\mathscr{E}}$ and $\vec{\mathscr{H}}$ (i.e., the shift in the "level" with $n=-1$ vanishes). Hence it follows that in all terms of the expansion (10), except the initial one, we can take a factor $(n+1)$ outside the brackets and this has been done in (10).

Without being able to go into more details we indicate solely that the existence of exact solutions for $n=-1, -2, \ldots$ is closely connected with the finite-dimensional non-unitary representations of the $O(2,1)$ group.

When $F>F_*(B)$ the radius of the classical orbit and the coefficients $\varepsilon^{(k)}$ become complex. Such a solution loses its meaning in classical mechanics, but when we go over to quantum mechanics it reveals in fact the possibility to describe (in the $1/n$ expansion framework) not only the shift but also the width of the levels in a strong field.

3. Results of the calculations. We give in Table I the first 11 coefficients $\varepsilon^{(k)}$ of the $1/n$ expansion (when $F<F_*$ all $\varepsilon^{(k)}$ are real, and when $F>F_*$ they are complex; $F_*(1)=0.345$). A typical behavior of the $\varepsilon^{(k)}$ coefficients is: initially (up to $k=3$–6) they decrease, and after that they increase. When $k\gg 1$ the increase of $|\varepsilon^{(k)}|$ becomes factorial so that for the evaluation of the energy with a high accuracy it is necessary to use the methods for summing divergent series (see Refs. 3, 14, 18, and 19 in that connection).

The results of the summation of the $1/n$ expansion for the reduced energy ε_n are given in Table II. When $F>F_*$ we used Padé approximants (PA) $[L/M]$, and for $F<F_*$ quadratic Padé-Hermite approximants (PHA) $[L,M,N]$. We have indicated only those decimal places which were stabilized for the [4/5] and [5/5] PA or for the [3,3,2] and [3,3,3] PHA. Even in the least favorable case (ground state, expansion parameter $1/n=1$) the accuracy of the determined energy was $\sim 10^{-4}$, and increases rapidly with increasing n. The results of the summation agree for $n=1$ with the results of a numerical integration of the Schrödinger equation.[20]

Some of the results are shown in Figs. 3 and 4 (for nodeless states: $n_1=n_2=0$, $m=n-1$, $n=3$ and 5; see also Ref. 10). The solid lines are the real ($\varepsilon_n'=2n^2\mathrm{Re}E_n$) and the imaginary ($\varepsilon_n''=n^2\Gamma_n$) parts of the reduced energy as functions of the electric field F for a few fixed values of B (the gaps in the ε_n' curves correspond to that range of F values close to F_* where the $1/n$ expansion converges poorly). For comparison the dashed curves show the real and imaginary parts of the classical energy $\varepsilon^{(0)}$. It is clear that $\mathrm{Re}\,\varepsilon^{(0)}$ shows already qualitatively the field-dependence of the energy; as to $\mathrm{Im}\,\varepsilon^{(0)}$, it is a rather rough approximation (see Fig. 3b), i.e., here we cannot avoid the summation of the series (5). On the whole it is clear that the $1/n$ expansion is an altogether efficient calculation method, especially for Rydberg states.

4. We make a few additional remarks.

a. The calculations show that the energy of a level increases with increasing B (see Figs. 3a and 4a). This is explained by the classical-orbit compression that brings the

TABLE II. Reduced energies of states with $m=n-1$ in parallel $\vec{\mathscr{E}}$ and $\vec{\mathscr{H}}$ fields.

n	$B=n^3\mathscr{H}$		
	0,1	0,5	1,0
1	1,246+1,292i	1,210+1,256i	1,084+1,155i
2	1,2717+0,9532i	1,2384+0,9218i	1,1274+0,8315i
3	1,27760+0,83750i	1,24573+0,80792i	1,13994+0,72186i
5	1,28150+0,74380i	1,25079+0,71568i	1,14931+0,63330i
10	1,283974+0,672744i	1,254163+0,645764i	1,155989+0,566273i

Note. We give in the table the values of ε_n for $F=n^4\mathscr{E}=1.0$ and various B.

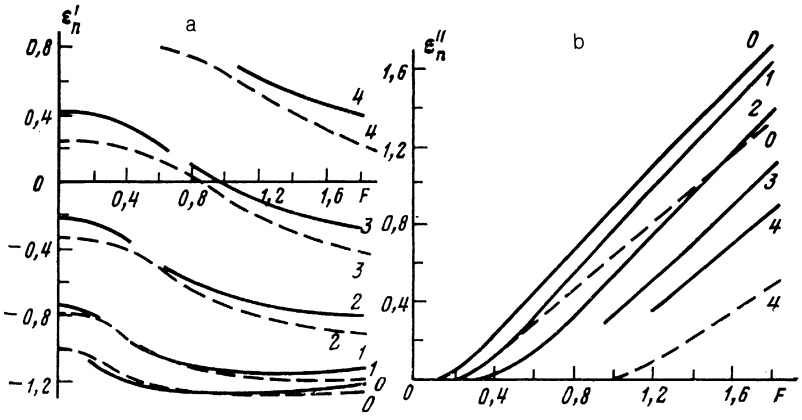

FIG. 3. Real (a) and imaginary (b) parts of the energy $\varepsilon_n = 2n^2E_n - \varepsilon_n' - i\varepsilon_n''$ for states with $m = n - 1$ ($n = 3$). The solid curves are obtained by summing the $1/n$ expansion using the PA method, the dashed curves give the classical approximation $\varepsilon^{(0)}$. The values of B are indicated at the curves.

electron closer to the nucleus. As $B \to \infty$ and for fixed F we have [see Eq. (A11)]

$$r_0(F,B) = \beta\Big[1 - \frac{1}{4}\beta - \frac{1}{32}\beta^2 + \frac{5}{256}\beta^3 + \frac{1}{2}\Big(\frac{7}{1\,024} + F^2\Big)\beta^4 + \ldots\Big], \qquad (11)$$

where $\beta = (B/2)^{-1/2} \to 0$. As to the width Γ_n (i.e., the probability for the decay of the atomic level under the action of the electric field), it is reduced by a magnetic field and increased by an electric field (see Fig. 3). We must note that in the $F > F_*$ region the F dependence of the width Γ_n is nearly linear, as in the case of the Stark effect.[12]

b. The results given in § 3 refer to states with $n = m + 1$ which go over in the limit as $n \to \infty$ into the ground state ($n_1 = n_2 = 0$) of the two-dimensional oscillator. However, the method considered can be generalized also to excited states and this does not meet with any difficulties of principle. The first term $\varepsilon^{(0)}$ in (5) and also the values of ω_1, ω_2, and ρ_0 are then unchanged, the term $\varepsilon^{(1)}$ reduces to (6) and the subsequent coefficients $\varepsilon^{(k)}$, although becoming more complex,[4)] can be evaluated using recurrence relations. Such a generalization is of interest for states with $n_1, n_2 \ll m$. We show the results of the calculations for the state $|2,0,0\rangle$ in Fig. 5.

The convergence of the $1/n$ expansion for states with different quantum numbers is illustrated in Table III.

c. For a hydrogen atom in parallel $\vec{\mathscr{E}}$ and $\vec{\mathscr{H}}$ fields one used earlier perturbation theory[5,6] and semiclassical methods[8] for states with $n \sim 30$ and $|m| = 0,1$ (apart from the reference given above we mention the review in Ref. 2 and the literature cited there). The results of the calculations for states with $m \sim n \gg 1$ are new.

5. In parallel $\vec{\mathscr{E}}$ and $\vec{\mathscr{H}}$ fields electron resonances appear not only in an attractive Coulomb center (proton), but also in a repulsive center (antiproton). Up to now ($\bar{p}e$) resonances have not been observed experimentally and not been studied theoretically. At the same time they may occur when electrons are scattered by antiprotons (or positrons by protons) in regions where $\mathscr{E}$ and $\mathscr{H}$ fields operate, and a theory of such resonances can be obtained by a simple generalization of the corresponding theory for the hydrogen atom.

A magnetic field stabilizes resonances in a repulsive center. In the classical limit, as $n \to \infty$, such states correspond for large $\mathscr{H}$ to an electron orbit with a small radius $\rho_0 = (2m/\mathscr{H})^{1/2}$ located on the cathode side of the antiproton at a distance $z_0 = \mathscr{E}^{-1/2}$

For a repulsive center Eqs. (2), (3), (5)–(8), and (B1)–(B4) of the $1/n$ expansion are valid as before if we replace in them r by $-r$. In Eq. (A13) which defines $F_*(B)$

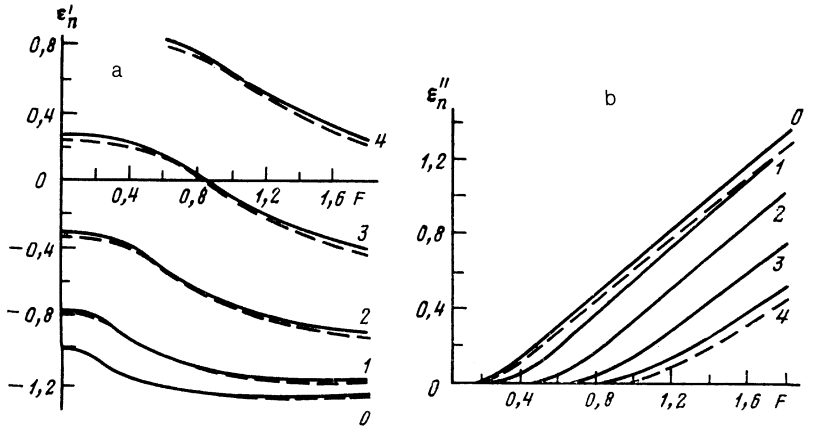

FIG. 4. The same as Fig. 3 for the state with $n = 5$ ($m = 4$).

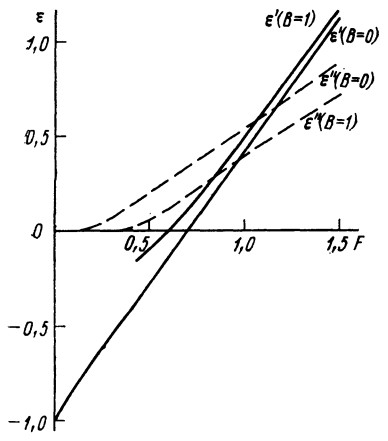

FIG. 5. Effect of a magnetic field on the position and the width of a Stark level (for the state $|2,0,0\rangle$, $n=3$). The curves are obtained by summing the $1/n$ expansion (for $B=0$ they refer to the normal Stark effect in a hydrogen atom).

we must put $1<\tau\leqslant 3$; the corresponding asymptotic formulæ have the form

$$F_r(B)=\begin{cases}(B/2)^{4/3}[1-a'B^{2/9}+O(B^{4/9})], & B\to 0, \quad (12)\\ c_1B-c_2B^{1/2}+c_3+O(B^{-1/2}), & B\to\infty, \quad (12')\end{cases}$$

where $a'=5\cdot 3^{-1/3}\cdot 2^{16/9}\approx 11.9$, while c_1, c_2, and c_3 are the same coefficients as in (9'). If we change to the field strengths $\mathscr{E}$ and $\mathscr{H}$, in a weak field, $n^3\mathscr{H}\ll 1.5\cdot 10^{-5}$, we have $\mathscr{E}_*\approx(\mathscr{H}/2)^{4/3}$, independently of n. For instance, a field $\mathscr{H}=100$ G corresponds for $n\ll 7$ to $\mathscr{E}_*=0.30$ V/cm.

As $\mathscr{H}\to\infty$ the electron motion becomes essentially one-dimensional and the energy equal to $E=\frac{1}{2}n\mathscr{H}+E_z$, where $E_z\approx 2\mathscr{E}^{1/2}$ is the energy in the one-dimensional potential $-1/z+\mathscr{E}z$. The coefficients $\varepsilon^{(k)}$ can be expanded in powers of B^{-1}:

$$\varepsilon^{(0)}=B+4F^{1/2}-2F^{1/2}B^{-1}-{}^3/_2F^{3/2}B^{-2}+O(B^{-3}), \quad (13)$$

$$\varepsilon^{(1)}=\sqrt{2}F^{3/4}-\frac{3\sqrt{2}}{2}F^{1/4}B^{-1}+\left(3F^{5/4}-\frac{63\sqrt{2}}{32}F^{11/4}\right)B^{-2}+O(B^{-3}).$$

As $\mathscr{E}\to 0$ we have $\varepsilon^{(0)}\to B$, and $\varepsilon^{(k)}\to 0\,(k\geqslant 1)$; the electron moves away from the antiproton and goes over into a Landau level with energy $\varepsilon=B$.

The F dependence of the ground state energy is for $B=1$ shown in Fig. 6. The solid curves are the results of the summation of the $1/n$ expansion and the dashed curves the classical energy $\varepsilon^{(0)}$. It turned out that the level width increases very slowly even beyond the classical ionization threshold [when $F>F_*(1)=0.14$].

6. For a single-electron atom the $1/n$ expansion coincides with that in powers of $1/n'$ for the ground state ($n'=(N-1)/2$), but in a space of dimensionality $N\gg 1$ (Ref. 9). For a two-electron atom this is no longer the case, but the $1/n'$ expansion is applicable as before. Putting $n'=1$ we can thus calculate the ground state of real three-dimensional atom.

Carrying out a scale transformation similar to (1), but with the substitution $n\to n'$, we find a Schrödinger equation with an effective potential

$$U_{eff}=-\frac{Z}{r_1}-\frac{Z}{r_2}+\frac{1}{r_{12}}+F(z_1+z_2)+\frac{B^2}{8}(\rho_1^2+\rho_2^2)+U_c, \quad (14)$$

in which $1/n'$ enters (in front of the second derivatives) in the same way as the Planck constant $\hbar$ (see also Ref. 9). In (14) Z is the charge of the nucleus and U_c the centrifugal potential,[5)]

$$U_c=(h_1^{-2}+h_2^{-2})/2,$$

where the h_i are the altitudes of a triangle with sides ρ_1, ρ_2, and ρ_{12} drawn to the sides ρ_i; $\rho_i=(r_i^2-z_i^2)^{1/2}\,(i=1,2)$,

$$\rho_{12}=(r_{12}^2-z_{12}^2)^{1/2}, \quad r_{12}=|\mathbf{r}_1-\mathbf{r}_2|.$$

In the limit as $n'\to\infty$ the energy is given by the minimum of the effective potential:

$${}^1/_2\varepsilon^{(0)}=U_{eff}(\rho_1^{(0)},\rho_2^{(0)},\rho_{12}^{(0)},z_1^{(0)},z_2^{(0)}).$$

In the harmonic-oscillator approximation

$$\varepsilon=\varepsilon^{(0)}+\varepsilon^{(1)}/n', \quad \varepsilon^{(1)}=\sum_{i=1}^{5}\omega_i-6U_c. \quad (15)$$

TABLE III. Convergence of the $1/n$ expansion for various states when $F=B=1$.

	(n_1n_2m)			
	(0, 0, 0)	(0, 0, 1)	(0, 1, 0)	(1, 0, 0)
ε_{osc}	−1,0980− 1,1784i	−1,13023− 0,83852i	−2,147− 1,616i	−0,0489− 0,7405i
[4/4]	−1,0843− 1,1541i	−1,12739− 0,83146i	−2,475− 1,258i	0,0822− 0,5802i
[4/5]	−1,0836− 1,1557i	−1,12736− 0,83148i	−2,486− 1,238i	0,0830− 0,5812i
[5/5]	−1,0843− 1,1545i	−1,12738− 0,83147i	−2,483− 1,233i	0,0828− 0,5817i

Note. For each state we have given in the table the oscillator approximation $\varepsilon_{osc}=\varepsilon^{(0)}+\varepsilon^{(1)}n^{-1}$ and three Padé approximants $[L/M]$. When $F=B=1$ for all states $\varepsilon^{(0)}=-1.16248-0.49863i$.

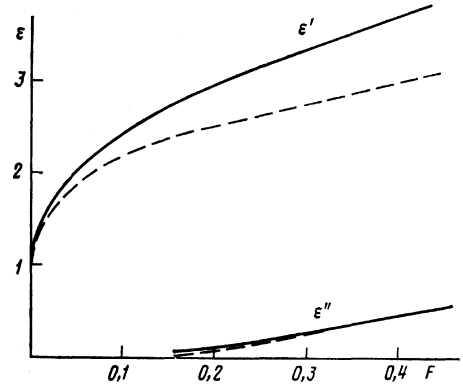

FIG. 6. Quasistationary state in a repulsive center ($Z = -1$) for $B = 1$. Here $\varepsilon = 2E = \varepsilon' - i\varepsilon''$, $F = \mathscr{E}$. The solid curves are the results of summing the $1/n$ expansion, the dashed curves give the classical energy $\varepsilon^{(0)}$.

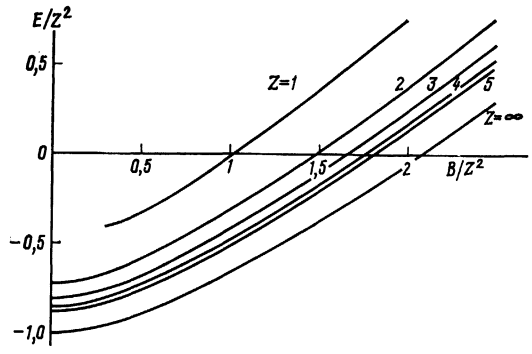

FIG. 7. Ground state energy of two-electron atoms in a magnetic field.

We calculated also the anharmonic correction $\varepsilon^{(2)}/n'^2$, but the formula for this is very cumbersome and we do not give it here.

Because of exchange symmetry, the potential U_{eff} can have symmetric minima ($\rho_1^{(0)} = \rho_2^{(0)}$ and $z_1^{(0)} = z_2^{(0)}$) or twofold asymmetric ones, which are typical of states with weakly bound electrons ($r_2^{(0)} \gg r_1^{(0)}$). The calculations were carried out only for the simplest case of a symmetric minimum.

When $F = 0$ a symmetric minimum exists for $Z \geqslant 1.228$ for any B, and when $Z = 1$ only when $B \geqslant 0.26$ (see Fig. 7). The results of summing three terms of the $1/n'$ expansion (PA [1/1]) for the ground state ($n = 1$) of H^- and He in a magnetic field are given in Table IV. PA [1/1] agree with variational calculations[21] within ± 0.03. An exception is the case $B = 2$ for helium. The bad accuracy for $\mathscr{H} = B = 2$ can be explained by the closeness of the pole in the PA [1/1] at $B = 2.1$. In that case the PA [2/0] $= -2.287$ will be more accurate. Using the PA [1/1] we obtained a value which was 86% of the value of the diamagnetic susceptibility for He and 90% for Li^+.

We show in Fig. 7 the ground-state energy of two-electron atoms in a magnetic field. Using the variables E/Z^2 and B/Z^2 enables us to cover in a single figure all nuclear charge values Z. We note that the curve with $Z = 1$ breaks off at $B = 0.26$ (for smaller values of B we must carry out the calculations for the asymmetric minimum of U_{eff}). This restriction is not present in the case $Z \geqslant 2$ and the curves start at $B = 0$.

When $B = 0$ the symmetric minimum of the potential U_{eff} exists only in sufficiently weak fields $F \leqslant F_c$ ($F_c = 0.795$ for He and 3.720 for Li^+). The sum of three terms of the $1/n'$ expansion gives 94% of the dielectric constant for He and 99% for Li^+.

We give a characteristic example of the summation of the $1/n'$ expansion for helium in parallel fields $\mathscr{E} = 0.5$ and $\mathscr{H} = 1$:

$$\varepsilon^{(0)} = -5{,}3493, \quad \varepsilon^{(1)} = -0{,}5458, \quad \varepsilon^{(2)} = 0{,}3424,$$

whence

$$E = \frac{1}{2}\varepsilon^{[1/1]} = \frac{1}{2}\left[\varepsilon^{(0)} + \frac{(\varepsilon^{(1)})^2}{\varepsilon^{(1)} - \varepsilon^{(2)}}\right] = -2{,}842.$$

7. At the present time the $1/n$ expansion (in its various variants differing in the choice of the expansion parameter $1/n$) is widely applied in quantum mechanics and field theory. However, in most papers only the case of a discrete spectrum is considered. Apparently, Ref. 15 was the first to show that this method is applicable also to calculating energies and widths ($E = \operatorname{Re} E - \frac{1}{2}i\Gamma$) of quasistationary levels if we take classical orbits into consideration which satisfy equations of motion but have complex coordinate values. This made it possible to use the $1/n$ expansion in the theory

TABLE IV. Ground state energy of two-electron atoms in a magnetic field. The first row gives the results of summing the $1/n$ expansion and the second row that of a variational calculation.[21]

$\mathscr{H}$	E(H⁻)	E(He)	$\mathscr{H}$	E(H⁻)	E(He)
0	–	−2,888	2	0,756	−2,447
	−0,528	−2,904		0,765	−2,327
0,2	–	−2,881	3	1,586	−1,820
	−0,479	−2,894		1,598	–
0,5	−0,329	−2,846	5	3,330	−0,598
	−0,329	−2,854		3,360	–
1	−0,009	−2,733	10	7,900	3,046
	−0,002	−2,727			

of the Stark effect in a strong field[3,11] which turned out to be especially useful in the case of Rydberg states.

In the present paper we used the $1/n$ expansion to solve the problem of a hydrogen atom in parallel $\mathscr{E}$ and $\mathscr{H}$ fields. The main results are Eq. (10) and the recurrence relations which enable us to calculate in principle any term of the $1/n$ expansion. The summation of this expansion enabled us to evaluate the position and width of various states in strong fields, which are comparable to atomic fields. We also (§ 6) considered the $1/n$ expansion for a two-electron atom.

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APPENDIX A. PERTURBATION THEORY SERIES AND OTHER EXPANSIONS

1. We denote by $x_0(\lambda)$ that root of the equation

$$x=1-\lambda x^{\alpha}, \tag{A1}$$

which tends to unity as $\lambda \to 0$. Applying Lagrange's theorem (see Ref. 22, p. 149) gives for any index ν

$$x_0^{\nu}=1+\nu\sum_{k=1}^{\infty}c_k\lambda^k, \tag{A2}$$

where

$$c_k=\begin{cases}(-1)^k\Gamma(k\alpha+\nu)/k!\;\Gamma(k(\alpha-1)+1+\nu), & \alpha>0,\\ -\Gamma(k(\alpha'+1)-\nu)/k!\;\Gamma(k\alpha'+1-\nu), & \alpha'=-\alpha\geqslant 0\end{cases}$$

(in particular, $c_1=-1$, $c_2=\alpha+(\nu-1)/2$, and so on). Here $\Gamma(x)$ is the gamma function.

We note that through the substitution $x=t^{-\alpha}$ the equation

$$x(1-\lambda x^b)^a=1 \tag{A3}$$

reduces to the previous one. In that case in (A2)

$$c_k=a^{-1}\Gamma\left(\frac{k(a+b)+\nu}{a}\right)\Big/k!\,\Gamma\left(\frac{kb+a+\nu}{a}\right),\quad a\neq 0, \tag{A4}$$

The expansions obtained converge for sufficiently small λ; for instance, the latter one for

$$|\lambda|<\frac{a}{a+b}\left(1+\frac{a}{b}\right)^{-b/a}. \tag{A5}$$

2. Equation (3) reduces for $F=0$ to (A3) with the parameters $a=1$, $b=3$, and $\lambda=-\frac{1}{4}F^2$, whence

$$r_0(0,B)=\sum_{k=0}^{\infty}(-1)^k\frac{(4k)!}{2^{2k}k!\,(3k+1)!}B^{2k}. \tag{A6}$$

Using also the fact that in this case

$$z_0=0,\quad \rho_0=r_0,\quad \varepsilon^{(0)}=\frac{1}{r_0^2}-\frac{2}{r_0}+\frac{1}{4}B^2r_0^2=\frac{2}{r_0^2}-\frac{3}{r_0},$$

we easily find that

$$\varepsilon^{(0)}(0,B)=-1+\sum_{k=1}^{\infty}(-1)^{k-1}\frac{(4k-3)!}{2^{2k-1}k!\,(3k-1)!}B^{2k} \tag{A7}$$

(these series converge when $|B|<3^{3/2}/8=0.6495$).

An expansion similar to (A7) was given in Ref. 16 [Eq. (24)] but with errors in the coefficients of B^4 and B^6.

3) If $B=0$, we have $a=2$, $b=4$, $\lambda=F^2$, and

$$r_0(F,0)=1+\frac{1}{2}\sum_{k=1}^{\infty}\frac{\Gamma(3k+1/2)}{k!\,\Gamma(2k+3/2)}F^{2k}, \tag{A8}$$

$$\varepsilon^{(0)}(F,0)=-1-6\sum_{k=1}^{\infty}\frac{(9k-4)!}{k!\,(8k-2)!}F^{2k} \tag{A9}$$

(the convergence range is: $|F|<0.2081$, see Refs. 3 and 11). We note that in a magnetic field the perturbation theory series are alternating whereas in the case of an electric field the coefficients of the expansion retain their sign. This is directly connected with the position of the closest singularity in B^2 (or F^2).

4) We give the first terms of the perturbation theory series for the coefficients of the $1/n$ expansion (5):

$$\begin{aligned}\varepsilon^{(0)}&=-1-F^2+\frac{1}{4}B^2-3F^4-\frac{1}{16}B^4+\frac{3}{4}F^2B^2+\dots,\\ \varepsilon^{(1)}&=-\frac{9}{4}F^2+\frac{1}{4}B^2-\frac{1\,125}{64}F^4-\frac{13}{64}B^4+\frac{99}{32}F^2B^2+\dots,\\ \varepsilon^{(2)}&=-\frac{5}{4}F^2-\frac{2\,483}{64}F^4-\frac{41}{192}B^4+\frac{135}{32}F^2B^2+\dots,\\ \varepsilon^{(3)}&=-\frac{1\,215}{32}F^4-\frac{7}{96}B^4+\frac{15}{8}F^2B^2+\dots,\\ \varepsilon^{(4)}&=-\frac{55}{4}F^4+\dots\end{aligned} \tag{A10}$$

(the next coefficients $\varepsilon^{(k)}$ no longer contain terms F^iB^j with $i+j\geqslant 4$). Hence the expansion (10) follows immediately [terms proportional to F^6, F^4B^2, F^2B^4, and B^6 in (10) are found similarly]. Equations (A10) were found on a computer using recurrence relations similar to the ones described in detail in Ref. 16 for the Stark effect. In view of the complexity of these relations we do not give them here. We note that the expansions (A7) and (A9) were used to control the numerical calculation.

5) It is convenient to carry out in (3) the substitution $r_0=\beta s^{1/4}$, where $\beta=(B/2)^{-1/2}\to 0$ in the strong magnetic field region. We get

$$s+\beta s^{3/4}-2\beta^4F^2s+O(\beta^8)=1. \tag{A11}$$

Hence follows Eq. (11) and also

$$\begin{aligned}\varepsilon^{(0)}&=2\beta^{-2}-2\beta^{-1}-\frac{1}{4}-\frac{1}{16}\beta-\frac{1}{64}\beta^2\\ &\quad-\left(\frac{3}{1\,024}+F^2\right)\beta^3+O(\beta^4),\\ \alpha_0&=\frac{2F}{B}\left[1-\frac{1}{2}\beta+O(\beta^3)\right].\end{aligned} \tag{A12}$$

The orbit is then strongly compressed, the classical energy $\varepsilon^{(0)}$ is mainly determined by the magnetic field, and the electric field leads only to small corrections.

6. The classical ionization threshold $F_*(B)$ is determined by the set (3) and (8). Putting

$$\xi=r_0^{-1}, \quad \eta=B^2r_0^3, \quad \tau=3F^2r_0^4,$$

we find ξ, η as functions of τ:

$$\xi=\frac{3}{4}\left(1-\frac{\tau}{3}\right)^3(1-\tau)^{-1}, \quad \eta=(3\tau-1)(1-\tau)^{-1}.$$

We can write the B dependence of F_* in parametric form:

$$F_*=\xi^2(\tau/3)^{1/2}, \quad B=(\xi^3\eta)^{1/2} \tag{A13}$$

($\frac{1}{3}\leqslant\tau<1$). Here $\tau=\frac{1}{3}$ corresponds to the absence of a magnetic field: $F_*(0)=2^{12}\cdot3^{-9}$, $r_*=\frac{81}{64}$ and for $F=0$ Eqs. (3) and (8) are incompatible (this corresponds to the fact that when there is no electric field present bound states do not remain quasistationary for any values of $\mathscr{H}$). From (A13) we easily find Eqs. (9) in the two limiting cases $\tau\to\frac{1}{3}$ and $\tau\to1$).

APPENDIX B

We briefly give an account of the more standard method of deriving the $1/n$ expansion. Using the axial symmetry of the problem we write the Schrödinger equation in cylindrical coordinates:

$$\left\{-\frac{1}{2}\left(\frac{\partial^2}{\partial\rho^2}+\frac{\partial^2}{\partial z^2}\right)+\frac{m^2-1/4}{2\rho^2}-\frac{1}{r}-\mathscr{E}z+\frac{1}{8}\mathscr{H}^2\rho^2-E\right\}\chi=0, \tag{B1}$$

where $r=(\rho^2+z^2)^{1/2}$, the wave function

$$\psi(\mathbf{r})=\rho^{-1/2}e^{im\varphi}\chi(\rho,z)$$

and (as in § 2) we have dropped the paramagnetic term $\frac{1}{2}\mathscr{H}(L_z+2S_z)$; its contribution to the energy is trivial. After scaling (1) we find an equation in which $1/n$ plays the role of Planck's constant $\hbar$:

$$\left\{-\frac{1}{2n^2}\left(\frac{\partial^2}{\partial\tilde\rho^2}+\frac{\partial^2}{\partial\tilde z^2}\right)-\frac{1}{\tilde r}-F\tilde z+\frac{1}{8}B^2\tilde\rho^2+\frac{1}{2\tilde\rho^2}\left(1-\frac{2p}{n}+\frac{p^2-1/4}{n^2}\right)\right\}\tilde\chi=\frac{1}{2}\varepsilon\tilde\chi, \tag{B2}$$

where $p=n-m$ and $\tilde\chi(\tilde\rho,\tilde z)=\chi(n^2\tilde\rho,n^2\tilde z)$. In the limit as $n\to\infty$ the effective potential in (B2) is

$$U(\tilde\rho,\tilde z)=-\frac{1}{\tilde r}+\frac{1}{2\tilde\rho^2}+F\tilde z+\frac{1}{8}B^2\tilde\rho^2. \tag{B3}$$

It has a minimum in the point $(\tilde\rho_0,\tilde z_0)$ determined by Eq. (3). The frequencies of the small oscillations of the electron around the equilibrium point are determined by diagonalizing the matrix $(\partial^2U/\partial x_i\partial x_j)_0$:

$$\omega_{1,2}=(a\pm b)^{1/2}, \tag{B4}$$
$$a=\tfrac{1}{2}(U_{\rho\rho}+U_{zz}), \quad b=\tfrac{1}{2}[(U_{\rho\rho}-U_{zz})^2+4U_{\rho z}^2]^{1/2},$$

where

$$U_{\rho\rho}=4/\tilde\rho_0^4-3\tilde\rho_0^2/\tilde r_0^5, \quad U_{\rho z}=-3\tilde\rho_0\tilde z_0/\tilde r_0^5,$$
$$U_{zz}=\frac{1}{\tilde r_0^3}(1-3\tilde z_0^2/\tilde r_0^2).$$

Hence follows Eq. (7).

When $\omega_2=0$ the two [stable $(\tilde\rho_0,\tilde z_0)$ and unstable] equilibrium points in the potential (B3) merge after which these points enter the complex plane. As in other problems[11,14,15] such a situation is of special interest in quantum mechanics as it enables us to evaluate (using the $1/n$ expansion) the width of quasistationary states.

[1)] We use in what follows atomic units $\hbar=m_e=e=1$. The unit of the electric field strength is $\mathscr{E}_0=m_e^2e^5/\hbar^4=5.142\times10^9$ V/cm, and that of the magnetic field strength $\mathscr{H}_0=m_e^2e^3c/\hbar^3=2.350\times10^9$ G.

[2)] This situation is a common one and occurred, for instance, for the calculation of $\varepsilon^{(0)}$ for Yukawa or Hulthén potentials.[15]

[3)] See Refs. 4–6 and also Ref. 7 for the case of an arbitrary angle between $\vec{\mathscr{E}}$ and $\vec{\mathscr{H}}$ (one should note that the expansion coefficients given in Ref. 6 contain errors; see Refs. 7 and 17 in that connection).

[4)] Compare Eq. (2.5) in Ref. 9 for the case of potentials with spherical symmetry.

[5)] It is similar to the term $\tilde\rho^{-2}/2$ in Eq. (B2) for the hydrogen atom arising after splitting off the angular variable φ.

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