Strong-field Stark effect

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The Stark shifts and the widths of the ground and excited states of the hydrogen atom are calculated. Two independent calculation methods are used: a summation of a divergent perturbation-theory series and a $1/n$ expansion.

1. The Stark effect is one of the best known problems in quantum mechanics but at the same time one of the most difficult (outside the weak-field region) (Refs. 1–10, for example). For a level with parabolic quantum numbers n_1, n_2, m in the hydrogen atom, the perturbation-theory series is[1]

$$E^{(n_1\ n_2\ m)}(\mathcal{E}) = \frac{1}{2n^2} \sum_{k=0}^{\infty} \epsilon_k^{(n_1, n_2, m)} F^k \qquad (1)$$

where $n = n_1 + n_2 + |m| + 1$ is the principal quantum number; $\epsilon_0 = -1$;

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$\epsilon_1 = 3(n_1 - n_2)/n,\ldots$; $F = n^4\mathscr{E}$; and $\hbar = m = e = 1$ (the unit of electric field is 1 a.u. $= m^2c^5/\hbar^4 = 5.142\times10^9$ V/cm. The recent development of new perturbation-theory methods has made it possible to calculate a large number of perturbation-theory coefficients[4-7] ϵ_k, up to $k = 160$ in the case of the ground state.[5,6] Series (1) has a zero convergence radius, however, and the energy $E(\mathscr{E})$ has an essential singularity at $\mathscr{E} = 0$ and a cut $0 < \mathscr{E}^2 < \infty$. For this reason, the use of perturbation theory to calculate the shift and width ($E = E_0 - i\Gamma/2$) of atomic levels in a strong electric field $\mathscr{E}$ would be impossible without corresponding methods for summing divergent series.

Using Padé approximants, one can determine E_0 and Γ up to $\mathscr{E} \approx 0.1$ (Ref. 6). The method of complex coordinates[9] and the Padé-Borel transformation[10] make it possible to sum perturbation-theory series highly accurately, but again only up to $\mathscr{E} = 0.1$ (and only for the ground state). The results in the literature[2,3,8] for $\mathscr{E} \sim 0.2$ are mutually contradictory (the discrepancy is particularly large for the width Γ). Developments in lasers and spectroscopy make it worthwhile to calculate E_0 and Γ for intense fields, $\mathscr{E} > 0.1$, also.

For this purpose, we use Padé-Hermite approximants[11] and a $1/n$ expansion.[12] Let us consider the case $n_1 = n_2 = 0$, $|m| = n - 1$, in which the odd orders of the perturbation theory vanish, and we have $\epsilon_{2k} < 0$ for all k (i.e., the perturbation-theory series is a constant-sign series). The ground level, $n = 1$, is one such state.

2. Calculation methods. The values of the Padé-Hermite approximants $f_N(\mathscr{E}^2)$ are calculated from the equation $P - Qf + Rf^2 = 0$, where P, Q, and R are polynomials of $\mathscr{E}^2$ of degree N, whose coefficients are determined unambiguously from the perturbation-theory coefficients through the condition

$$P - QE + RE^2 = O(\mathscr{E}^{2(3N+2)}),\ \mathscr{E} \to 0 \tag{2}$$

where $E(\mathscr{E}^2)$ is series (1). The ordinary Padé approximants are the special case of (2) with $R \equiv 0$. It is clear that $f_N(\mathscr{E}^2)$, in contrast with the Padé approximant $[P/Q](\mathscr{E}^2)$, can have an imaginary part even when the coefficients of the polynomials P, Q, and R are real.[3)]

The other approach, independent from that just described, is based on a $1/n$ expansion.[12] We make use of the fact that at $n \gg 1$ the Bohr model of the atom is applicable. In the absence of an electric field, the state $(0,0,m)$ corresponds to a circular electron orbit, perpendicular to the z axis (the direction of the field $\mathscr{E}$). When the field is turned on, the classical orbit shifts along z and changes in radius, remaining circular. Working from these considerations, and imposing the scaling $r \to n^2 r$, $\epsilon = 2n^2E$, $F = n^4\mathscr{E}$, we find the equations

$$\epsilon = \epsilon^{(0)} + \frac{\epsilon^{(1)}}{n} + \frac{\epsilon^{(2)}}{n} + \ldots, \tag{3}$$

where

$$\epsilon^{(0)} = 3u^3 - 4u^2,$$
$$\epsilon^{(1)} = u^3[(1 + 3\sqrt{1-u})^{1/2} + (1 - 3\sqrt{1-u})^{1/2} - 2], \tag{4}$$

TABLE I. Value of $-\epsilon_n$.

F	$n = 1$	$n = 10$
0.1	1.054 84 + i 0.014 54	1.012 97
	1.054 836 + i 0.014 538 [10,11]	1.012 976 $(1/n)$
0.25	1.170 + i 0.189	1.099 766 + i 0.032 154
	1.172 + i 0.188 [2]	1.100 + i 0.032 $(1/n)$
1.0	1.3 + i 1.29	1.2851 + i 0.6739
	1.235 + i 1.286 $(1/n)$	1.285 178 + i 0.673 874 $(1/n)$

and $u = u(F)$ is that root of the equation

$$u^4(1-u)^{1/2} = F,$$

which approaches unity in the limit $F \to 0$. The succeeding corrections $\epsilon^{(k)}$ are calculated by means of recurrence relations. With $u = 8/9$ or $F = F_* = 2^{12} \times 3^{-9} = 0.2081$, there is a "clash" of two classical solutions,[4] at which point $\epsilon^{(k)}$ acquires an imaginary part. Expansion (3) could also be found for other states if the conditions $n_1, n_2 \ll n$ hold.

The $1/n$ expansion converges rapidly at $n \gtrsim 5$, while the method of Padé-Hermite approximants has advantages at small values of n. An important point is that there is an overlap region in which the two methods agree with each other quite closely (and at $F \leqslant 0.1$ they agree with the results of other calculations[9,10]). The $1/n$ expansion thus supports the procedure which we have selected for summing divergent perturbation-theory series. See Table I, where the first line corresponds to the method of Padé-

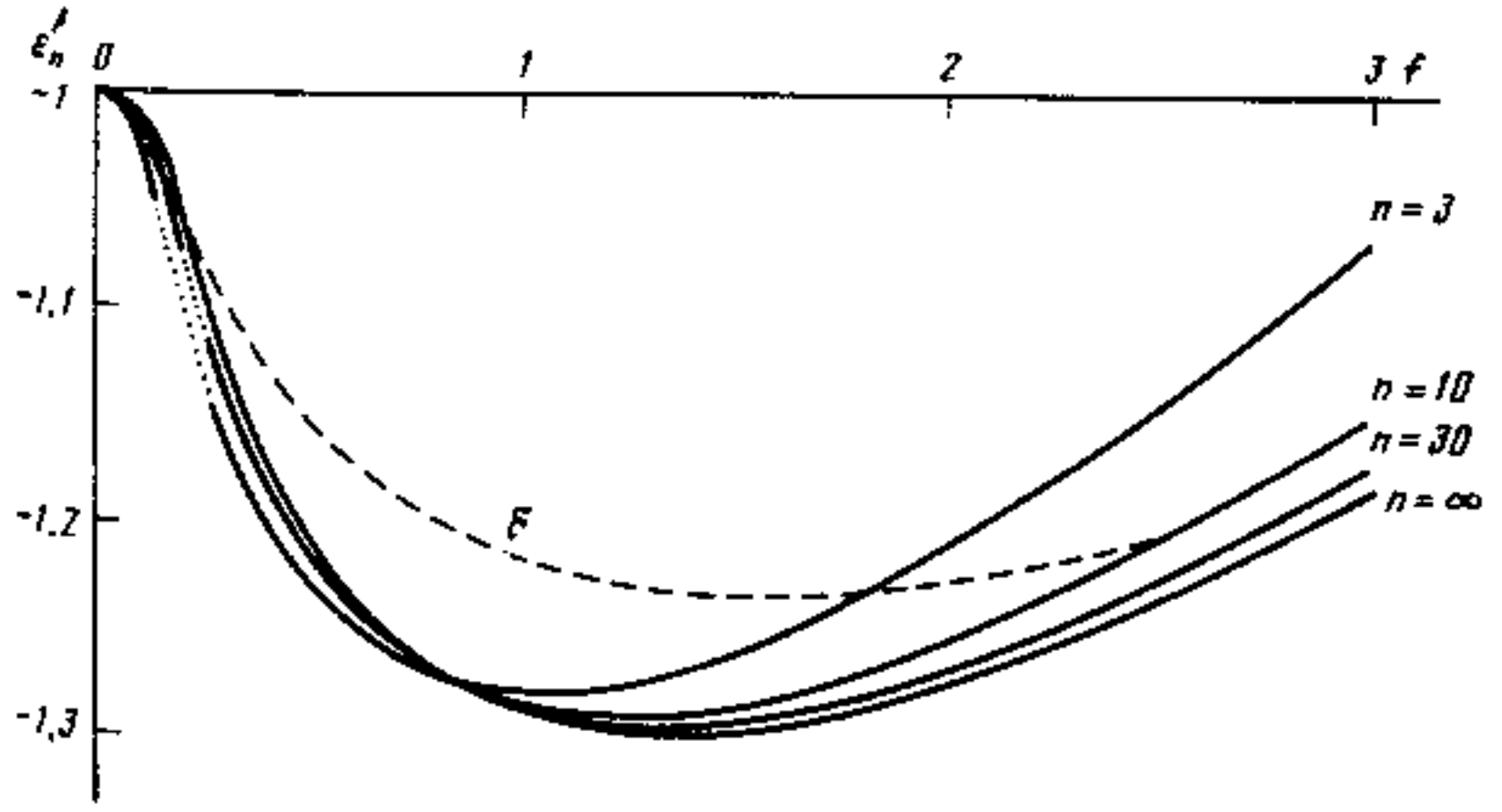

FIG. 1. Real part of the level energy, $\epsilon'_n = 2n^2 \mathrm{Re} E^{(0,0,n-1)}$, for $(0,0,n-1)$ states. Curve δ corresponds to a one-dimensional δ-function potential.

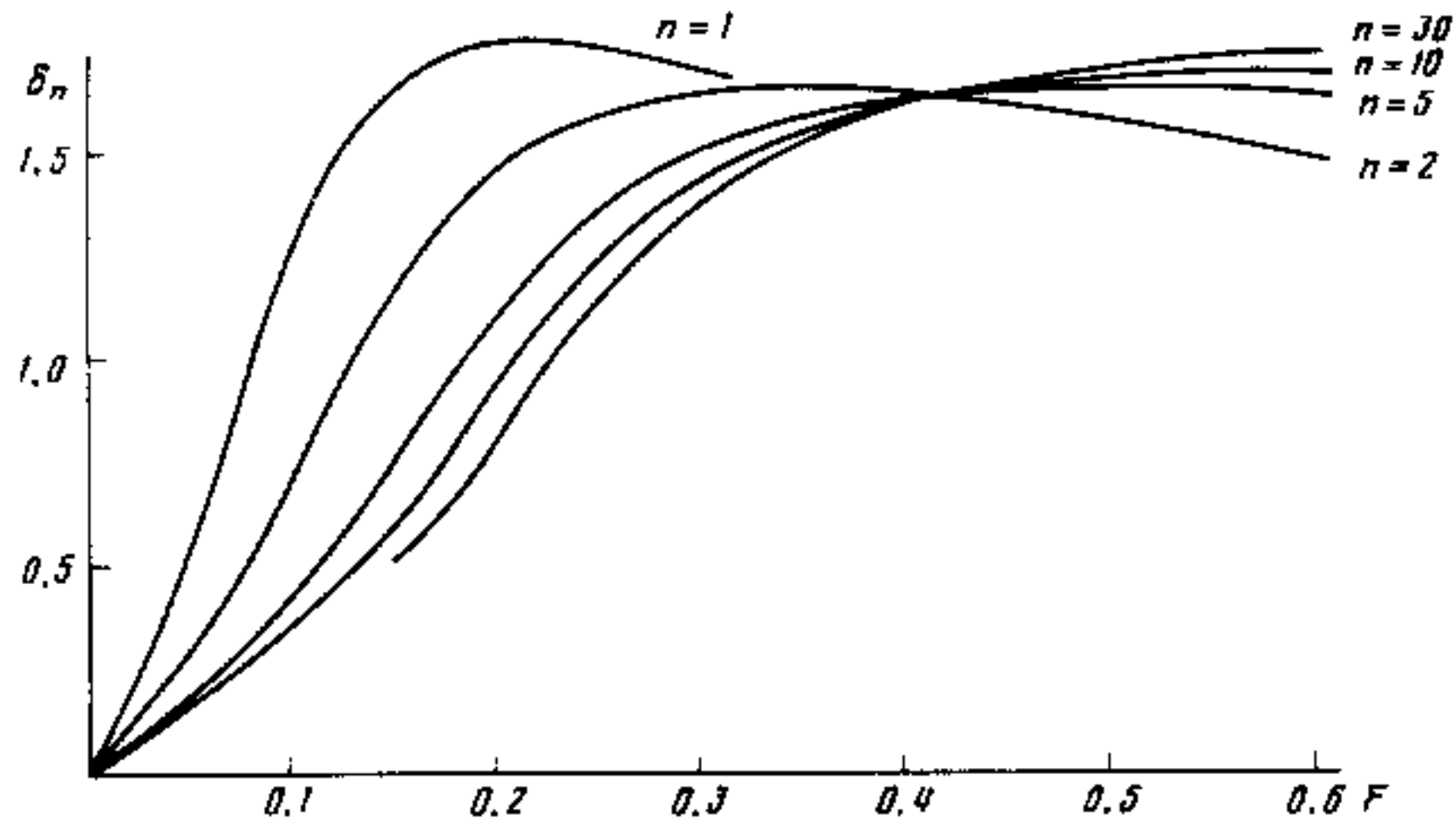

FIG. 2. The function $\delta_n(F)$; see Eq. (6).

Hermite approximants, and the second corresponds to other methods (in particular the $1/n$ expansion).

3. Figures 1 and 2 show results calculated on the real and imaginary parts of the "reduced energy" of a level, $\epsilon_n = 2n^2 E^{(0,0,n-1)}$. In very strong fields, the Stark shift of the levels $(0,0,n-1)$ changes sign. The width of the levels is conveniently written in the form

$$\Gamma^{(n_1 n_2 m)}(\mathscr{E}) = \tilde{\Gamma}^{(n_1 n_2 m)}(\mathscr{E}) \exp\{-n\delta_{n_1 n_2 m}(\mathscr{E})\}, \tag{6}$$

where $\tilde{\Gamma}$ corresponds to the semiclassical formula,[1] which is asymptotically exact in the limit $\mathscr{E} \to 0$; the second factor includes corrections to the semiclassical results. For the states considered we have

$$\tilde{\Gamma}^{(0,0,n-1)}(\mathscr{E}) = \frac{2^{2n}}{n!\, n^{3n+2}}\, \mathscr{E}^{-n} \exp\left\{-\frac{2}{3n^3\mathscr{E}}\right\} \tag{7}$$

and $\delta_n = c_1 F + 0(F^2)$ in the limit $F \to 0$, where $c_1 = (33n^2 + 54n + 20)/12n^2$. At small values of $\mathscr{E}$, only the factor $\tilde{\Gamma}(\mathscr{E})$, which depends very strongly on the field and which varies by many orders of magnitude, is important in (6). Our calculations shows, however, that the range of applicability of (7) is quite narrow: $\mathscr{E} \lesssim 0.1n^{-3}$. The term with δ_n would have to be taken into account for stronger fields, especially in the case of Rydberg states ($n \gg 1$). Correspondingly, the ionization probability $\Gamma^{(0,0,n-1)}(\mathscr{E})$ is much smaller than the value that follows from semiclassical estimate (7).

We have considered only states with $n_1 = n_2 = 0$ here. There are no fundamental difficulties in generalizing the arguments to arbitrary n_1, n_2, and m. The results of such calculations will be reported in a more detailed publication.

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Since all the ϵ_k in (1) are real, the polynomials P, Q, and R found from (2) have only real coefficients. The energy E, on the other hand, has an imaginary part $\Gamma/2$, which corresponds to the probability for ionization of the level by the electric field, for any $\mathscr{E} \neq 0$. This circumstance represents an advantage of the method of Padé-Hermite approximants over Padé approximants in the Stark-effect problem. A similar event occurs in other problems, e.g., those of the Yukawa and Hulthén potentials.[12]

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