Critical fields and above-barrier Stark resonances

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Exact values of the critical field $\mathscr{E}_c$ are calculated for a hydrogen atom, including the case of the ground state. The widths Γ_n of Stark resonances at $\mathscr{E}=\mathscr{E}_c$ are also calculated. In the above-barrier region ($\mathscr{E}>\mathscr{E}_c$) the widths $\Gamma_n(\mathscr{E})$ are essentially linear functions of the electric field strength.

1. Experiments on near-threshold Stark states[1–3] are attracting interest to values of the electric field $\mathscr{E}=\mathscr{E}_c(n_1,n_2,m)$ at which an atomic level "touches" the top of a potential barrier (following Shakeshaft *et al.*,[4] we will call these "critical fields"). The value $\mathscr{E}_c$ separates two characteristic regions: a "weak-field" region, in which the levels are below-barrier levels, with exponentially small widths (and in which a semiclassical asymptotic behavior prevails as $\mathscr{E}\to 0$; Ref. 5), and a "strong-field" region ($\mathscr{E}>\mathscr{E}_c$), in which the resonances are above-barrier resonances. Both experimental data and numerical calculations show that the transition from one region to the other is exceedingly sharp. Consequently, the critical fields $\mathscr{E}_c$, which are strictly determined in the semiclassical case, $n\gg 1$, remain meaningful at small quantum numbers.

In the problem of the Stark effect in the hydrogen atom, variables can be separated in parabolic coordinates, and there is a barrier along the variable $\eta=r-z$. Since the wave function $\chi_2(\eta)$ is defined on the semiaxis $0<\eta<\infty$, the point $\eta=0$ is a singular point. A Langer transformation[6]

$$\eta=\exp(x), \quad \chi_2(\eta)=\exp(x/2)\varphi(x) \tag{1}$$

moves this singularity off to $-\infty$ and allows one to correctly incorporate the boundary condition $\chi_2(0)=0$ in the semiclassical approach. The Schrödinger equation becomes

$$\frac{1}{n^2}\frac{d^2\varphi}{dx^2}+p^2\varphi=0, \quad p^2=-\frac{\mu^2}{4}+\beta_2 y+\frac{1}{2}\epsilon y^2+\frac{1}{4}Fy^3, \tag{2}$$

where $y=n^{-2}\eta$; β_2 is a separation constant; ϵ, F, and μ are the "reduced" variables

$$\epsilon=\epsilon'-i\epsilon''=2n^2E_n(\mathscr{E}), \ \epsilon''=n^2\Gamma_n, \quad F=n^4\mathscr{E}, \ \mu=\frac{|m|}{n}; \tag{2a}$$

$E=E_r-i\Gamma/2$ is the energy of the resonance; and n_1, n_2, and m are parabolic quantum numbers (we are using atomic units and the standard notation[5]).

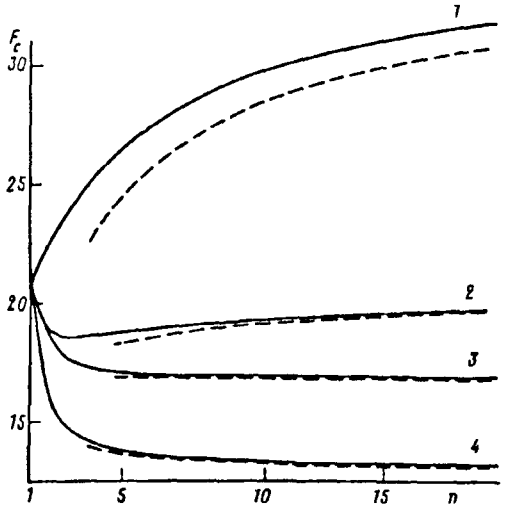

FIG. 1. The critical fields $F_c(n_1,n_2,m)$ for the hydrogen atom. Solid curves: Calculated through the introduction of a Langer correction. Dashed curves: Without this correction. Curves 1–4 refer to the following series of states: $(n-1,0,0)$, $(0,0,n-1)$, $(n_1,n_1,0)$, and $(0,n-1,0)$, where $n_1=n_2=(n-1)/2$, and n is the main quantum number of the level.

The condition that a level "touches" the top of the barrier (i.e., $E_r=U_m$) is expressed by the equations

$$\mathrm{Re}\ p^2(y_m)=\mathrm{Re}\frac{dp^2}{dy}\Big|_{y=y_m}=0. \tag{3}$$

Using (2), we can put these equations in the form

$$\epsilon'+2Fy+\mu^2y^{-2}=0,\quad y=-\frac{\epsilon'}{3F}\left[1+(1-\zeta)^{1/2}\right], \tag{4}$$

where $y=y_m$, $\zeta=12\beta_2' F/\epsilon'^2$, $\beta_2'=\mathrm{Re}\beta_2$ and $\epsilon'<0$. The quantities ϵ' and β_2' depend on the reduced electric field F and on the quantum numbers of the state. These quantities are calculated by summing the divergent perturbation-theory series with the help of the Pade–Hermite approximant (this method is described in Ref. 7). The calculations were carried out up to 80th-order perturbation theory and achieved an accuracy $\sim 10^{-4}$ for ϵ and β_2. The critical field $F_c(n_1, n_2, m)$ was then determined from Eqs. (4).

Figure 1 shows results calculated for F_c for four series of (n_1,n_2,m) states of the hydrogen atom. The Langer correction turns out to be extremely important at small values of n, particularly for the ground state. In this case we have $F_c=\mathscr{E}_c=0.2082$, while we would find $F_c'=0.1587$ without this correction. The effect of the Langer correction on the value of F_c can be estimated with the help of the parameter

$$\delta=\delta U_2/U_2|_{\eta=\eta_m}\sim F_c^2/n^2(-\epsilon_c)^3. \tag{5}$$

We thus have $\delta\sim n^{-2}\to 0$. Exceptional cases are the states $(n-1, 0, 0)$, for which we have $-\epsilon_c\propto\nu_2^{2/3}\sim n^{-2/3}$, so the correction δ falls off very slowly as $n\to\infty$.

As n increases, the values of F_c approach the classical ionization threshold F_*, which depends on only the ratios $\nu_i=(n_i+1/2)/n$. Here are their numerical values:

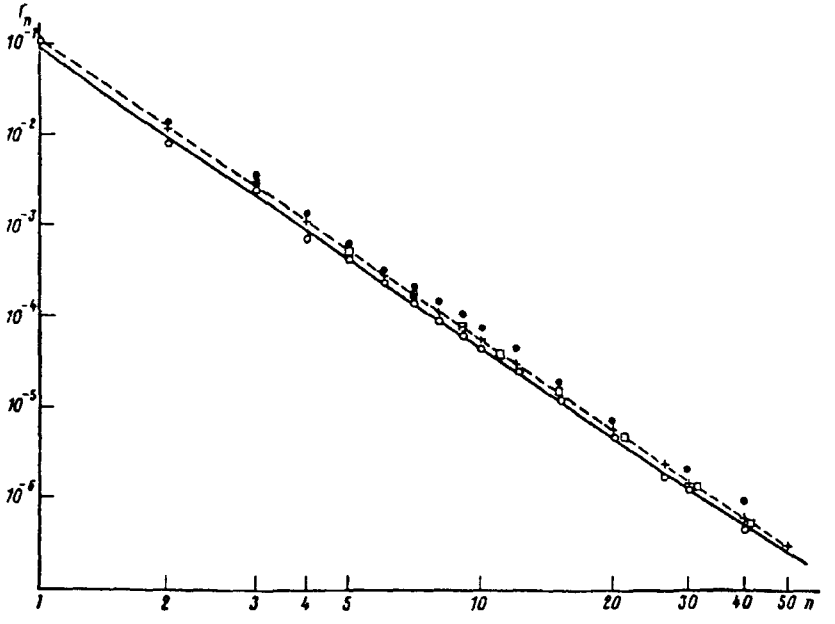

FIG. 2. The Stark widths $\Gamma_n(\mathscr{E} = \mathscr{E}_c)$ versus n. The scale along each axis is logarithmic. The quantity log (n^3) is plotted along the abscissa. ○—The widths Γ_n for the $(0,n-1,0)$ states; +—for the $(0,0,n-1)$ series; □—for $(n_1,n_1,0)$; ●—for $(n-1,0,0)$. The solid curve was plotted from Eq. (7) for the $(0,n-1,0)$ series, while the dashed curve corresponds to the series of states $(0,0,n-1)$, which correspond (in the limit $n \to \infty$) to circular electron orbits.

$F_*=0.3834$, 0.2081, 0.1674, and 0.1298, respectively, for the series of states $(n-1, 0, 0)$, $(0, 0, n-1)$, $[(n-1)/2, (n-1)/2, 0]$, and $(0, n-1, 0)$, as $n \to \infty$. For Rydberg $(n \gg 1)$ resonances we find[1)]

$$F_c/F_* = 1 + \frac{c_1}{n} + \frac{c_2}{n(\ln n + l_0)} + \dots , \tag{6}$$

where, for the $(0, n-1, 0)$ series, for example, we have $F_* = 2^{10}(3\pi)^{-4}$, $c_1 = 2 - 2^{5/2}\pi^{-1} = 0.199$, $c_2 = \ln 2/2 = 0.347$ and $l_0 = 2.286$. Equations (5) and (6) give a qualitative explanation of the results of the numerical calculations shown in Fig. 1.

2. The positions and, especially, the widths Γ_n of the Stark resonances at $\mathscr{E} = \mathscr{E}_c$ are of interest. Using the semiclassical quantization condition, and incorporating the barrier transmission,[8,9] we can show that we have

$$\Gamma_n(\mathscr{E} = \mathscr{E}_c) = \gamma n^{-3}(\ln n + l_0)^{-1}, \quad n \gg 1, \tag{7}$$

where γ and l_0 are constants which depend on the quantum numbers. For the $(0, n-1, 0)$ states, for example, we find $\gamma = 2^8(3\pi)^{-3} \ln 2 = 0.212$ and $l_0 = 2.286$. Figure 2 shows that the asymptotic behavior in (7) agrees well with the results of

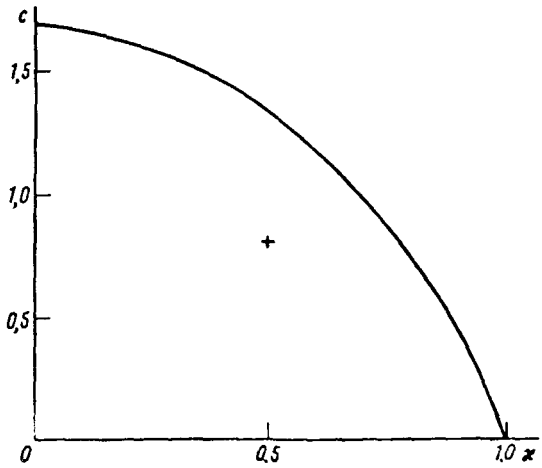

FIG. 3. The slope c of the reduced width of the $(n_1,n_2,0)$ levels in the above-barrier region. $\kappa=(n_1-n_2)/n$, $n\to\infty$. The plus sign shows the value of the coefficient c for circular orbits, i.e., for $(0,0,n-1)$ states.

numericalcalculations even at $n\geqslant 3$. We see that the Stark resonances at the time of the touching have a small width, particularly in the case of Rydberg ($n\gg 1$) states.[2)]

In the general case in which the potential binding the particle has the behavior $V(r)\propto r^{-\alpha}$ at short range, we find, in place of (7),

$$\Gamma_n(E_r=U_m)\approx\text{const}/n^{(2+\alpha)/(2-\alpha)}\log n,\quad 0<\alpha<2. \tag{7a}$$

3. Numerical calculations show[7,10] that the Stark widths in the above-barrier region are essentially linear functions of the electric field[3)]:

$$\epsilon''(F)\equiv n^2\Gamma_n=c(F-F_0),\quad F\gtrsim 1,2F_c. \tag{8}$$

Using generalized quantization conditions for the above-barrier resonances (for states of the hydrogen atom with $m=0$, $n\gg 1$, we can write these conditions in analytic form[7,9]), we have calculated the constants c and F_0 in (8). The results of these calculations (Fig. 3) show, in particular, that we have $c\to 0$ as $\kappa=(n_1-n_2)/n\to 1$, i.e., for Rydberg states $(n-1,0,0)$. The explanation for this result is that the widths Γ_n of the states are smaller by another order of n .

In the limit of a very strong field, we find $\Gamma_n\propto\mathscr{E}^{2/3}$ as $\mathscr{E}\to\infty$ (Ref. 9). The linear dependence in (8) is thus an "intermediate asymptotic behavior." This dependence has recently been used to calculate the electron energy spectrum in the process of above-barrier ionization.[12]

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[1)]Here, as in (5), this asymptotic behavior ceases to hold for state $(n-1,0,0)$.

[2)]This situation corresponds to the circumstance that (within the framework of a $1/n$ expansion[10]) the reduced width ϵ_n'' vanishes as long as the condition $F<F^*$ holds, i.e., up to the point at which the classical solutions collide.

[3)]A qualitative explanation of this fact is provided by the semiclassical $1/n$ expansion.[10] The use of that

expansion makes it possible to write ϵ''as a function of F (in the limit $n \to \infty$) in a simple parametric form; see Eqs. (5) in Ref. 11.

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