

Critical fields and above-barrier Stark resonances

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Exact values of the critical field \mathcal{E}_c are calculated for a hydrogen atom, including the case of the ground state. The widths Γ_n of Stark resonances at $\mathcal{E} = \mathcal{E}_c$ are also calculated. In the above-barrier region ($\mathcal{E} > \mathcal{E}_c$) the widths $\Gamma_n(\mathcal{E})$ 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 $\mathcal{E} = \mathcal{E}_c(n_1, n_2, m)$ 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 \mathcal{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 $\mathcal{E} \rightarrow 0$; Ref. 5), and a “strong-field” region ($\mathcal{E} > \mathcal{E}_c$), 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 \mathcal{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 transformation⁶

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

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

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

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

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

$E = E_r - i\Gamma/2$ 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 notation⁵).

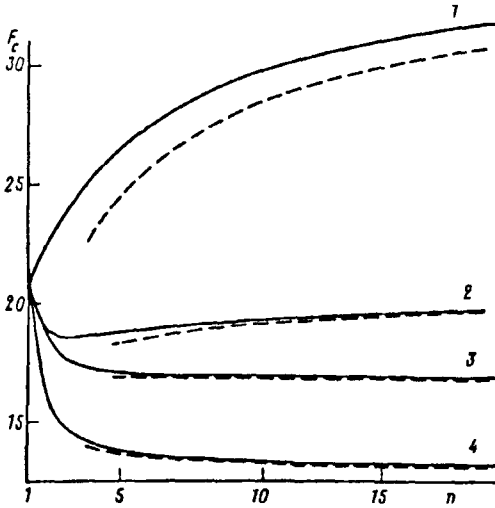


FIG. 1. The critical fields $F_c(n_1, n_2, m)$ for the hydrogen atom. Solid curves: Calculated through the introduction of a Langer correction. Dashed curves: Without this correction. Curves 1-4 refer to the following series of states: $(n-1, 0, 0)$, $(0, 0, n-1)$, $(n_1, n_1, 0)$, and $(0, n-1, 0)$,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

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

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

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

where $y = y_m$, $\xi = 12\beta_2' F / \epsilon'^2$, $\beta_2' = \operatorname{Re}\beta_2$ 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 $F_c = \mathcal{E}_c = 0.2082$, 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

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

We thus have $\delta \sim n^{-2} \rightarrow 0$. Exceptional cases are the states $(n-1, 0, 0)$, for which we have $-\epsilon_c \propto v_2^{2/3} \sim n^{-2/3}$, so the correction δ falls off very slowly as $n \rightarrow \infty$.

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

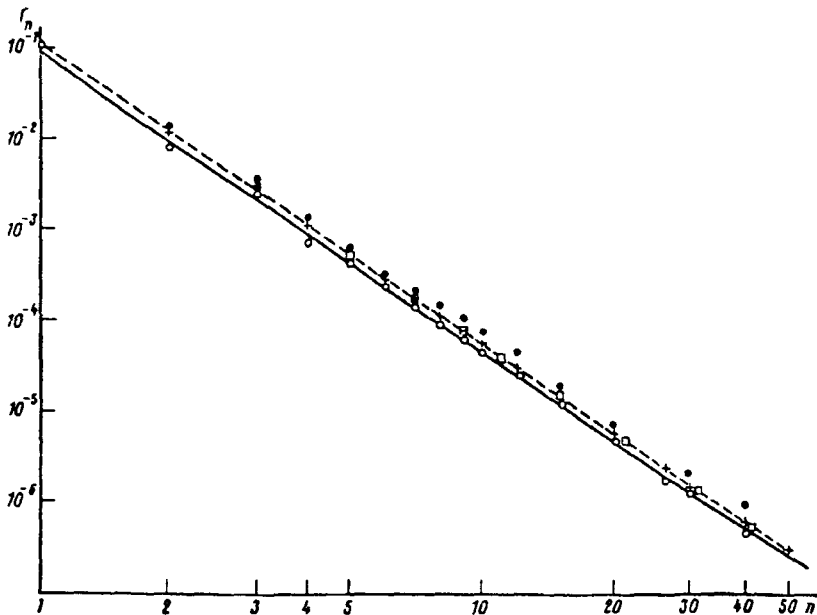


FIG. 2. The Stark widths $\Gamma_n(\mathcal{E} = \mathcal{E}_c)$ versus n . The scale along each axis is logarithmic. The quantity $\log(n^3)$ is plotted along the abscissa. \circ —The widths Γ_n for the $(0, n-1, 0)$ states; $+$ —for the $(0, 0, n-1)$ series; \square —for $(n_1, n_1, 0)$; \bullet —for $(n-1, 0, 0)$. 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 $n \rightarrow \infty$) 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 $n \rightarrow \infty$. For Rydberg ($n \gg 1$) resonances we find¹⁾

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

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 $\mathcal{E} = \mathcal{E}_c$ are of interest. Using the semiclassical quantization condition, and incorporating the barrier transmission,^{8,9} we can show that we have

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

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

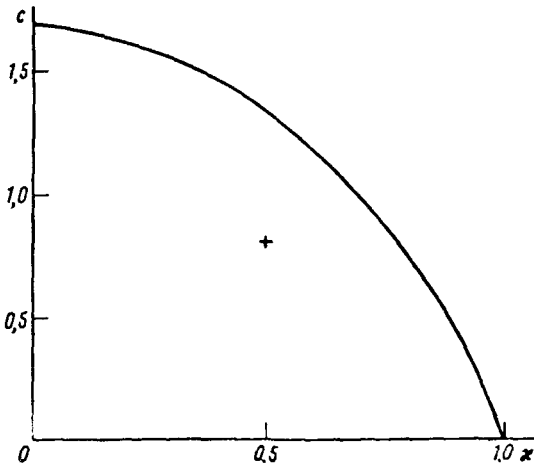


FIG. 3. The slope c of the reduced width of the $(n_1, n_2, 0)$ levels in the above-barrier region. $\kappa = (n_1 - n_2)/n$, $n \rightarrow \infty$. The plus sign shows the value of the coefficient c for circular orbits, i.e., for $(0, 0, n-1)$ states.

numerical calculations even at $n \geq 3$. 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),

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

3. Numerical calculations show^{7,10} that the Stark widths in the above-barrier region are essentially linear functions of the electric field³⁾:

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

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 $c \rightarrow 0$ as $\kappa = (n_1 - n_2)/n \rightarrow 1$, 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 $\Gamma_n \propto \mathcal{E}^{2/3}$ as $\mathcal{E} \rightarrow \infty$ (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 $1/n$ expansion¹⁰) 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 $n \rightarrow \infty$) in a simple parametric form; see Eqs. (5) in Ref. 11.

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