Top energy levels of the hydrogen atom in an electric field

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The energy levels on the top of the potential barrier are considered for a hydrogen atom located in an electric field. The critical field intensity, the level energy position, and the level width are calculated in the quasiclassical approximation.

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1. INTRODUCTION

The energy levels of a hydrogen atom in an electric field, which lie exactly on the top of the potential barrier, and which can be called top levels (see, e.g., Ref. 1 and the references therein), have attracted much attention recently. In this article these levels are considered on the basis of a quasiclassical approximation in the parametric form developed in Ref. 2. We confine ourselves to zero projection of the angular momentum on the field direction, $m=0$.

We use the atomic system of units. We introduce the effective quantum number ν connected with the electron energy E by the relation

$$\nu=(-2E)^{-1/2}, \tag{1.1}$$

and denote by n the principal quantum number into which ν goes over when the field intensity $\mathscr{E}$ vanishes. As shown in Ref. 2, the ratio ν/n is a universal function of two quantities:

$$T=4n^4\mathscr{E},\quad S=(n_1-n_2)/n, \tag{1.2}$$

where n_1 and n_2 are parabolic quantum number, and in our case ($m=0$) $n=n_1+n_2+1$. The quantity S has a simple physical meaning: it describes the well-known asymmetry of the distribution of the charge of the excited atom (in the absence of the field) which takes place at $n_1\neq n_2$ (Ref. 3).

The use of the quasiclassical approximation presupposes that $n_{1,2}\gg 1$, and we put therefore approximately $n=n_1+n_2$.

In this approximation we have

$$1-S=2\frac{n_2}{n}=2\left(1-\frac{n_1}{n}\right),\quad 1+S=2\frac{n_1}{n}=2\left(1-\frac{n_2}{n}\right). \tag{1.3}$$

The dependence of ν/n on S and T is expressed with the aid of two parameters, z_1 and z_2, which range from 0 to 1. They are determined from a system of equations[2] which we represent in the form

$$z_1(1-z_1)^{-3/2}F\left(-\frac{1}{2},\frac{1}{2},2;-z_1\right)=\frac{1+S}{1-S}z_2(1+z_2)^{-3/2}F\left(-\frac{1}{2},\frac{1}{2},2,z_2\right) \tag{1.4}$$

$$T=\left[\frac{2z_2}{1-S}F\left(-\frac{1}{2},\frac{1}{2},2,z_2\right)\right]^4\frac{(1-z_1)^6}{[z_1(1+z_2)^2+z_2(1-z_1)^2]^3}, \tag{1.5}$$

where F is a hypergeometric function.

By obtaining z_1 and z_2 from the given S and T, we determine ν/n from the relation

$$\frac{\nu}{n}=\frac{1+S}{2(1-z_1)^{1/2}F(-1/2,1/2,2,-z_1)}+\frac{1-S}{2(1+z_2)^{1/2}F(-1/2,1/2,2,z_2)}. \tag{1.6}$$

2. TOP LEVEL

The top level corresponds[2] to $z_2=1$. In this case ν/n and T become functions of a single quantity S and are expressed in parametric form in terms of z_1. Recognizing that $F(-\frac{1}{2},\frac{1}{2},2,1)=8/3\pi$, we obtain from (1.4) an equation for z_1 in terms of the given S:

$$z_1(1-z_1)^{-3/2}F\left(-\frac{1}{2},\frac{1}{2},2,-z_1\right)=\frac{4}{3\sqrt{2}\pi}\frac{1+S}{1-S}. \tag{2.1}$$

As seen from (2.1), positive S that are close to 1 correspond to values of z_1 likewise close to 1, while negative S close to -1 correspond to small z_1 close to zero.

Equation (1.5) for T takes at $z_2=1$ the form

$$T=\left(\frac{16}{3\pi}\right)^4\frac{1}{(1-S)^4}\left(\frac{1-z_1}{1+z_1}\right)^6. \tag{2.2}$$

Finally, Eq. (1.6) takes at $z_2=1$ the form

$$\frac{\nu}{n}=\frac{1+S}{2(1-z_1)^{1/2}F(-1/2,1/2,2,-z_1)}+\frac{3\pi}{16\sqrt{2}}(1-S). \tag{2.3}$$

In the limiting cases of small n_1/n or small n_2/n we can obtain in explicit form approximate equations for z_1 in terms of n_1/n and for $1-z_1$ in terms of n_2/n, respectively. At small n_1/n it suffices to retain in the left-hand side of (2.1) the factor z_1, put $z_1=0$ in the remaining term, and replace $(1+S)/(1-S)$ in the right-hand side by n_1/n. We obtain

$$z_1=\frac{4}{3\sqrt{2}\pi}\left(\frac{n_1}{n}\right). \tag{2.4}$$

At small n_2/n we expand in the left-hand side the hypergeometric function in powers of $1-z_1$, retaining terms not higher than linear.

In the right-hand side we replace $(1+S)/(1-S)$ by n/n_2. Using the known expression for the derivative of the hypergeometric function, we get

$$(1-z_1)^{-3/2}F\left(-\frac{1}{2},\frac{1}{2},2,-1\right)-(1-z_1)^{-1/2}\left[F\left(-\frac{1}{2},\frac{1}{2},2,-1\right)+\frac{1}{8}F\left(\frac{1}{2},\frac{3}{2},3,-1\right)\right]=\frac{4}{3\sqrt{2}\pi}\left(\frac{n}{n_2}\right).$$

An approximate solution of this equation with respect to $1-z_1$, in which account is taken of the leading term and of the most significant correction for it, is

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$$(1-z_1)=a_1\left(\frac{n_2}{n}\right)^{2/3}\left[1-a_2\left(\frac{n_2}{n}\right)^{2/3}\right], \tag{2.5}$$

where

$$a_1=\left[\frac{3\pi\sqrt{2}}{4}F\left(-\frac{1}{2},\frac{1}{2},2,-1\right)\right]^{2/3},$$
$$a_2=\frac{2}{3}a_1\left[1+\frac{F(1/2,3/2,3,-1)}{8F(-1/2,1/2,2,-1)}\right]. \tag{2.6}$$

The hypergeometric functions contained in a_1 and a_2 can be expressed in terms of gamma functions by using Eqs. (15.3.3), (15.1.21), and (15.1.22) of the Abramovitz and Stegun handbook.[4] The gamma functions in Eqs. (15.1.21) and (15.1.22) can in turn be expressed, using known relations, in terms of $\Gamma(1/4)$ and $\Gamma(3/4)$. Without dwelling on these elementary operations, we present the final expressions for the coefficients a_1 and a_2:

$$a_1=\pi[\Gamma(3/4)]^{-4/3}=2.41\ldots,$$
$$a_2={}^1/_2\pi[\Gamma(3/4)]^{-4/3}[1+4(\Gamma(3/4)/\Gamma(1/4))^2]=1.75\ldots \tag{2.7}$$

Equation (2.5) is valid at $a_2(n_2/n)^{2/3}\ll 1$ or $n_2/n\ll 0.4$. With the aid of (2.4) and (2.5) we can now use (2.2) and (2.3) to calculate T and ν/n for both limiting cases.

Small n_1/n. We consider first the quantity T defined by expression (2.2).

To first order of smallness in z_1 we have

$$\left(\frac{1-z_1}{1+z_1}\right)^6\approx 1-12z_1,$$

which equals, according to (2.4),

$$1-(16/\sqrt{2}\,\pi)\,(n_1/n).$$

Representing $1-S$ in the form $2(1-n_1/n)$ and calculating $(1-S)^{-4}$ we obtain, accurate to terms of first order in n_1/n,

$$T=b_1(1+b_2n_1/n);\quad b_1=(8/3\pi)^4=0.519\ldots,\quad b_2=4-16/\sqrt{2}\,\pi=0.398\ldots \tag{2.8}$$

We turn now to the quantity ν/n defined by (2.3). We put in the first term $z_1=0$, since $1+S$ is proportional to n_1/n and is small by assumption.

We then obtain

$$\nu/n=b_3(1+b_4n_1/n);$$
$$b_3=3\pi/8\sqrt{2}=0.833\ldots,\quad b_4=8\sqrt{2}/3\pi-1=0.200. \tag{2.9}$$

2. *Small* n_2/n. Substituting in (2.2) the approximate expression (2.5) for $1-z_1$ and replacing $1+z_1$ by 2 and $1-S$ by $2n_2/n$, we obtain

$$T=c_1[1-a_2(n_2/n)^{2/3}]^6,\quad c_1=(8\pi/9)^2[\Gamma(3/4)]^{-8}=1.534\ldots \tag{2.10}$$

Turning to Eq. (2.3) for ν/n, we note that the second term can be discarded, since it contributes only in the corrections of higher order of smallness than included in this case. As for the first term, it is convenient to consider its reciprocal, i.e., n/ν. Expanding the hypergeometric function in powers of $1-z_1$ and proceeding in a manner similar to that above, we obtain

$$\frac{n}{\nu}=c_2\left(\frac{n_2}{n}\right)^{1/3}\left[1-c_3\left(\frac{n_2}{n}\right)^{2/3}\right],$$
$$c_2=\frac{4\pi}{3\sqrt{2}}\left[\Gamma\left(\frac{3}{4}\right)\right]^{-8/3}=1.722\ldots,\quad c_3=\frac{4\pi[\Gamma(3/4)]^{2/3}}{[\Gamma(1/4)]^2}=1.094\ldots. \tag{2.11}$$

3. LEVEL WIDTH

The level width Γ is defined in terms of the imaginary part of the complex zero of the Jost function[2,5] and can be represented in accord with Ref. 2 in the form

$$\Gamma=\frac{4}{\nu^3h(z_2)}\frac{[1+\exp(-2K)]^{1/2}-1}{[1+\exp(-2K)]^{1/2}+1}. \tag{3.1}$$

Expressions for $K(z_2)$ and $h(z_2)$ are given in Ref. 2.[1)]

For a level far from the top of the barrier, expression (3.1) coincides with the asymptotic Damburg-Kolosov formula[6] at large quantum numbers, if their factorials are expressed by using Stirling's formula.

In the case of a level close to the top of the barrier, expression (3.1) agrees with the exact solution of the standard problem for a parabolic barrier.

For the boundary level $z_2=1$ it follows from the equations of Ref. 2 that

$$K=0,\quad h(1)=\sqrt{2}(d+\ln n_2), \tag{3.2}$$

where

$$d=8\ln 2-4/3-\ln(32/3\pi)-\psi(1/2)\approx 5, \tag{3.3}$$

and ψ is the logarithmic derivative of the gamma function. Recognizing that

$$\frac{4}{\sqrt{2}}\frac{\sqrt{2}-1}{\sqrt{2}+1}\approx\frac{1}{2}$$

we have

$$\Gamma=1/2\nu^3(5+\ln n_2). \tag{3.4}$$

We note also that it follows from (3.4) that

$$\Gamma/E=1/\nu(5+\ln n_2). \tag{3.5}$$

4. COMPARISON WITH THE RESULTS OF REF. 1.

We compare now our present results with the corresponding equations of Ref. 1. It must be recognized here that our n_1 is designated n_2 in Ref. 1, and our n_2 by n_1.

1. Kadomtsev and Smirnov[1] calculated a quantity $\mathscr{E}n^4$ equal to $T/4$. When this is taken into account, our Eq. (2.8) agrees fully with the results of Ref. 1. Our Eq. (2.10) differs from the corresponding result of Ref. 1 in that it contains the factor

$$[1-a_2(n_2/n)^{2/3}]^6.$$

2. In Ref. 1 they calculated the quantity En^2, i.e., $(1/2)(n/\nu)^2$ in our notation. A comparison of the results shows that their Eq. (10b) contains an obvious misprint, viz., 2^7 in place of 2^6. Equation (11 b) of Ref. 1 does not contain the factor

$$[1-\mathrm{const}(n_2/n)^{2/3}]$$

which follows from our Eq. (2.11). In addition, the coefficient

$$\frac{64}{9\pi^2}\left[\Gamma\left(\frac{7}{4}\right)\Big/3\sqrt{\pi}\,\Gamma\left(\frac{5}{4}\right)\right]^{8/3},$$

contained in Eq. (11b) of Ref. 1 does not agree with the indicated numerical value 1.48. Comparison with our Eq. (2.11) shows that the literal expression for this coefficient is incorrect, but the numerical value is correct and agrees with that following from our Eq. (2.11).

3. The lifetime calculated in Ref. 1 is $\tau = 1/\Gamma$. For the top level, according to Eq. (2.1) of Ref. 1, we have in our notation

$$\tau = \frac{1}{\sqrt{2}\mathscr{E}^{3/4}} \ln(2^{3/2}\nu),$$

whereas our Eq. (3.4) yields

$$\tau = 2\nu^3(5 + \ln n_2).$$

In the particular case $n_1 \ll n$ the result of Ref. 1 can be reduced to the form

$$\tau = Bn^3(A + \ln n).$$

Our equation can be reduced to the same form. The constants, however, differ substantially.

It follows from Ref. 1 that $A = 0.857$, $B = 3.27$, whereas our values are $A = 5$, $B = 1.156$. It is possible that the discrepancy is due to the fact that the calculation in Ref. 1 is with logarithmic accuracy, and in addition, cannot be matched to the asymptotic formula of Ref. 6 in the region where the latter is valid.

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[1)]We call attention to the following misprints in Ref. 2: A factor 1/8 was left out from the term $z_2(1+z_2)$ in Eqs. (5.4) and (5.7). The value 6 in expression (5.13) for $h(1)$ should be replaced by $8 \ln 2 - 4/3$. A factor π was left out of the expression for the mean distance between the levels.

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