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A NEW APPROACH TO THE STARK EFFECT IN HYDROGEN

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Abstract

A new iteration procedure for the studying of the Stark effect in hydrogen is proposed. The method is very accurate numerically for any value of the electric field strength. The approximate explicit expression obtained for the ground state energy eigenvalue has analytic properties similar to those known for the exact solution.

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The hydrogen atom behaviour in an electric field was recently subjected to a considerable attention [1-9]. For small values of the field strengh E the perturbation expansion in powers of E gives sufficiently accurate results. This power series is known [5,10] to be divergent, however, and for $E > 0.1$ a.u. the perturbation theory does not work. The Stark splitting calculations outside the framework of the perturbation theory were done with various numerical methods [6-9] being in mutual contradiction for $E \gtrsim 0.15$ a.u.

In what follows we will describe a new iteration procedure which results in analytic expressions for the energy eigenvalues and are applicable to strong as well as to weak fields. We confine ourselves here to the calculation of the shift and width of the ground state energy level. The method can be easily generalized to the exited states too. Our results agrees with the numerical calculation of ref.[7].

In essential features the method presented coincides with that of ref. [11] where it was applied to the one dimentional anharmonic oscillator problem.

The Schrödinger equation for hydrogen atom in external electric field is

$$\left(\frac{\Delta}{2} + \varepsilon + \frac{1}{r} - Ez\right)\psi = 0 \qquad (1)$$

where ε is the energy and E is the electric field strength in atomic units. In terms of the parabolic coordinates $\xi = r + z$ and $\eta = r - z$ eq. (1) is splitted into two equations for the ground state wave

function (see e.g. ref. [12])

$$\xi F'' + F' + \left(\frac{1}{2}\varepsilon\xi - \frac{1}{4}E\xi^2 + \alpha\right)F = 0, \tag{2a}$$

$$\eta G'' + G' + \left(\frac{1}{2}\varepsilon\eta + \frac{1}{4}E\eta^2 + \beta\right)G = 0 \tag{2b}$$

where the substitution $\Psi = F(\xi)G(\eta)(\xi\eta)^{-1/2}$ was made. The separation constants α and β satisfy the condition

$$\alpha + \beta = 1. \tag{3}$$

Function G and parameter β are the analytic continuations in E of F and α respectively:

$$G(E) = F(-E) \quad \text{and} \quad \beta(E) = \alpha(-E). \tag{4}$$

The basic point is the dealing with the Riccati equation instead of eq. (2a). By the substitution $f = F'/F$ we obtain

$$f' + f^2 + \frac{1}{4\xi^2} + \frac{\varepsilon}{2} - \frac{E\xi}{4} + \frac{\alpha}{\xi} = 0. \tag{5}$$

A perturbation theory for this equation is developed. As the zero order approximation we chose the function

$$f_0 = \frac{1}{2\xi} - \frac{1}{2}\sqrt{1 + E\xi} \tag{6}$$

which tends to the exact solution when $\xi \to \infty$ and $\xi \to 0$. The deviation of $f(\xi)$ from $f_0(\xi)$ being small, the perturbation series is constructed with subsequent neglect of the nonlinear term in eq. (5). We define

$$f(\xi) - f_0(\xi) = \sum_{n=1}^{\infty} f_n(\xi), \quad \alpha = \sum_{n=1}^{\infty} \alpha_n, \quad \varepsilon = \sum_{n=1}^{\infty} \varepsilon_n \tag{7}$$

where $f_n(\xi)$, α_n and ε_n are determined order by order through the following recurrent relations

$$f_1' + f_n\left(\frac{1}{\xi} - \sqrt{1+E\xi}\right) = \varkappa_n - \frac{\alpha_n}{\xi} - \varphi_n(\xi) \quad (8)$$

Here $\varkappa_n = -(2\varepsilon_n + \delta_{n1})/4$, $\varphi_1(\xi) = -\sqrt{1+E\xi}/2\xi - E/4\sqrt{1+E\xi}$ and $\varphi_n = \sum_{\ell=1}^{n-1} f_\ell(\xi)\, f_{n-\ell}(\xi)$ for $n > 1$.

The solution of eq (8) vanishing as $\xi \to \infty$ is

$$f_n(\xi) = -\frac{1}{\xi}\exp\{K(\xi)\}\int_{\xi}^{\infty} dt\, t\, e^{-K(t)}\left\{\varkappa_n - \varphi_n(t) - \frac{\alpha_n}{t}\right\} \quad (9)$$

where $K(t) = (2/3E)(1+Et)^{3/2}$. From the condition $\xi f_n(\xi) \to 0$ as $\xi \to 0$ the parameter α_n can be found:

$$\alpha_n = \langle t(\varkappa_n - \varphi_n)\rangle \quad (10)$$

where the notation is introduced

$$\langle\varphi\rangle = \int_0^{\infty} dt\, e^{-K(t)}\varphi(t) \Big/ \int_0^{\infty} dt\, e^{-K(t)}.$$

Using conditions (3) and (4) we find for the separate terms in the energy eigenvalue expansion

$$\varkappa_n = \frac{\langle t\varphi_n\rangle + \overline{\langle t\varphi_n\rangle} + \delta_{n1}}{\langle t\rangle + \overline{\langle t\rangle}} \quad (11)$$

where δ_{n1} is the Kronecker symbol and the bar means analytic continuation from E to (-E). Recall that $\varepsilon_n = -(\delta_{n1}/2) - 2\varkappa_n$.

The coefficients $\varkappa_n$ are complex and determine the shift as well as the width of the ground state energy level of hydrogen atom. The expansion of $\sum \varkappa_n$ in powers of E reproduces the standard series of perturbation theory, each term of this being determined by a finite number of

$\varkappa_n$'s . Imaginary part of $\varkappa_n$ is exponentially small when $E \to 0$ and differs from the quasiclassical expression [10] in *nonexponential* factor only. For large field values it follows from eq. (11) that

$$\varkappa_n = C_n e^{-i\pi/3} E^{2/3} \left\{ 1 + O(E^{-1/3}) \right\} \qquad (12)$$

where $C_1 = -\frac{1}{2}\left(\frac{3}{2}\right)^{2/3} / \Gamma(4/3)$ and $C_2 \simeq 0.2\, C_1$.

If the series $\sum C_n$ were convergent, the result (12) would be in contradiction to that of ref. [5] where it was claimed that $\varkappa \sim E^{2/3} \ln E$. We can show that our procedure is convergent for sufficiently small E and it seems probable that it is convergent for large E too. In the latter case, however, we failed to get a rigorous proof.

Numerical results for the energy shift and the width of the ground state are presented in figs. 1 and 2 respectively, first two orders of the described iterative procedure being taken into account. In fig. 3 the ratio of the second order term to the first order one for real and imaginary parts of the energy eigenvalue are presented. These ratios are small and so the method proved to be numerically accurate. There is some increase of these ratios at larger values of E; eq. (12) shows however that asymptotically, as $E \to \infty$, the ratio of ε_2 to ε_1 is about 0.2.

The application of this method to the higher levels of hydrogen atom will be published elsewhere.

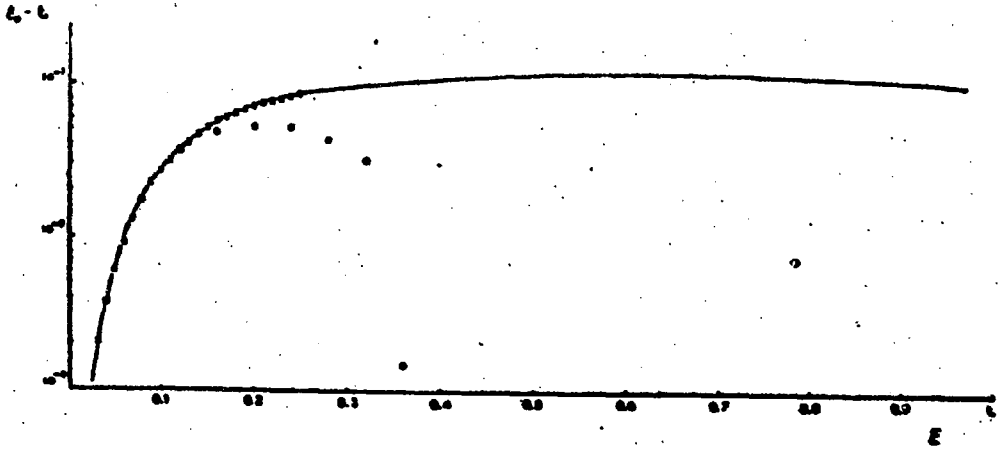

Fig. 1. Ground state energy shift vs.electric field $\mathcal{E}$ $(\mathcal{E}_0 = -1/2)$. The numerical results of ref. [7] are shown by crosses, that of ref. [9] are shown by circles. The solid curve is our result.

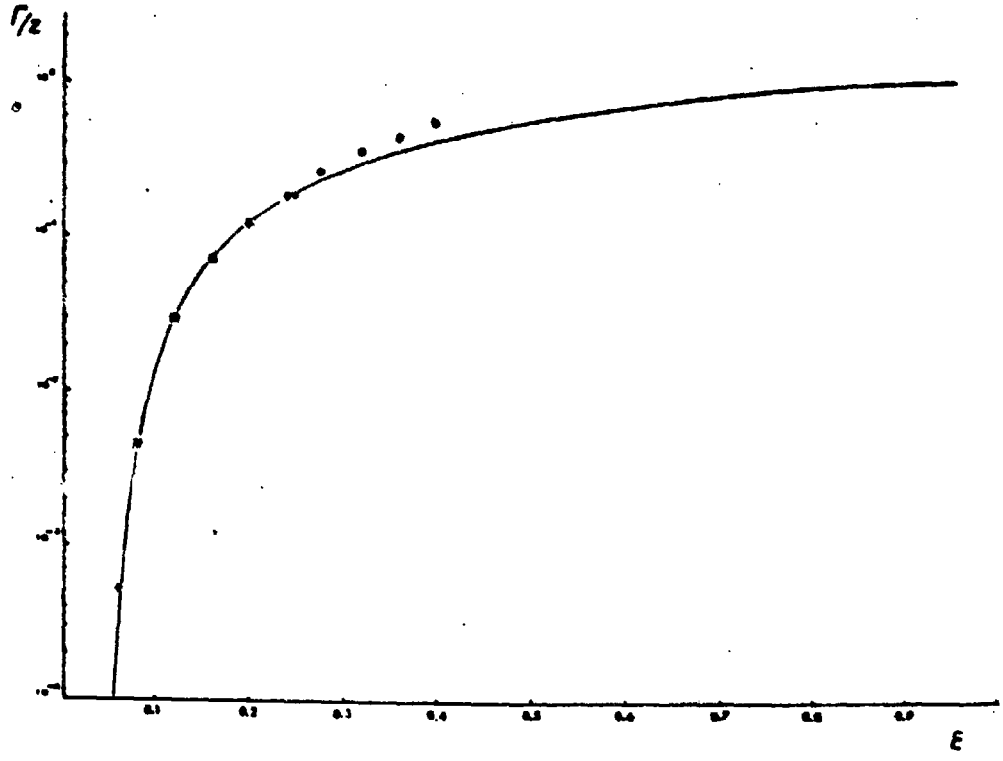

Fig. 2. Width of the ground state level vs.electric field E . The notations are the same as in fig.2.

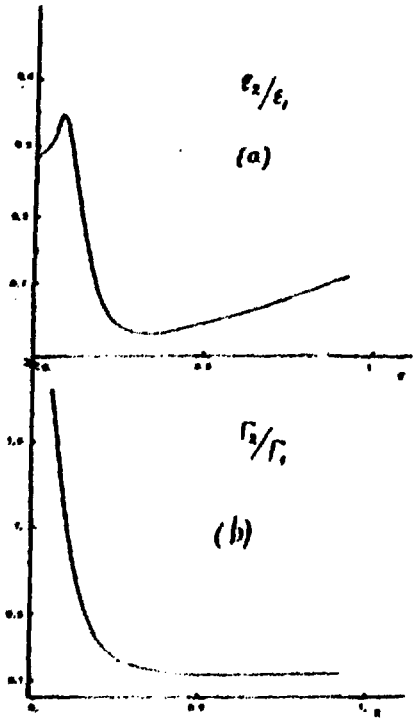

Fig. 3. The ratio of the second order term to the first order one for the shift and width ((a) and (b) respectively).

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