HYDROGEN ATOM IN A STRONG UNIFORM ELECTRIC FIELD: MODIFIED OPERATOR PERTURBATION THEORY METHOD

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The shifts and widths of the Stark resonances for hydrogen atom in a uniform electric field are calculated within the modified operator perturbation theory. We have studied the influence of the electric potential model function choice in the operator perturbation theory on the values of the resonance energies and widths. It is shown that the use of an asymptotically correct, new form for the electric potential model function in the operator perturbation theory calculation scheme leads to a quite reasonable agreement of theory with experiment and does not significantly change the final results for resonance characteristics. The comparison of the calculated Stark resonance widths and shifts with other theoretical and experimental data is presented.

Calculation of characteristics of atom in a strong electric field remains very important problem of modern atomic physics [1–21]. As it is well known, external electric field shifts and broadens the bound state atomic levels. The standard quantum-mechanical approach relates complex eigenenergies (EE) $E = E_r + 0.5iG$ and complex eigenfunctions (EF) to the shape resonances. The calculation difficulties in the standard quantum-mechanical approach are well known. The WKB approximation overcomes these difficulties for the states, lying far from the "new continuum" boundary and, as a rule, is applied in the case of relatively weak electric field. The same regards the widespread asymptotic phase method [2, 3], based on the Breit-Wigner parameterisation for the phase shift dependence on scattering energy. Some modifications of the WKB method are introduced in [9, 19, 20]. Quite different calculation procedures are used in the Borel summation of the divergent perturbation theory (PT) series [4] and in the numerical solution of the differential equations following from the expansion of the wavefunction over a finite basis [1, 17, 21]. In [7] a consistent uniform quantum-mechanical approach to the non-stationary state problems solution including the Stark effect and scattering problems has been developed. The essence of the method is the inclusion of the well known method of "distorted waves approximation" in the framework of the formally exact PT. The zeroth-order Hamiltonian H_0 of this PT corresponds only to stationary bound and scattering states. To overcome formal difficulties, the zeroth-order Hamiltonian was defined by a set of orthogonal EF and EE without specifying the explicit form of the corresponding zeroth-order potential. In the case of the optimal zeroth-order spectrum , the PT smallness parameter is of the order of G/E, where G and E are the field width and bound energy of the state level. One can see that $G/E \le 1/n$ even in the vicinity of the "new continuum" boundary (n is the principal quantum number). This method is called the operator PT (OPT) method [7]. It is very important that the Hamiltonian H_0 is defined so that it coincides with the total Hamiltonian H at $\varepsilon \Rightarrow 0$. ($\varepsilon$ is the electric field strength). Note that perturbation in OPT [7] does not coincide with the electric field potential though they disappear simultaneously. The present paper is devoted to the calculation of the Stark resonance energies and widths for hydrogen atom in a uniform electric field on the basis of OPT method and studying the problem of

influence of the corresponding electric potential model function choice on the values of energies and widths. We will show that the use of an asymptotically correct, new form for the electric potential model function results in a quite reasonable agreement of theory with experiment and does not significantly change the final results for the resonance shifts and widths.

As usually, the Schrödinger equation for the electron function with taking into account the uniform electric field and the field of the nucleus (Coulomb units are used: 1 unit is $h^2/Ze^2 m$; for energy 1 unit is $mZ^2 e^4/h^2$) is given by (Coulomb units are used: a unit of $h^2/Ze^2 m$ and a unit of $mZ^2 e^4/h^2$ for energy)

$$[-(1 - N/Z)/r + \varepsilon z - 0{,}5\Delta - E]\,\psi = 0\,, \quad (1)$$

where E is the electron energy, Z — the nucleus charge, N — the number of electrons in atomic core. Here we only deal with the hydrogen atom, i.e. Z=1, N=0. After the separation of variables equation (1) in parabolic coordinates is transformed into a system of two equations for the functions f, g:

$$f'' + \frac{|m|+1}{t} f' + [0{,}5E + \\ + (\beta_1 - N/Z)/t - 0{,}25\,\varepsilon(t)\,t]\,f = 0 \quad (2)$$

$$g'' + \frac{|m|+1}{t} g' + [0{,}5E + \\ + \beta_2/t + 0{,}25\,\varepsilon(t)\,t]\,g = 0 \quad (3)$$

coupled through the constraint on the separation constants: $\beta_1+\beta_2$= 1. For the uniform electric field $\varepsilon(t) = \varepsilon$. The potential energy in equation (4) has the barrier. Two turning points for the classical motion along the η axis, t_1 and t_2 , at a given energy E are the solutions of the quadratic equation ($\beta = \beta_1, E = E_0$). In [7] the uniform electric field ε in (3) and (4) was substituted by a model function $\varepsilon(t)$ with a parameter τ (τ = 1.5 t_2). Here we use another function, which satisfies the required asymptotic conditions [7]:

$$\varepsilon(t) = \frac{1}{t}\,\varepsilon\left[(t-\tau)\frac{\tau^2}{\tau^2+t^2} + \tau\right], \quad (4)$$

The final results do not depend on the parameter τ .To calculate the width G of the specific quasi-stationary state in the lowest PT order one should know two zeroth-order EF of H_0: the bound state function Ψ_{Eb} (ε, ν, φ) and the scattering state function Ψ_{Es} (ε, η, φ) with the same EE. First, one has to determine the EE of the expected bound state. It is the well known problem of state quantification in the case of the penetrable barrier. Following Ref. [7], we solve the system of (2 , 3) with the total Hamiltonian H under the conditions:

$$f(t) \to 0 \text{ at } t \Rightarrow \infty \text{ and } \partial x(\beta, E)/\partial E = 0 \quad (5)$$

with

$$x(\beta, E) = \lim_{t\Rightarrow\infty} [\,g2\,(t) + \{g'(t)/\mathrm{k}\}2\,]\,t|\,m| + 1.$$

These two conditions quantify the bound energy E, the separation constant β_1. The further procedure for this two-dimensional eigenvalue problem results in solving the system of ordinary differential equations (2, 3) with probe pairs of E, β_1. The bound state EE, eigenvalue β_1 and EF for the zeroth-order Hamiltonian H_0 coincide with those for the total Hamiltonian H at $\varepsilon \Rightarrow 0$, where all the states can be classified due to the quantum numbers: n, n_1 , n_2 , m (principal, parabolic, azimuthal) that are related to E, β_1, m by the well known expressions. We preserve the n, n_1 ,m states classification in the $\varepsilon \neq 0$ case . The scattering state functions must be orthogonal to the above defined bound state function and to each other. According to the OPT ideology [7], the following form of $g_{E's}$:is possible:

$$g_{E's}(t) = g_1\,(t) - z_2'\,g_2(t) \quad (6)$$

with $f_{E's}$, and $g_1(t)$ satisfying the differential equations (2) and (3). The function g_2(t) satisfies the non-homogeneous differential equation, which differs from (3) only by the right hand term, disappearing at $t \Rightarrow \infty$. The coefficient z_2' ensures the orthogonality condition and can be defined as

$$z_2' = \{ \iint d\zeta d\eta\, (\zeta+\eta) f^2_{Eb}(\zeta) g_{Eb}(\eta) g_1(\eta) \} / \{ \iint d\zeta d\eta\, (\zeta+\eta) f^2_{Eb}(\zeta) g_{Eb}(\eta) g_2(\eta) \}$$

The imaginary part of the state energy in the lowest PT order is

$$\mathrm{Im}\, E = G/2 = \pi \langle \Psi_{Eb} | H | \Psi_{Es} \rangle$$

with the total Hamiltonian H. The state functions Ψ_{Eb} and Ψ_{Es} are assumed to be normalized to unity and by the $\delta(k - k')$-condition , respectively. The whole calculation procedure at known resonance energy E and separation parameter β has been reduced to the solution of one system of the ordinary differential equations.

Table 1. The energies and widths of Stark resonances of the hydrogen atom:
Notation: a – [7]; b – [2]; c – [13]; d – [1]; e – [21]; f – [19]; g – the present paper.

$(n\, n_1\, n_2\, m)$	ε	Method	E_r (at.units)	G (at.units)
2 0 1 0	0.005	G	O.1425	0.101×10^{-3}
	0.005	A	O.1426	0.102×10^{-3}
		C	O.1426	0.106×10^{-3}
		E	O.1426	0.106×10^{-3}
2 0 1 0	0.010	g	O.1660	0.107×10^{-1}
		a	O.1661	0.108×10^{-1}
		c	O.1661	0.109×10^{-1}
		d	O.1661	0.109×10^{-1}
		e	O.1661	0.109×10^{-1}
2 0 0 1	0.005	g	0.1270	0.266×10^{-4}
		A	0.1272	0.267×10^{-4}
		C	0.1272	0.262×10^{-4}
		E	0.1272	0.262×10^{-4}
2 0 0 1	0.010	G	0.1342	0.636×10^{-2}
		A	0.1345	0.637×10^{-2}
		C	0.1345	0.628×10^{-2}
		e	0.1345	0.628×10^{-2}
2 0 1 0	1.8×10^{-4}	g	0.2061	0.277×10^{-5}
		A	0.2062	0.278×10^{-5}
		b	0.2062	0.228×10^{-5}
		d	0.2062	0.228×10^{-5}
		f	0.2062	0.222×10^{-5}

The calculation results for some states of the hydrogen atom are presented in Table 1. For comparison we have shown the similar data, obtained within another approaches: the WKB-approximation, the summation of divergent PT series, the numerical solution of the differential equations, standard OPT [1–3, 7, 19, 21]. One can see that there is a reasonable agreement between theory and experiment. It is important to note that the use of a new, asymptotically correct form for the electric potential model function within the OPT method does not significantly change the final values of the Stark resonance energies and widths.

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АТОМ ВОДНЮ В СИЛЬНОМУ ОДНОРІДНОМУ ЕЛЕКТРИЧНОМУ ПОЛІ: МОДИФІКОВАНИЙ МЕТОД ТЕОРІЇ ЗБУРЕНЬ

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На основі модифікованої операторної теорії збурень розраховано енергії та ширини штарківських резонансів для атома водню в однорідному електричному полі. Досліджено вплив вибору форми модельної функції для електричного потенціалу в операторній теорії збурень на значення енергій та ширин резонансів. Показано, що використання асимптотично коректної, нової форми модельної функції для електричного потенціалу в операторній теорії збурень дає добре узгодження теорії з експериментом і не змінює суттєво остаточних результатів для характеристик резонансів. Наведено порівняння значень розрахованих зсувів та ширин штарківських резонансів з іншими теоретичними та експериментальними даними.