

**Stark resonances of the Yukawa potential: Energies and widths, crossings and avoided crossings**

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The resonance energy spectrum of a system interacting with the Yukawa potential and embedded in an external homogeneous and static electric field is investigated. The positions and widths of levels have been computed by using the complex coordinate rotation method. Interesting avoided-crossing and crossing effects appear.

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**I. INTRODUCTION**

The influence of a static electric field on the hydrogen atom has been one of the most investigated subjects. For a review of this problem see [1–7]. Bound and resonance states supported by the Yukawa potential, in which the Coulomb attraction is shielded, have also been investigated [8–13]. It seems, however, that the problem of both the shielding and the electric-field effects on the hydrogen atom has only been considered for the ground state [14]. In this work we extend the investigation of both the screening of the Coulomb attraction, described by the Yukawa potential, and the effect of a homogeneous static field to excited states.

General expectation as regards the solution for the energy spectrum of such a system is rather obvious: There are no strict discrete levels, i.e., no strictly bound states. There are broadened levels instead, corresponding to resonances of finite lifetime. The degeneracy characteristic to the isolated hydrogen atom is removed by both the shortening of the potential and by the electric field. The split levels are shifted either down or up by the electric field. This causes levels that originate from different field-free levels to meet one another and interact. Following the bound-state-based intuition one can expect avoided crossings in such cases. However, since the broadened resonance levels are represented by complex energies, the positions of levels may also cross. The problem of crossings and avoided crossings in the context of the Stark effect in a hydrogen atom has been investigated for several decades [15–17]. The papers of Rotter and coworkers [16,17] indicate that, in general, for quantum systems embedded in a continuum the complex energies may cross either in the real or imaginary part, including a possibility of complex degeneracy. Our computations revealed many energy crossing cases with no interaction of widths and a few cases of strong interaction causing avoided crossings either in energy or width.

The paper is organized as follows: In Sec. II the method involving the complex coordinate rotation technique is described. This includes details on the basis set used and convergence of computations. In Sec. III the results are discussed. The paper is summarized in Sec. IV.

**II. METHOD OF COMPUTATION**

We consider an axially symmetric system of one particle subjected to the Yukawa potential and an external homogeneous static electric field of strength  $F$ . This may correspond

to the Stark problem of a hydrogen atom in a medium that screens the Coulomb interaction. The system is described by the Hamiltonian (in a.u.)

$$\hat{H} = -\frac{1}{2}\nabla^2 - \frac{e^{-\lambda r}}{r} + Fz. \quad (1)$$

Because of the field term the energy continuum covers the whole range from  $-\infty$  to  $+\infty$ . The zero of the energy scale is kept at the continuum threshold of the field-free system.

We compute resonance energy levels (embedded in the continuum) and their widths by using the complex coordinate rotation (CCR) technique [18], which has been applied to the Stark problems for over three decades [1]. The coordinate vector  $\vec{r}$  is transformed to  $e^{i\theta}\vec{r}$ . Hence, instead of the Hamiltonian given in Eq. (1) we have a non-Hermitian operator

$$\hat{H}(\theta) = -e^{-i2\theta}\frac{1}{2}\nabla^2 - e^{-i\theta}\frac{1}{r}e^{-\lambda r e^{i\theta}} + e^{i\theta}Fz. \quad (2)$$

The spectrum of such an operator consists of complex eigenvalues, which are  $\theta$  dependent. However, among them there are some eigenvalues independent of  $\theta$  in a range of  $\theta$ . They are isolated in the complex plane and therefore they are easy to identify. They correspond to resonances. Their imaginary parts are negative and are related to the half widths of the resonance levels. Thus, a resonance eigenvalue is

$$E - i\frac{\Gamma}{2}, \quad (3)$$

where  $E$  is the position of the resonance level and  $\Gamma$  is its width.

We have computed the eigenspectrum of the Hamiltonian (2) by searching for approximate solutions of

$$\hat{H}(\theta)\Psi = \left(E - i\frac{\Gamma}{2}\right)\Psi \quad (4)$$

in a large trial space spanned by 1500 Slater-type orbitals (STO) of angular momentum  $l = 0, \dots, 5$  (250 STOs of each value of  $l$ ) and  $m = 0$ . Since the symmetry is axial (with respect to  $z$  axis), the  $z$  component of the angular momentum is a constant of motion, i.e.,  $m$  is a good quantum number. In this work we consider  $m = 0$  states only. We use STOs of different spherical symmetry (of different  $l$ ) and allow them to mix so as to represent axially symmetric functions. The radial parts of orbitals are of the form

$$\phi_k(r) = r^n e^{-\alpha_k r}, \quad k = 1, \dots, 250. \quad (5)$$

The main question is how the spectrum of resonance levels of such a system changes versus the screening parameter  $\lambda$  or

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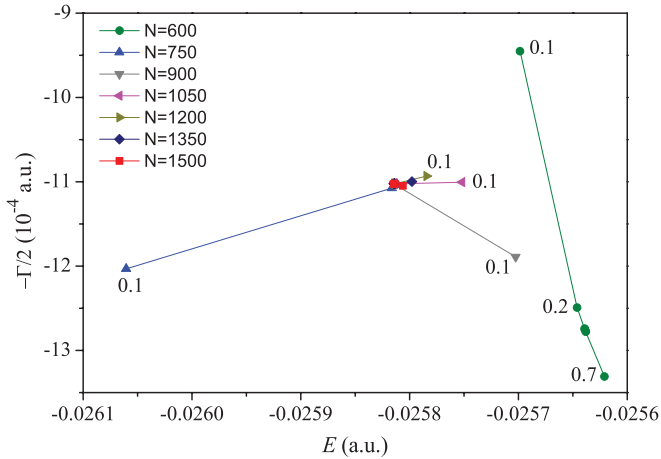


FIG. 1. (Color online) The  $\theta$  trajectories (dependence of a resonance complex eigenvalue on variation of  $\theta$ ) obtained for one of the  $n = 4$  resonances in seven basis sets of different size,  $N$ . Labels at specific points denote values of  $\theta$ . Each  $\theta$  trajectory consists of seven points corresponding to  $\theta = 0.1, 0.2, \dots, 0.7$  ( $F = 0.0015$  a.u.,  $\lambda = 0.01$  a.u.).

versus the field strength  $F$ . Therefore, the computations were performed for various values of  $F$  and several values of  $\lambda$ . For a given set of  $F$  and  $\lambda$ , we built the overlap and  $H(\theta)$  matrices and solved the generalized eigenvalue problem repeatedly for eight equidistant values of  $\theta$  in the range from 0 to 0.7. The resonance energies were identified by searching for complex eigenvalues stable against the variation of  $\theta$ .

The stability of a resonance eigenvalue against the variation of  $\theta$  and the convergence with respect to the size,  $N$ , of the basis set is illustrated in Fig. 1. One can see that with the basis length increasing the  $\theta$  trajectory length decreases, i.e., the  $\theta$  stabilization becomes better, and the eigenvalue converges to a well-defined value. The latter is also shown in Table I. Here one more basis-set result is given, for  $N=450$ . The corresponding  $\theta$  trajectory lies outside the region covered by Fig. 1. The case shown in Fig. 1 and in Table I is a typical one; for all resonances considered in this work the  $\theta$  stabilization and convergence were similar to this case.

TABLE I. Convergence of computations for one of the  $n = 4$  resonances with respect to the number of basis functions,  $N$ . The real and imaginary parts of the complex energy, i.e., the energy position,  $E$ , and half of the width,  $\Gamma/2$ , are given in a.u. The electric-field strength is  $F = 0.0015$  a.u. and the screening is  $\lambda = 0.01$  a.u.

$N$	$-E$	$\Gamma/2$
450	0.0245198	0.00306851
600	0.0256389	0.00110536
750	0.0258126	0.00110365
900	0.0258140	0.00110238
1050	0.0258140	0.00110241
1200	0.0258140	0.00110237
1350	0.0258140	0.00110237
1500	0.0258140	0.00110237

TABLE II. The energy,  $E$ , and width,  $\Gamma$ , of the  $n = 1$  Stark resonance of a hydrogen atom for various values of the dc field strength,  $F$  (all quantities in a.u.; (-x) denotes  $\times 10^{-x}$ ).

$F$	Reference	$-E$	$\Gamma/2$
0.05	This work	0.506105	0.38715(-4)
	[4,6]	0.506105	0.38592(-4)
0.07	This work	0.513077	0.92386(-3)
	[7]	0.513077	0.92358(-3)
0.1	This work	0.527418	0.72695(-2)
	[4,6]	0.527418	0.72690(-2)
	[7]	0.527419	0.72683(-2)
0.15	This work	0.551063	0.30021(-1)
	[7]	0.551067	0.30020(-1)
0.2	This work	0.570124	0.60612(-1)
	[4,6]	0.570124	0.60614(-1)
	[7]	0.570145	0.60600(-1)
0.3	This work	0.596729	0.13065
	[7]	0.596701	0.13059
0.5	This work	0.623116	0.27976
	[4,6]	0.623068	0.27974
	[7]	0.623068	0.28022
0.7	This work	0.630802	0.42893
	[4,6]	0.630711	0.42882
	[7]	0.631312	0.42845
1.0	This work	0.624432	0.64717
	[4,6]	0.624336	0.64682
	[7]	0.626772	0.65332

### III. RESULTS

Before presenting and discussing our results let us explain the notation we use for labeling states. Obviously, when the effects considered here are on, the hydrogenic principal quantum number,  $n$ , is no longer a strict quantum number. Nevertheless, if one increases the electric-field strength and shielding very slowly, one can observe how the hydrogen states labeled with  $n$  (and corresponding energy levels) evolve. In this sense hereafter we use  $n$  to label the states under consideration. Because of possible avoided-crossing disturbances, we mean here proximity of the wave function rather than a continuous character of the level dependence on the field or screening. Briefly, labeling a state with  $n$  means that following the wave function down the shielding and the field to the point where they vanish one ends at a state  $n$  of field-free and screening-free hydrogen.

The computations were done for three screening-parameter values:  $\lambda = 0.001, 0.01, \text{ and } 0.1$  a.u. and for the field strength in the range from 0 to 0.002 a.u. (extended up to 0.05 a.u. for the ground  $n = 1$  state, which responds to the field very weakly). Our aim is to investigate both effects together. However, to show the quality of our results, by their accuracy, we compare them with the literature data for two separate cases: for the screening-free hydrogen atom in an electric static field and for the field-free Yukawa problem. In Tables II, III, and IV our results for energy positions and widths of the ground state and the first excited state are shown together with the results of Kolosov [4], Telnov [6], and Nicolaidis and Themelis [7]. The agreement is satisfactory. In general, our results agree better

TABLE III. The energy,  $E$ , and width,  $\Gamma$ , of one of the  $n = 2$  Stark resonances (the one denoted as  $2s + 2p_0$  in [7]) of hydrogen atom for various values of the dc field strength,  $F$  (all quantities in a.u.; (-x) denotes  $\times 10^{-x}$ ).

$F$	Reference	$-E$	$\Gamma/2$
0.01	This work	0.166093	0.5442(-2)
	[4,6]	0.166094	0.5442(-2)
	[7]	0.166088	0.5448(-2)
0.015	This work	0.187622	0.1688(-1)
	[4]	0.187622	0.1688(-1)
	[7]	0.187636	0.1688(-1)
0.02	This work	0.206684	0.3039(-1)
	[4,6]	0.206682	0.3039(-1)
	[7]	0.206667	0.3041(-1)
0.025	This work	0.224042	0.4483(-1)
	[4]	0.224035	0.4483(-1)
	[7]	0.223978	0.4480(-1)
0.03	This work	0.240157	0.5982(-1)
	[4,6]	0.240147	0.5982(-1)
	[7]	0.240435	0.5984(-1)
0.035	This work	0.255297	0.7522(-1)
	[7]	0.255222	0.7525(-1)
0.04	This work	0.269614	0.9095(-1)
	[4,6]	0.269592	0.9092(-1)
0.05	This work	0.296052	0.1232
	[4,6]	0.296011	0.1231

with those of Kolosov [4] and Telnov [6], whose results are, within the digits given, identical. (The accuracy of Refs. [4,6] is much better than quoted here.) In Table V our results for the bound states of the spherically symmetric Yukawa system are

TABLE IV. The energy,  $E$ , and width,  $\Gamma$ , of one of the  $n = 2$  Stark resonances (the one denoted as  $2s - 2p_0$  in [7]) of the hydrogen atom for various values of the dc field strength,  $F$  (all quantities in a.u.).

$F$	Reference	$-E$	$\Gamma/2$
0.01	This work	0.103893	0.1637(-2)
	[4,6]	0.103894	0.1639(-2)
	[7]	0.103888	0.1632(-2)
0.015	This work	0.096946	0.7540(-2)
	[4]	0.096933	0.7526(-2)
	[7]	0.096899	0.7566(-2)
0.02	This work	0.088950	0.1549(-1)
	[4,6]	0.088983	0.1544(-1)
	[7]	0.088966	0.1539(-1)
0.025	This work	0.080025	0.2419(-1)
	[4]	0.080165	0.2418(-1)
	[7]	0.080177	0.2434(-1)
0.03	This work	0.070473	0.3313(-1)
	[4,6]	0.070723	0.3326(-1)
	[7]	0.069980	0.3279(-1)
0.035	This work	0.060526	0.4207(-1)
	[7]	0.060240	0.4181(-1)
0.04	This work	0.050344	0.5092(-1)
	[4,6]	0.050617	0.5169(-1)
0.05	This work	0.029682	0.6818(-1)
	[4,6]	0.029526	0.6998(-1)

TABLE V. Energies of lower lying bound states of the Yukawa potential.

State	$\lambda$ (a.u.)	$-E$ (a.u.)	
		This work	Ref. [9]
1s	0.1	0.40705863	0.40705803
	0.2	0.32680836	0.32680851
	0.3	0.25763894	0.25763858
	0.5	0.14811689	0.14811702
	1	0.010286071	0.010285789
2s	0.01	0.11529345	0.11529328
	0.02	0.10614875	0.10614832
	0.05	0.081771444	0.081771195
	0.1	0.049928015	0.049928271
	0.2	0.012107881	0.012107865
2p	0.01	0.11524537	0.11524522
	0.02	0.10596377	0.10596339
	0.05	0.080740317	0.080740387
	0.1	0.046534212	0.046534390
	0.2	0.0041019987	0.0041016465
3s	0.025	0.034329318	0.034329509
	0.05	0.019352734	0.019352554
	0.08	0.0077760441	0.0077758770
	0.025	0.034078634	0.034078910
3p	0.05	0.018557569	0.018557751
	0.08	0.0063298847	0.0063299954
	0.025	0.033572948	0.033573122
3d	0.05	0.016914928	0.016915570
	0.08	0.0032484515	0.0032483604
	0.025	0.012503268	0.012503238
4s	0.05	0.0030917043	0.0030916599
	0.025	0.012294315	0.012294320
4p	0.05	0.0025980548	0.0025980588
	0.025	0.011870454	0.011870448
4d	0.05	0.0015808677	0.0015808716
	0.01	0.022099216	0.022098770
4f	0.02	0.014492080	0.014491978

compared with the results of Stubbins [9]. Again the agreement is good. In the worst case the relative difference defined as  $\delta \equiv (E - E_{\text{Stubbins}})/E$  is  $\delta \simeq -4 \times 10^{-5}$ . These results also agree very well with those of Bylicki *et al.* [13].

Tables II, III, IV, and V give an idea about accuracy of our results. Now we present in a graphical form the results for the case where both the screening and the electric field are on. The results for the  $m = 0$  states of  $n = 1, \dots, 5$  are shown in Figs. 2–6, respectively. The first characteristics presented are the energy-level positions plotted as functions of the electric-field strength. One can see how the hydrogen levels split and how they are shifted up by the screening. It seems that this shift is just parallel; i.e., it is field independent. This is an illusion only caused by a low resolution of plots. In Fig. 7 we plot the shift, i.e., the difference

$$\Delta E = E_\lambda(F) - E_{\lambda=0}(F), \tag{6}$$

for levels of  $n = 1, 2, 3$ , for  $\lambda = 0.1$  a.u. It is clearly visible now that the shifts depend on the field in a nonmonotonic way different for different states. Thus there are cross screening-field effects that cause the screening and field effects not to be

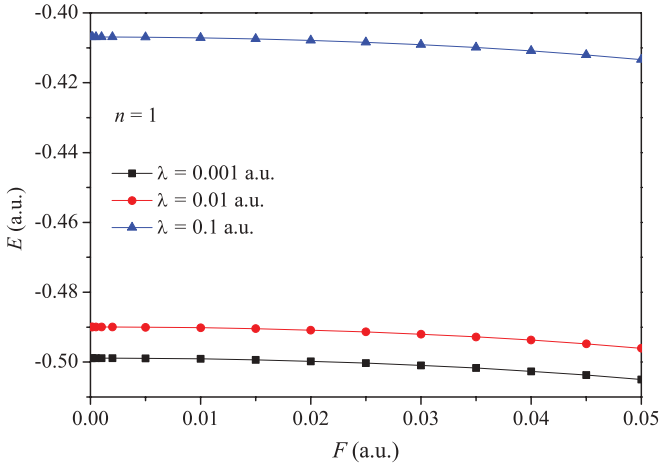


FIG. 2. (Color online) The energy level of the  $n = 1$  Stark resonance as a function of the field strength, for three values of the screening parameter,  $\lambda$ .

additive. The shifts vary in a quite narrow range similar for all states associated with a given  $n$  but different for different  $n$ . Since the screening shortens the range of the potential and decreases its depth, it is rather obvious that the lower the level the higher the shift. Figure 7 shows also clearly the zero-field splitting of levels due to the screening, which is difficult to see in Figs. 3–6.

The widths of levels are shown in the lower panels of Figs. 4, 5, and 6, for states of  $n = 3, 4$ , and  $5$ , respectively. (For  $n = 1$  and  $2$  the widths are extremely small so they are not very interesting; on the other hand they are very difficult to compute accurately.) The plots confirm an obvious expectation that the widths increase significantly as the field and screening increase. Another feature is that within a family of levels of a given  $n$  the less stable, i.e., those having the largest width, are the lowest in energy. For all  $n$ -families of the Stark levels presented in Figs. 4–6 we observe that the lower the level the wider it is. The higher levels are very narrow. Moreover, they seem to be stabilized by the field; i.e., in some ranges their

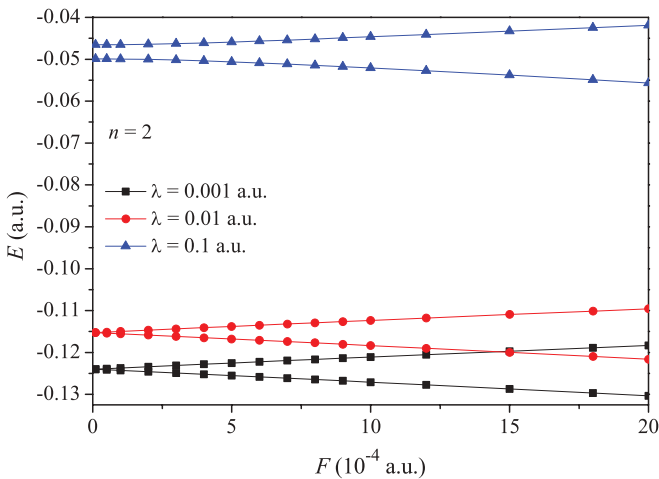


FIG. 3. (Color online) The energy levels of two  $m = 0$  components of  $n = 2$  Stark resonances for three values of the screening parameter,  $\lambda$ .

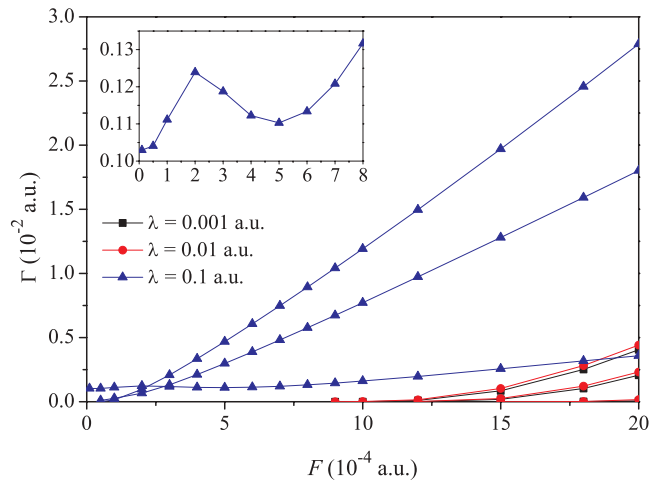
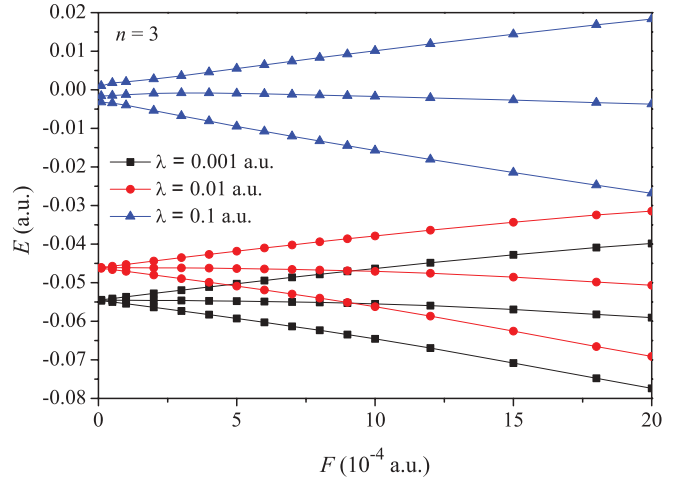


FIG. 4. (Color online) The energy levels (upper panel) and widths (lower panel) of the  $m = 0$  members of the  $n = 3$  family.

widths decrease as the field increases. This can be seen in Fig. 4 and Fig. 6 for  $n = 3$  and  $n = 5$ , respectively (the details are shown in the insets). In the case of  $n = 4$  the effect is not visible in Fig. 5; however, we have checked that it takes place for a stronger field. The fact that the highest Stark components are narrower than the other nearest  $n$ -manifold members was already noticed for highly excited states of hydrogen (no screening) of  $n = 18, \dots, 28$  by Kolosov [5]. The fact that they are narrower than the separation between them even when pushed by the field above the zero-field ionization threshold allowed Kolosov [5] to explain the appearance of sharp resonances observed [3] in the photoionization spectrum in that energy region. Recently, Pawlak *et al.* [19] predicted similar resonances caused by the highest components of the Stark manifolds of  $n = 3, \dots$  for much stronger electric fields.

In Figs. 3–6 the Stark  $n$ -manifolds are shown separately, selected from all other levels present in the spectrum. In fact they are not separated from one another and when the field and screening increase they overlap, causing interesting interactions of levels. In Fig. 8 the Stark  $n$ -families are plotted (for  $\lambda = 0.001$  a.u.) as if the levels that approached one another were simply crossing. It is well known that in most similar diabatic situations such levels should avoid crossings.

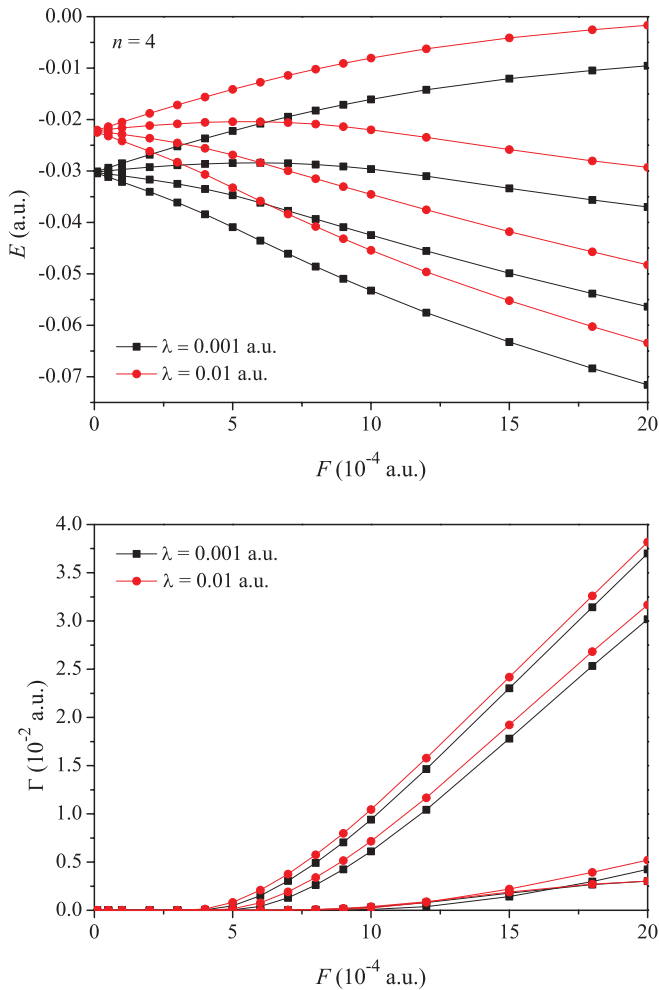


FIG. 5. (Color online) The energy levels (upper panel) and widths (lower panel) of the  $m = 0$  members of the  $n = 4$  family.

However, the states we consider here are resonances and their energies are complex. This opens more possibilities for the behavior of levels at “crossings.” These problems have been studied and are reviewed by Okołowicz, Płoszajczak, and Rotter in [17]. To summarize, such meeting levels do not have to avoid crossing. Their complex energies may avoid degeneracy in the complex plane by repelling in widths. Moreover, in an extreme case, for very specific strength of interaction (though nonzero) between levels they may cross both in energy and width (at the so-called double pole of the  $S$  matrix or a branch-point) [17].

Regarding our results, two typical cases are shown in Figs. 9 and 10 where the energies and widths of two states interacting at approach are plotted against the field strength. An avoided crossing (repelling in energy), typical for a bound state level interaction, is shown in Fig. 9, whereas Fig. 10 contains a crossing (in energy) case where the widths do not cross. It is worth noting that though eventually at the energy crossing point the widths repel each other, in a wider vicinity of the crossing point they attract each other. It should be stated here that in most cases among our results where the widths of two levels approaching in energy are extremely different, as the lowest one of one  $n$ -manifold and the highest one of another

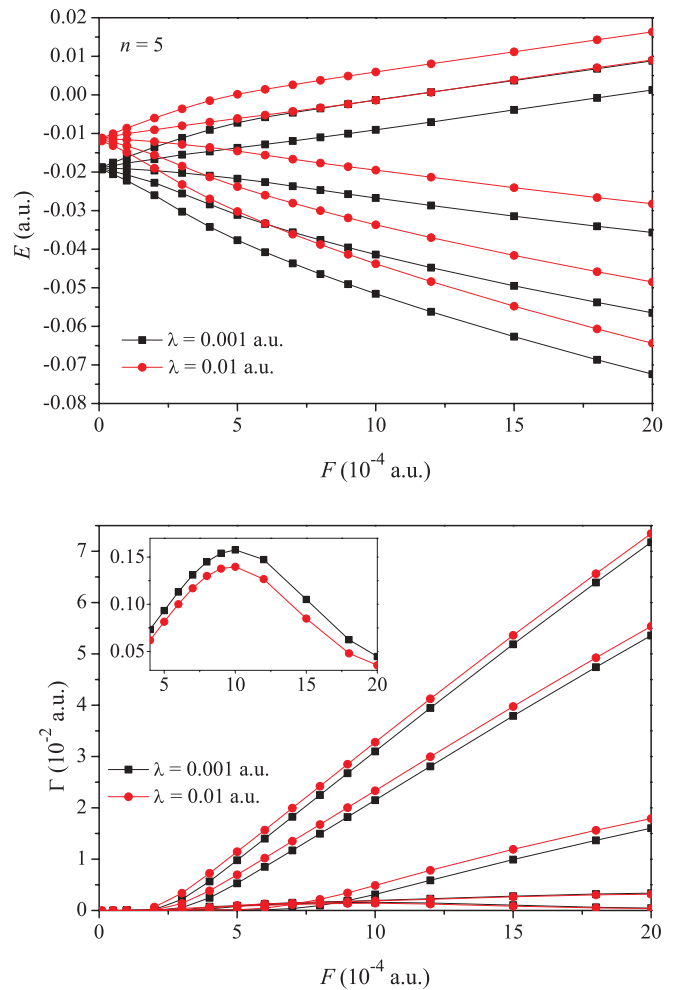


FIG. 6. (Color online) The energy levels (upper panel) and widths (lower panel) of the  $m = 0$  members of the  $n = 5$  family.

$n$ -manifold, the levels do not interact; they simply cross in energy without a visible disturbance of widths.

It is well known that at avoided crossings the wave functions are exchanged so that beyond the interaction region things look like there was no interaction and the levels simply crossed. In Figs. 11 and 12 the wave functions of interacting states are illustrated by partial wave decomposition. The contributions coming from different groups of spherically symmetric orbitals of  $l = 0, \dots, 5$  (from different partial waves) to the normalization unity are plotted there. (It should be mentioned here that due to large trial expansion of 1500 terms, we cannot follow the amplitudes that could give information on how the phase of the wave function changes.) From Fig. 11 one can see that the composition of the wave function does change dramatically at the avoided crossing (one state function takes the form of the other one involved in the avoided crossing), whereas Fig. 12 shows that when the energies are crossing, the wave functions though disturbed significantly in the interaction region return to the form they had before. In both cases the character of the wave function is preserved along the curves plotted in Fig. 8. Due to the resolution of the figures, the avoided crossings are not shown but can be seen in a close-up as that in Fig. 9.

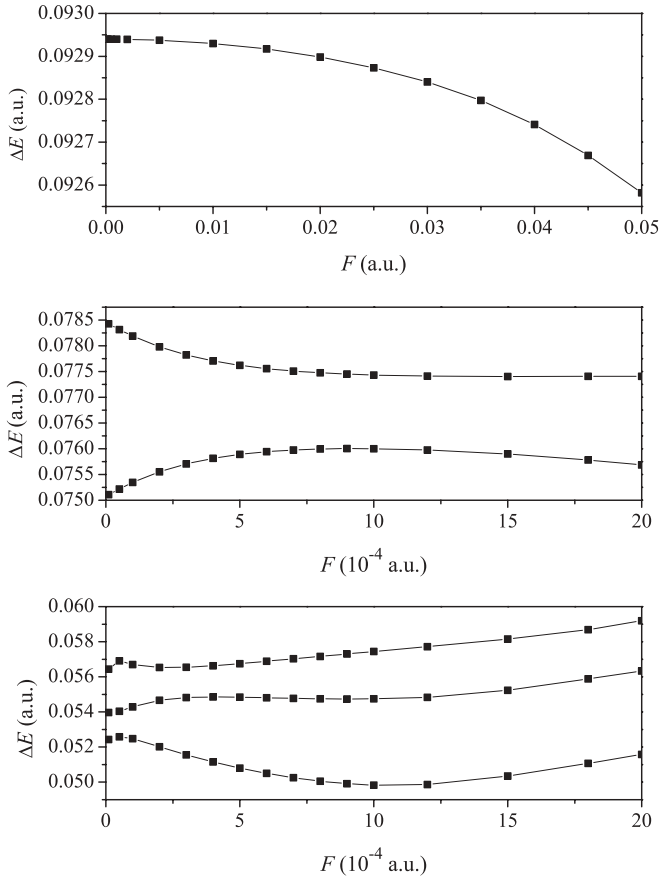


FIG. 7. The energy shift due to the screening at  $\lambda = 0.1$  a.u. defined in Eq. (6) for states of  $n = 1, 2, 3$ .

IV. SUMMARY

Resonances of a charged particle attracted by the Yukawa potential and under the influence of a static homogeneous electric field have been investigated. The energies and widths have been computed by the complex coordinate rotation method for three values of the screening parameter and a field strength in the range up to 0.002 a.u. The  $m = 0$  Stark

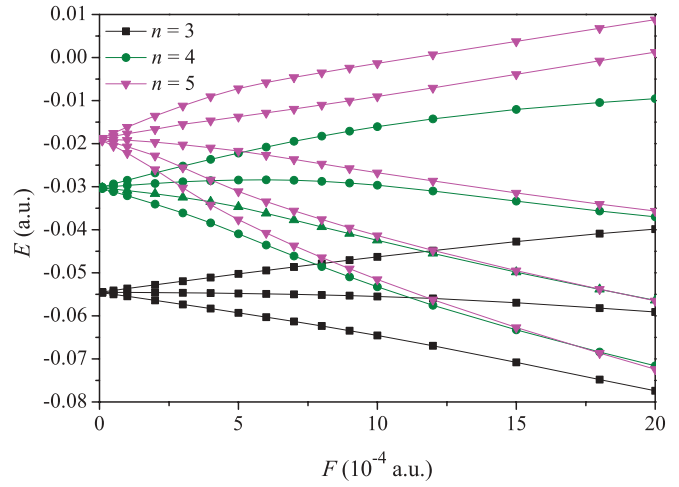


FIG. 8. (Color online) The  $n = 3, 4$ , and  $5$  manifolds of Stark resonances for the screening parameter  $\lambda = 0.001$  a.u.

components of the  $n = 1, \dots, 5$  families of states have been considered. It turned out that the widths are very different within an  $n$ -family of states. The upper components are by an order of magnitude more stable. Moreover, in the case of higher components of  $n$ -manifolds the results exhibit a kind of stabilization, i.e., decrease of the width in a range of field-strength values. It has been found that in contrast to real-energy (bound) states in most cases the energy levels cross with no significant disturbance of widths. Two cases when the levels do interact are presented. One is the avoided-crossing case in which the wave functions and widths of the interacting states are exchanged. The other one is the crossing in energies and avoided crossing in widths. In this case the wave functions and widths of both states involved are preserved outside the interaction region. Although for a very specific value of coupling between the approaching levels a crossing in both energies and widths may occur [17], we have not come across such a situation in the present work. A similar two-parameter case of the hydrogen atom in crossed external electric and

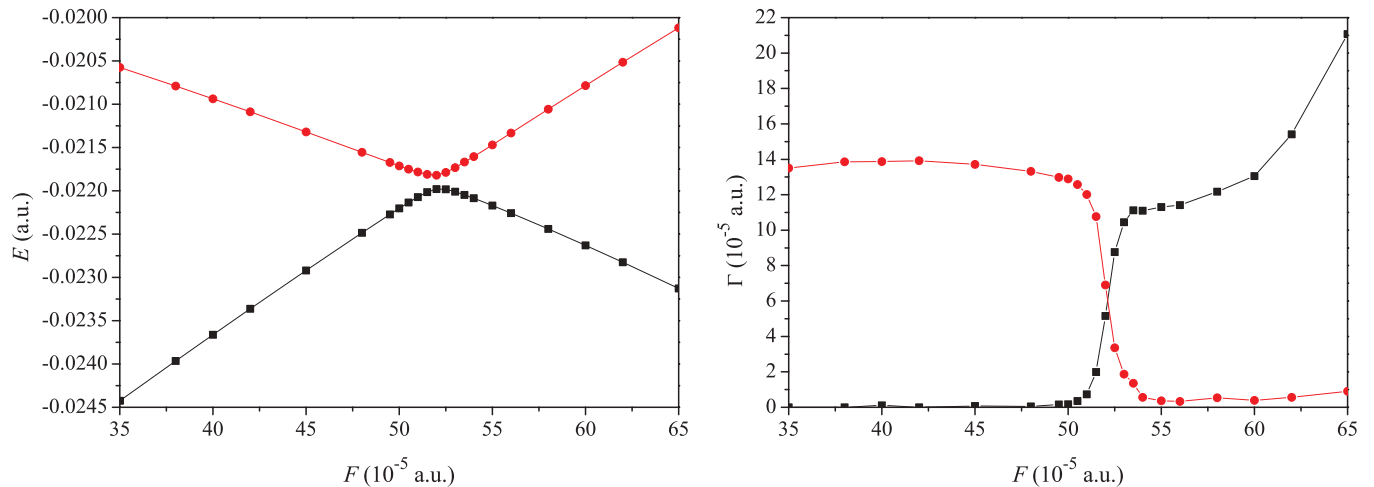


FIG. 9. (Color online) Avoided crossing of the middle Stark component of  $n = 5$  and the highest one of  $n = 4$ .

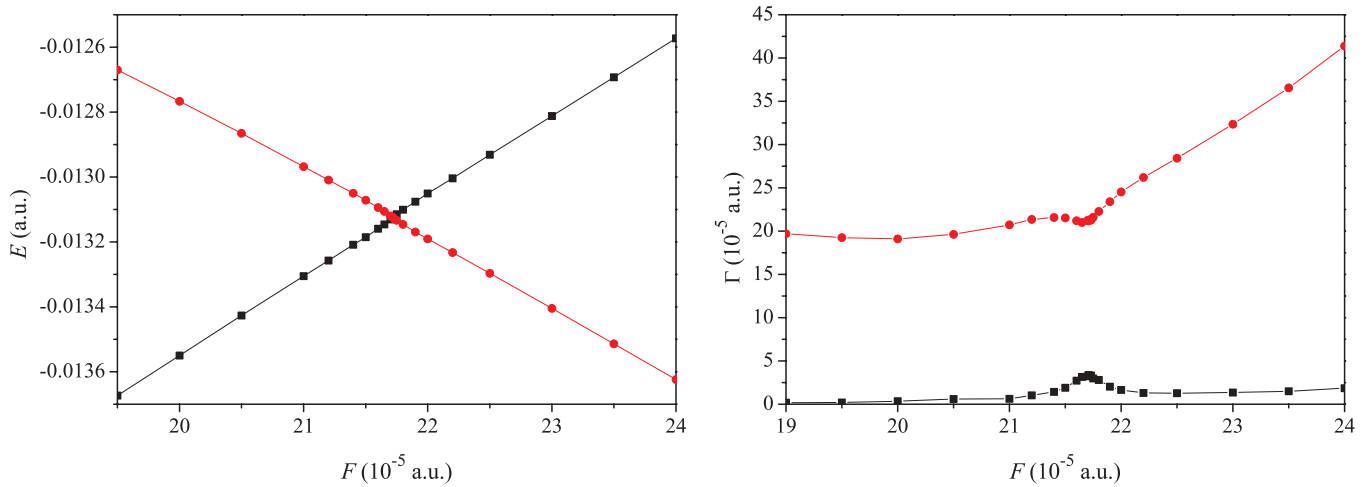


FIG. 10. (Color online) Crossing of the highest Stark component of  $n = 5$  and one of components of  $n > 5$ .

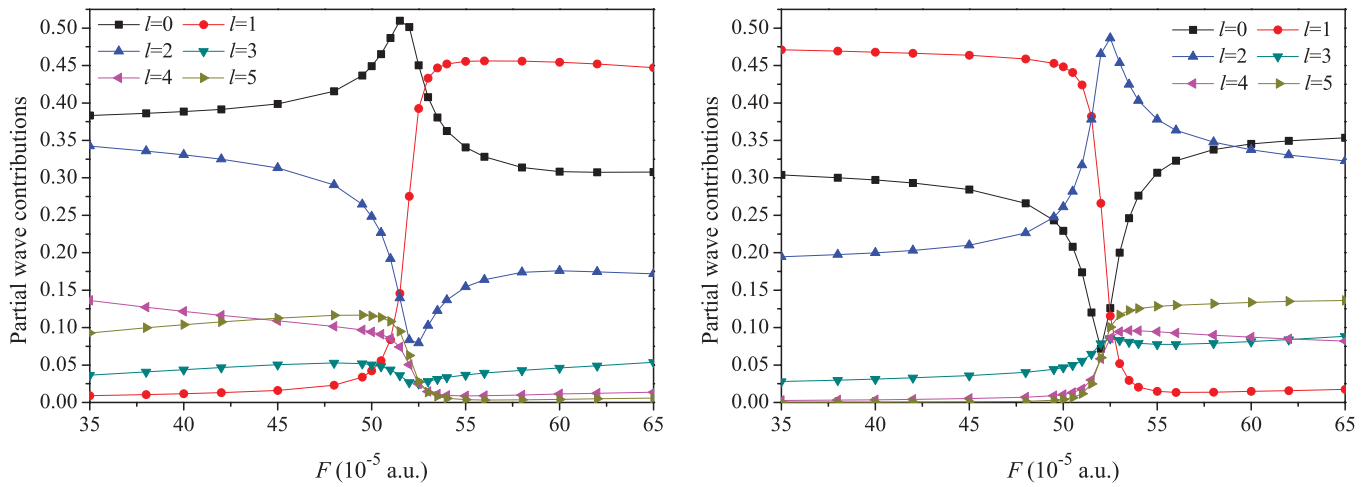


FIG. 11. (Color online) Contributions of spherically symmetric partial waves to the normalization of states that avoid crossing in energy, in Fig. 9. Left panel: The middle Stark component of the  $n = 5$  manifold. Right panel: The highest component of the  $n = 4$  manifold. The character of the wave functions is exchanged.

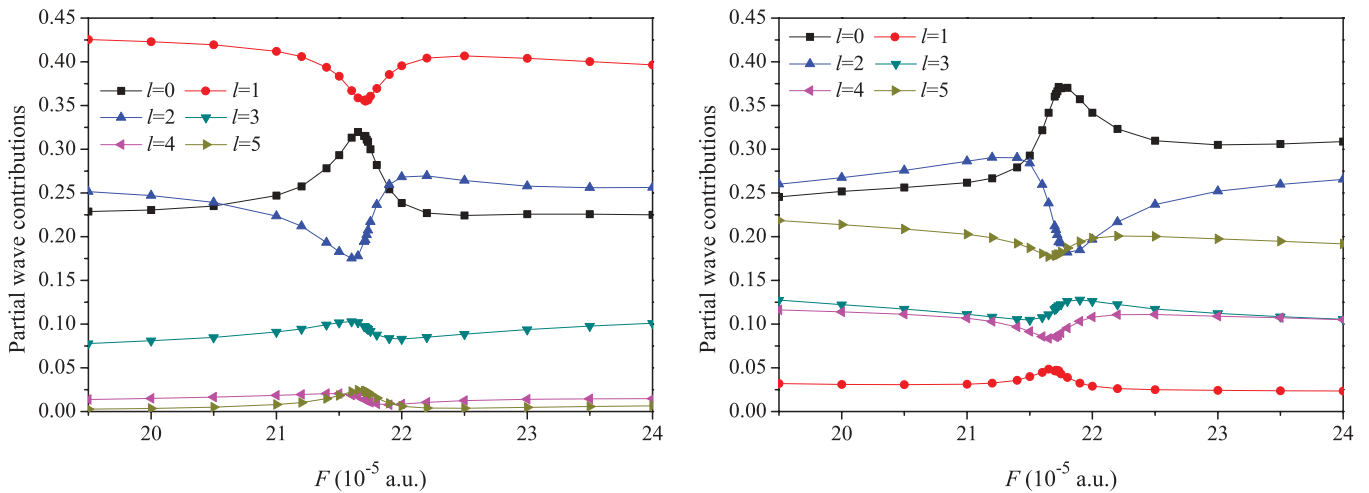


FIG. 12. (Color online) Contributions of spherically symmetric partial waves to the normalization of states whose energy levels cross in Fig. 10. Left panel: The highest Stark component of the  $n = 5$  manifold. Right panel: One of the components of  $n > 5$ . The wave functions character remains almost unchanged after crossing.

magnetic fields has been considered by Cartarius, Main, and Wunner [20]. They have proven the existence of such exceptional points in their case and presented a procedure for a

systematic search for them. We believe that a similar procedure could also reveal branch points for the system considered in this work.

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