Atoms in hydrogen plasma in strong electric fields

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Two-particle states of a hydrogen plasma under the influence of a homogeneous strong electric field and of the density are investigated. The complex rotated Stark-Coulomb-Schrödinger equation was solved analytically using complex power series expansions. In this technique one works with square integrable eigenfunctions. Density effects were taken into account as a second-order perturbation of those polynoms. Real and imaginary parts of the energies are determined which give information about location and width of the states.

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I. INTRODUCTION AND BASIC IDEAS

In dense plasmas, atomic bound state energies are drastically influenced by the many-particle effects, i.e., screening, self-energy, and phase space occupation. At sufficiently high densities, bound states decay and will have a finite lifetime $\tau \sim -\hbar/[2\,\mathrm{Im}(E)]$ corresponding to "complex eigenvalues." In addition, the continuum edge is changed so that bound states may disappear (Mott effect) [1,2]. We want to mention here that the behavior of bound states in strongly coupled plasmas is of great interest in the discussion of reaction and ionization kinetics [3,4]. The influence of external strong electric fields leads, already for low density systems, to complex eigenvalues, too, because the electric field gives rise to a finite tunnel probability. The related Schrödinger equation has no stationary solutions and no square integrable eigenfunctions at the complex energies because the Hamiltonian of the system is Hermitian and its eigenvalues have to be real. The former bound states will now become resonances and move into the complex energy plane. The energy plane consists of two Riemann sheets, the physical and the nonphysical ones; the branch cut represents the continuum. Points belonging to square integrable eigenfunctions can be found on the upper sheet. But resonances are located in the nonphysical plane. A way out is given by the Aguilar-Balslev-Combes complex scaling method [5,6], which allows one to rotate the continuous spectrum over the resonances, so they will be uncovered and be found in the upper half-plane. This method developed into a powerful tool of mathematical physics during the last 20 years [9]. The basic idea is the unitary transformation $\hat{U}_\theta$; it changes the asymptotic divergence behavior of the resonance eigenfunction:

$$\hat{U}\Psi_R = \Psi_R(re^{\theta}) \underset{r\to\infty}{\longrightarrow} 0\ , \quad \theta \in \mathbb{C}\ . \tag{1}$$

Carrying out the similarity transformation,

$$\{\hat{U}\hat{H}\hat{U}^{-1}\}\{\hat{U}\Psi_R\} = [E_1 + iE_2]\hat{U}\Psi_R\ , \tag{2}$$

one generates a complex rotated Hamiltonian $\hat{H}(\theta) = \hat{U}\hat{H}\hat{U}^{-1}$:

$$H(\theta) = H_0(\theta) + V(\theta)$$

or

$$H(\theta) = e^{-2\theta}(H_0 + e^{2\theta}V(\theta))\ . \tag{3}$$

From the potential $V(r)$ we have to demand dilatation analyticity [5,6]. The operator $e^{2\theta}V(\theta)$ is compact; that means it has only a finite or an enumerably infinite number of discrete eigenvalues:

$$\sigma_k(H_0 + e^{2\theta}V(\theta)) = \mathbb{R}_+\ ,$$
$$\sigma_k(H(\theta)) = e^{-2\theta}\mathbb{R}_+\ . \tag{4}$$

(σ_k stands for the continuous spectrum, $\mathbb{R}_+$ terms the positive real axis.) The transformation rotates the continuous spectrum over the resonances with the angle $-2\theta_2$, so that they become "uncovered" [7] and hence eigenvalues of $H(\theta)$. The real part of the transformation angle θ_1 causes a stretching along the new direction given by θ_2 (see Fig. 1). The calculated eigenvalues are independent of the angle θ, but it has to be big enough to turn the branch cut over the resonances. It is not necessary to take into account the real part of θ when solving two-body problems, but it may be useful in numerical calculations supporting the convergence of the procedure calculating eigenvalues. Now complex eigenvalues are associated with square integrable functions, and computational techniques originally developed for bound states

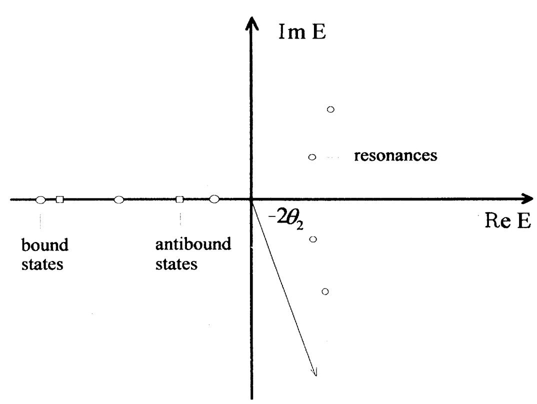

FIG. 1. Complex energy plane after scaling procedure.

can be used. The complex coordinate method has been successfully applied to atomic and molecular autoionization resonances, predissociation resonances, positronium hydrogen scattering resonances, van der Waals molecules, gas surface scattering resonances nuclear multiparticle systems, and for determining tunneling rates in bound systems [8]. An overview is given in [15,16].

The Schrödinger equation for hydrogen embedded in an ionized background described by an Ecker-Weizel potential [10], see also [11,12], with an additional external electric field F (static, homogeneous) reads

$$\left[\frac{\hbar^2}{2\mu}\Delta+\frac{e^2}{4\pi\varepsilon_0}\frac{e^{-\kappa r}}{r}-eFz+E+\frac{\kappa e^2}{4\pi\varepsilon_0}\right]\Psi=0\ , \qquad (5)$$

with

$$\kappa=\sum_a\left[\frac{n_a e_a^2}{\varepsilon_0 kT}\right]^{1/2}\ , \quad \mu=\text{reduced mass}\ .$$

Taking into account both $F>0$ and $\kappa>0$, the problem is not separable in the general case. In [13] the screening along the x-y plane was specialized. Other results for the real parts of the energy calculated by perturbation theory (electric field as a perturbation of Debye eigenfunctions and both the electric field and density as a perturbation of Coulomb eigenfunctions) expire for strong fields.

In the present work another way is shown. Eigenfunctions of the complex scaled Stark Hamiltonian are determined as analytic complex power series. These functions have no direct physical meaning, but they are normalizable so that we can use them as a basic system for a perturbation theory in the complex rotated plane with the density effects as perturbation. Now strong fields can be taken into account, and real and imaginary parts of the spectrum are determined.

II. THE FIELD DEPENDENT BASIC SYSTEM

Without the density effects, (5) was complex transformed to

$$\left[\frac{\hbar^2 e^{-2\theta}}{2\mu}\Delta+\frac{e^2 e^{-\theta}}{4\pi\varepsilon_0 r}-eFze^{\theta}+E\right]\Psi=0\ . \qquad (6)$$

This problem is usually separated by means of parabolic coordinates. With hartree units $\hbar=1$, $\mu=1$, $e^2=1$, $4\pi\varepsilon_0=1$, and the ansatz $\Psi=\Phi(\xi)X(\eta)e^{im\varphi}$, it follows that

$$e^{-\theta}\frac{d}{d\xi}\left[\xi\frac{d}{d\xi}\Phi(\xi)\right]+\left[\frac{E}{2}\xi e^{\theta}+\alpha-\frac{F}{4}\xi^2e^{2\theta}-\frac{m^2}{4\xi}e^{-\theta}\right]\Phi(\xi)=0\ ,$$
$$e^{-\theta}\frac{d}{d\eta}\left[\eta\frac{d}{d\eta}X(\eta)\right]+\left[\frac{E}{2}\eta e^{\theta}+\beta+\frac{F}{4}\eta^2e^{2\theta}-\frac{m^2}{4\eta}e^{-\theta}\right]X(\eta)=0\ . \qquad (7)$$

Here, m is the magnetic quantum number, and the separation constants α and β represent the parabolic quantum numbers

$$n=|m|+n_1+n_2+\alpha+\beta\ , \quad \alpha+\beta=1\ , \quad \alpha,\beta\in\mathbb{C}\ . \qquad (8)$$

Eigenvalues of the system (7) are the resonances (complex energy values E) and the complex separation constant α (β depends on α); i.e., we have finally a coupled eigenvalue problem of four equations with four eigenvalues. Now we consider a complex power series for the functions $\Phi(\xi)$ and $X(\eta)$,

$$\Phi(\xi)=\sum_{n=0}^{\infty}a_n\xi^{n+|m|}\ , \quad X(\eta)=\sum_{n=0}^{\infty}b_n\eta^{n+|m|}\ , \quad a_n,b_n\in\mathbb{C}\ . \qquad (9)$$

Equation (9) in (7) gives the following expressions for the coefficients:

$$a_n=\frac{-1}{3m^2+8n|m|+(2n)^2}[4\alpha e^{\theta}a_{n-1}+2Ee^{2\theta}a_{n-2}-Fe^{3\theta}a_{n-3}]\ ,$$
$$b_n=\frac{-1}{3m^2+8n|m|+(2n)^2}[4\beta e^{\theta}b_{n-1}+2Ee^{2\theta}b_{n-2}+Fe^{3\theta}b_{n-3}]\ . \qquad (10)$$

For a_2 and b_2, the terms with index $n-3$ (and for a_1 and b_1 additionally the $n-2$ terms) disappear. Now real and imaginary parts are separated. Let us denote real parts with the index 1 and imaginary parts with the index 2:

$$\theta=\theta_1+i\theta_2\ ,$$
$$\alpha=\alpha_1+i\alpha_2\ , \quad \beta=\beta_1+i\beta_2\ ,$$
$$E=E_1+iE_2\ ,$$
$$a_n=a_{n,1}+ia_{n,2}\ , \quad b_n=b_{n,1}+ib_{n,2}\ .$$

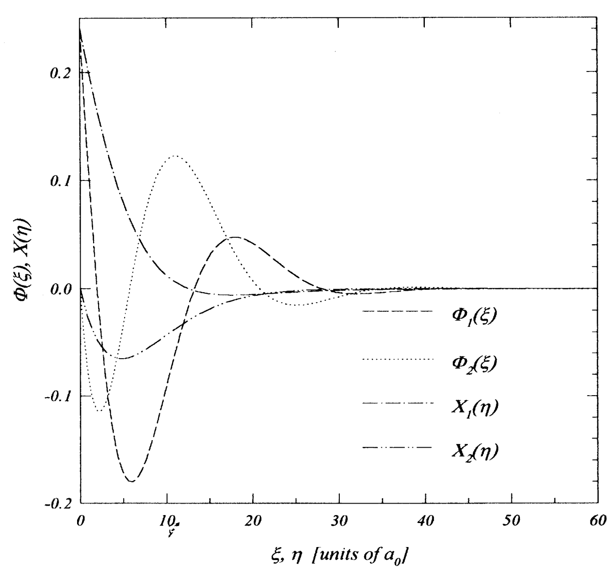

FIG. 2. Components of the eigenfunction $\Psi_{2,1,0,0}(\xi,\eta)$ ($\mathrm{Im}(\theta)=0.7$ rad).

With

$$\begin{aligned} &e_{c1}=e^{\theta_1}\cos\theta_2\ , \quad e_{s1}=e^{\theta_1}\sin\theta_2\ ,\\ &e_{c2}=e^{2\theta_1}\cos2\theta_2\ , \quad e_{s2}=e^{2\theta_1}\sin2\theta_2\ ,\\ &e_{c3}=e^{3\theta_1}\cos3\theta_2\ , \quad e_{s3}=e^{3\theta_1}\sin3\theta_2\ , \end{aligned} \tag{11}$$

it follows that

$$\begin{aligned} a_{n,1}&=\frac{-1}{3m^2+8n|m|+(2n)^2}\left[\begin{array}{c} 4(\alpha_1e_{c1}-\alpha_2e_{s1})a_{n-1,1}-4(\alpha_2e_{c1}+\alpha_1e_{s1})a_{n-1,2}\\ +2(E_1e_{c2}-E_2e_{s2})a_{n-2,1}-2(E_2e_{c2}+E_1e_{s2})a_{n-2,2}\\ -Fe_{c3}a_{n-3,1}+Fe_{s3}a_{n-3,2}\end{array}\right]\ ,\\ a_{n,2}&=\frac{-1}{3m^2+8n|m|+(2n)^2}\left[\begin{array}{c} 4(\alpha_2e_{c1}+\alpha_1e_{s1})a_{n-1,1}+4(\alpha_1e_{c1}-\alpha_2e_{s1})a_{n-1,2}\\ +2(E_2e_{c2}+E_1e_{s2})a_{n-2,1}+2(E_1e_{c2}-E_2e_{s2})a_{n-2,2}\\ -Fe_{s3}a_{n-3,1}-Fe_{c3}a_{n-3,2}\end{array}\right]\ ,\\ b_{n,1}&=\frac{-1}{3m^2+8n|m|+(2n)^2}\left[\begin{array}{c} 4(\beta_1e_{c1}-\beta_2e_{s1})b_{n-1,1}-4(\beta_2e_{c1}+\beta_1e_{s1})b_{n-1,2}\\ +2(E_1e_{c2}-E_2e_{s2})b_{n-2,1}-2(E_2e_{c2}+E_1e_{s2})b_{n-2,2}\\ +Fe_{c3}b_{n-3,1}-Fe_{s3}b_{n-3,2}\end{array}\right]\ ,\\ b_{n,2}&=\frac{-1}{3m^2+8n|m|+(2n)^2}\left[\begin{array}{c} 4(\beta_2e_{c1}+\beta_1e_{s1})b_{n-1,1}+4(\beta_1e_{c1}-\beta_2e_{s1})b_{n-1,2}\\ +2(E_2e_{c2}+E_1e_{s2})b_{n-2,1}+2(E_1e_{c2}-E_2e_{s2})b_{n-2,2}\\ +Fe_{s3}b_{n-3,1}+Fe_{c3}b_{n-3,2}\end{array}\right]\ . \end{aligned} \tag{12}$$

The function Ψ determined thus is normalizable for the correct complex eigenvalues α and E:

$$\Psi(\xi,\eta,\varphi,\theta)=\left[\sum_{n=0}^{\infty}a_{n,1}\xi^{n+|m|}+i\sum_{n=0}^{\infty}a_{n,2}\xi^{n+|m|}\right]\times\left[\sum_{n=0}^{\infty}b_{n,1}\eta^{n+|m|}+i\sum_{n=0}^{\infty}b_{n,2}\eta^{n+|m|}\right]e^{im\varphi}\ . \tag{13}$$

The normalization can be calculated analytically. With the help of this function Ψ, which has to be a square integrable, one can find the resonances E_1, E_2 and the separation constants belonging to them. Figure 2 shows an example for $n=2$, $n_1=1$, $n_2=0$, $m=0$, $F=0.005$ a.u., $\theta=0.7i$ rad, $E_1=-0.112061$ hartree, and $E_2=-2.8\times10^{-6}$ hartree.

III. PERTURBATION THEORY FOR DENSITY EFFECTS

Let us consider the perturbation

$$V=\frac{1}{r}-\frac{e^{-\kappa r}}{r}=\frac{2}{\xi+\eta}-\frac{2e^{-\kappa[(\xi+\eta)/2]}}{\xi+\eta}\ , \tag{14}$$

in second-order terms of the functions (13); that means the unperturbed problem is the Stark-hydrogen case discussed above. The self-energy shift $-\kappa e^2/4\pi\varepsilon_0$ from (5) will be added after the perturbation calculation. Because the m degeneracy, also with the existing screening term, remains, the energy corrections are given by

$$E_\nu^{\{2\}}=\langle\Psi_\nu|V|\Psi_\nu\rangle+\sum_{\mu\neq\nu}\frac{\langle\Psi_\mu|V|\Psi_\nu\rangle\langle\Psi_\nu|V|\Psi_\mu\rangle}{E_\nu^{\{0\}}-E_\mu^{\{0\}}}\ . \tag{15}$$

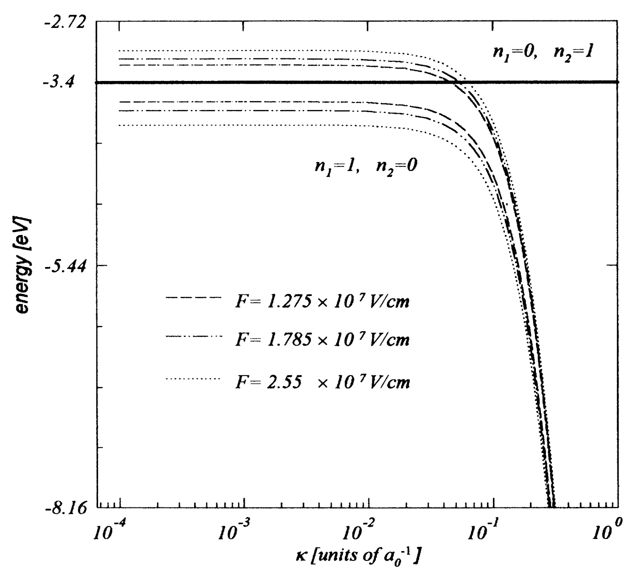

FIG. 3. κ dependence of $n=2$, $m=0$ states (real parts) with F as parameter.

The matrix elements are determined using the normalized power series from Sec. II:

$$\langle \Psi_\nu | V | \Psi_\mu \rangle = \pi \delta_{m_\nu, m_\mu} \int_0^\infty \int_0^\infty \Phi_\nu(\xi) X_\nu(\eta) \Phi_\mu^*(\xi) X_\mu^*(\eta) \times [1 - e^{-\kappa[(\xi+\eta)/2]}] d\xi \, d\eta \, . \tag{16}$$

After expansion the integrand K was split into real and imaginary parts:

$$\mathrm{Re}(K) = A(\xi,\eta)[1 - e^{-(\kappa/2)\xi} e^{-(\kappa/2)\eta}] \, ,$$
$$\mathrm{Im}(K) = B(\xi,\eta)[1 - e^{-(\kappa/2)\xi} e^{-(\kappa/2)\eta}] \, , \tag{17}$$

wherein the collection of ξ and η terms as Cauchy products leads to the sums

$$A(\xi,\eta) = \sum_{j=1}^{8} \left[\lim_{N\to\infty} \sum_{n=0}^{2N} c_{j,n} \xi^{n+2|m|} \sum_{n=0}^{2N} d_{j,n} \eta^{n+2|m|} \right] ,$$
$$B(\xi,\eta) = \sum_{j=9}^{16} \left[\lim_{N\to\infty} \sum_{n=0}^{2N} c_{j,n} \xi^{n+2|m|} \sum_{n=0}^{2N} d_{j,n} \eta^{n+2|m|} \right] , \tag{18}$$

with the new coefficients c and d (Cauchy products of a_i and b_i). Here the convergence criterion of Cauchy products has to be satisfied; that means the convergence radius of the product sum is the smallest one of those of the factors [14]. The physical conditions demand that the series decay for $\xi, \eta \to \infty$, so there is no problem left. Carrying out some integrals of the structure

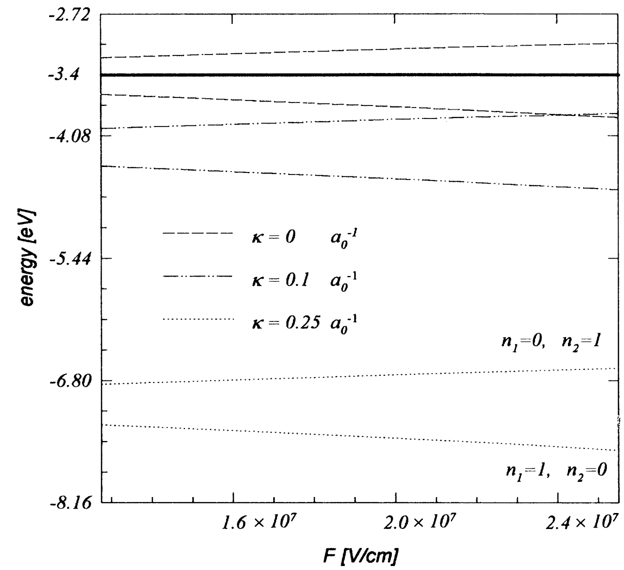

FIG. 4. Field dependence of $n=2$, $m=0$ states (real parts) with κ as parameter.

$$I = \int_0^\infty \int_0^\infty A(\xi,\eta) e^{-(\kappa/2)\xi} e^{-(\kappa/2)\eta} d\xi \, d\eta$$

$$= \lim_{N\to\infty} \left[\sum_{j=1}^{8} \left[\sum_{n=0}^{2N} c_{j,n} \int_0^\infty \xi^{n+2|m|} e^{-(\kappa/2)\xi} d\xi \sum_{n=0}^{2N} d_{j,n} \int_0^\infty \eta^{n+2|m|} e^{-(\kappa/2)\eta} d\eta \right] \right]$$

$$= \lim_{\xi,\eta,N\to\infty} \left[\sum_{j=1}^{8} \left[\sum_{n=0}^{4N} \sum_{k=0}^{n} c_{j,k} \frac{(-\kappa/2)^{n-k}}{(n-k)!} \frac{\xi^{n+2|m|+1}}{(n+2|m|+1)} \sum_{n=0}^{4N} \sum_{k=0}^{n} d_{j,k} \frac{(-\kappa/2)^{n-k}}{(n-k)!} \frac{\eta^{n+2|m|+1}}{(n+2|m|+1)} \right] \right] , \tag{19}$$

one gets the perturbation matrix elements (16), and the complex energy corrections can be written as

$$\left.\begin{matrix}\mathrm{Re}\\ \mathrm{Im}\end{matrix}\right\}(E_\nu^{\{2\}}) = \left\{\begin{matrix}\mathrm{Re}\\ \mathrm{Im}\end{matrix}\right\} \langle \Psi_\nu | V | \Psi_\nu \rangle \pm \sum_{\mu\neq\nu} \left[\frac{[(\mathrm{Re}\langle \Psi_\mu | V | \Psi_\nu \rangle)^2 + (\mathrm{Im}\langle \Psi_\mu | V | \Psi_\nu \rangle)^2](E_{2,\nu}^{\{0\}} - E_{2,\mu}^{\{0\}})}{(E_{1,\nu}^{\{0\}} - E_{1,\mu}^{\{0\}})^2 + (E_{2,\nu}^{\{0\}} - E_{2,\mu}^{\{0\}})^2} \right] . \tag{20}$$

TABLE I. Electron density for different κ and temperatures.

κ (units of a_0^{-1})	10^{-4}	10^{-3}	10^{-2}	10^{-1}	2.5×10^{-1}
n_e (cm^{-3}) at $T=80\,000$ K	6.8×10^{14}	6.8×10^{16}	6.8×10^{18}	6.8×10^{20}	4.2×10^{21}
n_e (cm^{-3}) at $T=100\,000$ K	8.5×10^{14}	8.5×10^{16}	8.5×10^{18}	8.5×10^{20}	5.3×10^{21}

TABLE II. Real and imaginary parts of the $n=1$ state dependent on κ and F.

F (10^7 V/cm)	Units of κ (a_0^{-1})	Re(E) (eV)	Im(E) (eV)
1.275	0	−13.6004	-8.8901×10^{-13}
1.275	0.0001	−13.6004	-8.8902×10^{-13}
1.275	0.001	−13.6004	-8.9037×10^{-13}
1.275	0.01	−13.6031	-1.0216×10^{-12}
1.275	0.1	−13.8511	-1.0985×10^{-11}
1.275	0.25	−14.9897	-4.3224×10^{-11}
1.275	0.45	−17.5083	-8.8538×10^{-11}
1.785	0	−13.6007	-3.3610×10^{-13}
1.785	0.0001	−13.6007	-3.9006×10^{-13}
1.785	0.001	−13.6008	-5.7167×10^{-12}
1.785	0.01	−13.6035	-5.2315×10^{-10}
1.785	0.1	−13.8540	-3.9836×10^{-8}
1.785	0.25	−15.0008	-1.6717×10^{-7}
1.785	0.45	−17.5310	-3.4636×10^{-7}
2.55	0	−13.6015	-1.7195×10^{-11}
2.55	0.0001	−13.6015	-3.2348×10^{-11}
2.55	0.001	−13.6016	-1.5281×10^{-9}
2.55	0.01	−13.6043	-1.4684×10^{-7}
2.55	0.1	−13.8594	-1.1152×10^{-5}
2.55	0.25	−15.0213	-4.7056×10^{-5}
2.55	0.45	−17.5733	-9.7648×10^{-5}

IV. RESULTS

The behavior of the $n=1$, $m=0$ and $n=2$, $m=0$ states is calculated using power series up to $N=521$. The convergence in ξ and η is still given at 100 Bohr radii. Electric fields from up to 2.55×10^7 V/cm and inverse Debye radii from 0 to 0.5 a_0^{-1} were taken into account. Figures 3 and 4 show the lowering of the real part of the energy levels in the $n=2$, $m=0$ case, dependent on κ and F, making clear the overlay effects of the external electric field and screening.

The problem of an avoided level crossing was not discussed. The dependence of the electron density on temperature and screening parameter κ at zero field strength is shown in Table I. Note that electrons in strong external electric fields have a Dawydov-like distribution function, so that κ will become field dependent, too [3].

In Table II are shown real and imaginary parts of some energy values of the $n=1$ state. For $\kappa=0$ we got an excellent agreement with data from [17]. In the case of nonzero electric field, there is always a finite tunnel probability; that means Im$E<0$. All states decay into the continuum, the imaginary parts being the relevant lifetimes.

V. CONCLUDING REMARKS

In this paper, the influence of strong electric fields on energy levels in hydrogen plasmas was considered. Power series determined by the complex scaling method were used as a basic system for perturbation calculations Within this technique, additional density effects described by the Ecker-Weizel potential were taken into account. Both the energy shift and the imaginary part of the resonances, which describes the decay rate of the levels, were calculated.

ACKNOWLEDGMENT

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