EFFECT OF DEBYE SCREENING ON IONIZATION
ENERGY OF COMPONENTS OF AIR PLASMA

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The effect of Coulomb interaction on the shift of energy levels of the components of air plasma is estimated. For illustrating the procedure of computation, the shift of the energy levels of hydrogen are computed. A simple method of computation of the shift of energy levels is given, which offers the possibility of cutting the computer time by a factor of 10-30. The dependence of the shift of the ground level of atoms of hydrogen, argon, nitrogen, and oxygen on Debye radius D is obtained for $20 \leq D \leq 2000$ atomic units.

1. Coulomb interaction results in a shift of the levels and a transition of the upper terms into a continuous spectrum. The shift of the ground state, which leads to a change of the ionization energy of the atoms, plays an especially important role.

A change of the ionization energy affects first of all the shift of the ionization equilibrium, i.e., the change of state of the plasma, which in turn affects all the other characteristics of the plasma. Furthermore, a change of the energy of the electronic levels can affect the thermophysical properties of the plasma also directly and not only through the effect on the composition. Thus a shift of the levels of electron excitation in atoms and cutoff of the upper terms lead to a shift of the threshold frequencies of photoionization in the absorption coefficient.

The computation of the energy shift of the ground state of an atom surrounded by charged particles can be done in two ways: first, considering the many-body problem and, second, considering an isolated particle located in an external effective field produced by the total effect of all the charged particles. The first approach involves considerable mathematical difficulties and is not suitable for practical computations. The reduction of the many-body problem to the description of the motion of a single particle in a certain field produced by other particles permits considerable simplification of the mathematical tool. In view of this, the single-frequency approximation, based on the introduction of the effective resultant field, was chosen for the computations of the level shifts of atoms.

2. For the determination of the eigenvalues of the energy of the atom, the Schrödinger equation with the potential energy depending on the parameters of the ambient plasma is solved.

For hydrogen and single-electron ions such computations have been done in [1-3] for Debye radii $D \leq 25$ (here and below all the quantities are expressed in atomic system of units); separate points for large D are given in [3]. These results are unsuitable for computations, since Debye radii are much larger in the ranges of temperature and pressure variations that are of practical interest. For example, for hydrogen plasma at a temperature of 10,000-50,000°K and pressure from 10 to 100 atm, the Debye radius lies in the range 25 to 600.

In [4], the Schrödinger equation for hydrogen with screened Coulomb potential is solved using the perturbation theory. It is noted that the computations are only for the upper states and are valid for sufficiently large Debye radii. For multielectron atoms two works are known. In [5] the computation of the energy level shifts of multielectron atoms with the use of the diagram method is discussed; numerical calculations are not given. In [6] a computation of the energy level shifts of iron for Thomas−Fermi potential is given for Debye radii $D \leq 50$.

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3. In view of the lack of data on the shift of the ground level of hydrogen for the range of variations of Debye radius that are of practical interest, and also for the development of the procedure of numerical calculation that could be applied to multielectron atoms in future, the shift of the ground level of hydrogen was computed for Debye radii from 20 to 2000.

The hydrogen atom is considered in the form of the stationary electron-proton system located in the external Debye-Hückel field. For the determination of the eigenvalues of the energy of the atoms, the Schrödinger equation with the potential energy in the form of screened coulomb potential is solved. The Schrödinger equation for the radial component P(r) of the wave function of the hydrogen atom has the form [7]

$$\frac{d^2P}{dr^2} - \frac{l(l+1)}{r^2} P - 2[u(r) - \varepsilon] P = 0 \tag{3.1}$$
$$(U(r) = -r^{-1}\exp(-r/D)) \,.$$

The problem reduces to the determination of the values of ε_n for which the solution of Eq. (3.1) satisfies the conditions

$$P(0) = 0, \qquad P(r) \to 0 \text{ for } r \to \infty$$
$$\int_0^\infty P^2(r)\,dr = 1 \,.$$

Estimates show that the second boundary condition $P(r) \to 0$ for $r \to \infty$ can be replaced by $P(r) = 0$, where R = 10 for the ground state of hydrogen.

Since in the computation of the ground state the maximum value of r is taken equal to 10, which is appreciably smaller than D in the investigated range, we can write

$$U(r) = -\frac{1}{r}\exp\left(-\frac{r}{D}\right) \approx -\frac{1}{r} + \frac{1}{D} \tag{3.2}$$

with sufficient degree of accuracy.

Substituting (3.2) into (3.1) we obtain

$$\frac{d^2P^*}{dr^2} - \frac{l(l+1)}{r^2} P^* - 2\left[-\frac{1}{r} + \frac{1}{D} - \varepsilon^*\right] P^* = 0 \tag{3.3}$$

where P* is the wave function of the hydrogen atom in screened Debye-Hückel field. It is obvious that the wave function remains practically constant for the chosen range of Debye radius, since in the region where the wave function is still appreciable, the change of the electric field intensity as a result of Debye screening is very small. This is evident from Fig. 1, in which the dependence of the radial wave function of state is of hydrogen atom and of the ratio E^*/E_0 (where E* is the field intensity taking into consideration the screening for D = 20 and E_0 is the intensity of the field of an isolated atom) on the distance from the center of the atom r is given. Let us consider Eq. (3.3) and the Schrödinger equation for an isolated hydrogen atom

$$\frac{d^2P}{dr^2} - \frac{l(l+1)}{r^2} P - 2\left[-\frac{1}{r} - \varepsilon\right] P = 0 \,. \tag{3.4}$$

Under the assumption that the wave functions P* and P are equal, Eqs. (3.3) and (3.4) will be equivalent under the condition of displacement of the eigenvalues of the energy by 1/D, i.e.,

$$\Delta\varepsilon_{1s} = 1/D \tag{3.5}$$

In order to check the assumptions made above, we computed the dependence $\Delta\varepsilon = f(D)$ for the state 1s of the hydrogen atom. Equation (3.1) with the boundary conditions was solved by the numerical method of Numerov [8, 9].

It was found that for a variation of Debye radius from 20 to 2000 the radial part of the wave function P(r) at the point r = 0.235 changes only by 0.001% and at the point r = 1.284 by 0.1%. The dependence (3.5) holds with an accuracy of ±1% for $20 \leq D \leq 2000$. Therefore, it can be hoped that the computation of $\Delta\varepsilon$ for the ground state of complex atoms will get considerably simplified if one starts from the condition of constancy of the wave function. The quantity $\Delta\varepsilon_{1s}$ for the hydrogen atom was calculated by the simplified method: successive change of ε was made so that the wave function of the atom in the plasma coincided
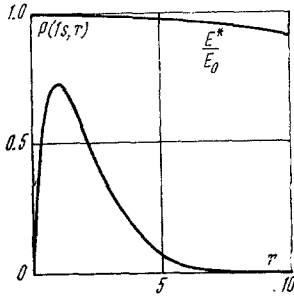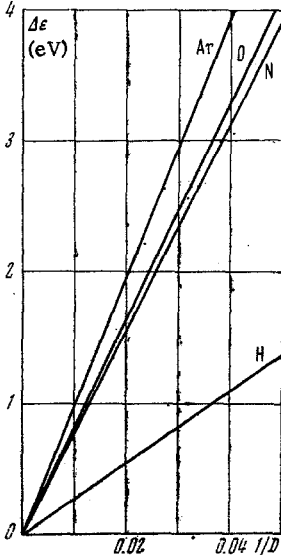
Fig. 1

Fig. 2

with the wave function of the isolated atom in the range $0 \le r \le r^*$, where r^* was chosen equal to 0.5. The dependence $\Delta\varepsilon_{1s} = f(D)$ was obtained as a result. In the entire range of variation of D the values of $\Delta\varepsilon$, computed by the method of V. B. Numerov, coincided with the results of the simplified method up to four significant figures. The computer time was reduced approximately by one order of magnitude.

4. The energy shifts of the ground states of nitrogen, oxygen, and argon (main components of air) were also computed for the variation of Debye radius from 20 to 2000.

Multielectron atoms were considered in the single-electron approximation by the method of self-consistent field with Hartree—Fock exchange [10]. The interaction of the atom with the ambient plasma was considered in Debye—Hückel approximation.

The interaction of an electron with the nucleus and all the remaining electrons was taken into consideration in the derivation of the equations for the radial components of single-electron wave functions of the atom. The interaction of the electrons among themselves reduces to the interaction of spherically symmetric space charges which may be reduced to the interaction of an electron with a certain effective point charge $z_e(r)$. Hence the potential energy of the electron is the energy of interaction of the electron with a certain point charge, which is determined in the following way:

$$z(r) = N - z_e(r) . \qquad (4.1)$$

It is obvious that with the increase of r the charge $z_e(r)$ approaches $N-1$. In the Debye—Hückel approximation the potential energy of the electron in the field of the nucleus, all other electrons, and the ambient plasma has the form

$$U(r) = \frac{N - z_e(r)}{r} \exp\left(-\frac{r}{D}\right) . \qquad (4.2)$$

The system of equations for the radial components of single-electron wave function [10] with (4.2) taken into consideration can be written in the form

$$\frac{d^2}{dr^2} + \frac{2}{r} Y(nl,r)\exp\left(-\frac{r}{D}\right) - 2\varepsilon_{nl,nl} - \frac{l(l+1)}{r^2} \ P(nl,r) = X(nl,r)\exp\left(-\frac{r}{D}\right) + 2\sum_{n\ne n'} \varepsilon_{nl,n'l}P(n'l,r) \qquad (4.3)$$

where the functions $Y(nl, r)$ and $X(nl, r)$ are determined for each specific electron configuration.

Thus, for the term ^4S of nitrogen atom (electron configuration $1s^2 2s^2 2p^3$) the system of equations (4.3) has the form

$$\left\{\frac{d^2}{dr^2} + [2N - 2Y_0(1s,1s,r) - 4Y_0(2s,2s,r) - 6Y_0(2p,2p,r)] \times \right.$$
$$\left. \times r^{-1}\exp(-r/D) - 2\varepsilon_{1s}\right\} P(1s,r) = - [2P(2s,r)Y_0(1s,2s,r) + P(2p,r)Y_1(1s,2p,r)] r^{-1}\exp(-r/D) ,$$

$$\left\{\frac{d^2}{dr^2} + [2N - 2Y_0(2s,2s,r) - 4Y_0(1s,1s,r) - 6Y_0(2p,2p,r)] \times \right.$$
$$\left. \times r^{-1}\exp(-r/D) - 2\varepsilon_{2s}\right\} P(2s,r) = - [2P(1s,r)Y_0(2s,1s,r) + P(2p,r)Y_1(2s,2p,r)] r^{-1}\exp(-r/D) ,$$

$$\left\{\frac{d^2}{dr^2} - \frac{2}{r} + [2N - 4Y_0(1s,1s,r) - 4Y_0(2s,2s,r) - 4Y_0(2p,2p,r) + \right.$$
$$\left. + 0.8Y_2(2p,2p,r)] r^{-1}\exp(-r/D) - 2\varepsilon_{2p}\right\} P(2p,r) =$$
$$= - {}^2/_3 [Y_1(1s,2p,r)P(1s,r) + Y_1(2s,2p,r)P(2s,r)] r^{-1}\exp(-r/D) , \qquad (4.4)$$

where for nitrogen N = 7

$$Y_k(nl,nl,r) = r\int_0^\infty U_k(r,s)P(nl,s)P(n'l',s)\,ds ,$$

$$U_k(r,s) = \begin{cases} r^k/s^{k+1} & \text{for } r < s \\ s^k/r^{k+1} & \text{for } r > s \end{cases}$$

For the nitrogen atom the energy shifts of the term ^4S were computed by a numerical solution of system (4.4) by the method of Numerov [9] on an M-220 computer for three values of Debye radius $D = 20, 200,$ and 2000. The wave functions from [11] were taken as the initial values.

The computation by the simplified method (see Sec. 3) gave values of $\Delta\varepsilon$ which coincided with the results obtained from the exact solution of the complete system of equations (4.4) within 0.5%.

The shift of the ground level for oxygen and argon was computed only by the simplified method.

It was established that the dependence of the shift of the ground level on Debye radius is well approximated by the expression

$$\Delta\varepsilon = z/D \tag{4.5}$$

where $z = 2.88$ for nitrogen, $z = 3.03$ for oxygen, and $z = 3.64$ for argon.

The results of the computations of the energy level shifts depending on D are shown in Fig. 2 for $20 \leq D \leq 2000$.

5. It is seen from these computations that the shift of the ionization equilibrium due to long-range Coulomb interactions are determined not only by the electron concentration and the gas temperature but also by the type of gas. With the increase of the charge of the nucleus of the atom the effect of Coulomb interaction on the ionization potential increases.

Experimental results for the displacement of the threshold of photoionization from 4s levels of argon atoms are given in [12]. A direct comparison of the results of the present work with the results of the experiment is difficult. But it must be noted that the results of the experiment are higher than the computation by Ecker—Weizel, which is true also for the computations given above.

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