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CONTRIBUTION TO THE THEORY OF ENERGY LEVELS OF ATOMS IN A PLASMA

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The energy spectrum of a hydrogenlike atom in a plasma is considered on the basis of the model of a cut-off Coulomb potential. The adiabatic solution for the bound states is investigated in detail in the case when $l = 0$. Approximate expressions are obtained for the S-state energies, showing the dependence of these energies on the cutoff radius. The critical Debye lengths at which the corresponding S levels vanish from the spectrum are obtained.

KNOWLEDGE of the energy spectrum of an atom perturbed by surrounding particles is essential for an experimental determination of the parameters of a partially ionized plasma (for example, by means of spectroscopic measurements), as well as for a correct theoretical description of the processes occurring in the plasma. Recently much progress has been achieved in the theory of the shift of atomic energy levels under the influence of a surrounding plasma, due to the application of methods of quantum field theory (the Green's function method and diagram techniques) to the quantum description of the plasma and to a consistent evaluation of its possible correlation with the atom (or ion) in question. In this approach, the screening effect of the plasma (regarded as a quasistatic perturbation) on the two-particle ion-electron interaction is taken into account by summing the corresponding diagrams.[1, 2] However, numerical results for the level shift can be obtained here only within the framework of perturbation theory.

1. In order to obtain a convenient model for an analytic calculation of the levels of the atom in the plasma, we can approximately reduce the problem to the two-body problem by introducing a certain effective pair-interaction potential between the ion and the electron to take into account the influence of the surrounding charged particles. The model considered for this purpose in [3, 4] is the Debye potential

$$V(r) = \frac{Ze\exp\{-\varkappa r\}}{r}, \qquad \varkappa = \frac{1}{D} = \left(\frac{4\pi}{kT}\sum_s n_s Z_s^2 e^2\right)^{1/2}, \tag{1}$$

where Ze is the ion charge, κ the reciprocal of the Debye radius, and n_s the density of the particles with charge $Z_s e$. Such a potential, as is well known, describes the screening influence of the charged environment on the Coulomb interaction in the self-consistent-field approximation for a weakly-nonideal plasma.[5] Of definite interest is also a consideration of another model of pair interaction in a plasma, namely, a Coulomb potential cut off at the Debye length:

$$V(r) = \begin{cases} Ze/r, & r \leqslant D \\ 0, & r \geqslant D. \end{cases} \tag{2}$$

Unlike the Debye potential, this potential admits of a solution of the corresponding Schrödinger equation in analytic form, thus greatly simplifying the determination of the dependence of the energy levels on the plasma parameters (density and temperature). In addition, this model deserves attention because, as shown by Alyamovskiĭ,[6] the influence of the charge interaction on the characteristics of the fluctuating micropole in the plasma can be described on the basis of the model of free particles that serve as sources for just this type of a potential (and not a Debye potential).

2. The radial part of the wave function R(r), which is a solution of the Schrödinger equation with potential (2) satisfying the requirement that it be bounded at $r = 0$ and that it decrease as $r \rightarrow \infty$, is

$$R_1(r) = Ae^{-kr} r^l F\left(l + 1 - \frac{1}{ka_0},\ \ 2l + 2;\ 2kr\right), \qquad r \leqslant D,$$

$$R_2(r) = Br^{-1/2} K_{l+1/2}(kr), \qquad r \geqslant D,$$

where

$$k^2 = \frac{2m|E|}{\hbar^2}, \qquad a_0 = \frac{\hbar^2}{me^2}, \qquad E < 0,$$

F(a, b; x) is a confluent hypergeometric function; $K_{l+1/2}(x)$ is a modified Bessel function of the second kind (Macdonald function), and A and B are normalization factors. Joining together the logarithmic derivatives of the wave functions R_1 and R_2 at the point $r = D$ and using the recurrence relations for $F'(a, b; x)$ and $K'_{l+1/2}(x)$, we obtain the

$$1-\frac{K_{l+3/2}(kD)}{K_{l+1/2}(kD)}=\frac{l+1-1/ka_0}{l+1}\times\frac{F[l+1+(1/ka_0),\,2l+3;\,-2kD]}{F[l+1+(1/ka_0),\,2l+2;\,-2kD]},\tag{3}$$

which determines the dependence of the energy of any bound state on the cutoff radius D. The determination of the energy levels entails calculation of the roots of this equation, which is rather difficult in the general case. The simplest relation is obtained for the S-levels, namely,

$$F\left(\varepsilon^{-1/2},\quad 1;\ -\frac{2D}{a_0}\varepsilon^{1/2}\right)=0,\tag{4}$$

where

$$\varepsilon=\frac{|E|}{|E_0|}=\frac{|E|}{me^4/2\hbar^2}.$$

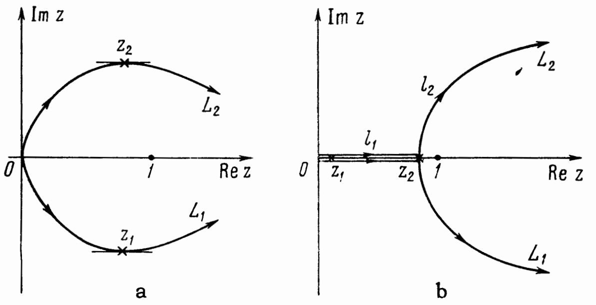

FIG. 1

3. To calculate the roots of F(a, 1; −x) we use a method proposed by Kolkunov[7] for functions having an integral representation. In the integral representation, (4) can be rewritten[8]

$$F(a,1;\,-x)\equiv\frac{1}{2\pi i}\int_0^{(1+)}e^{-xz}z^{a-1}(z-1)^{-a}\,dz=0.\tag{5}$$

Here $a = \epsilon^{-1/2}$ and $x = 2D\epsilon^{1/2}/a_0$. The integration contour L is chosen to pass through the saddle point

$$z_{1,2}=\frac{1}{2}\left\{1-\frac{1}{x}\pm\left[\left(1+\frac{1}{x}\right)^2-\frac{4a}{x}\right]^{1/2}\right\}$$

and to coincide with the constant-phase line of the integrand function, circling around the point Z = +1 in the positive direction (Fig. 1a). The contour L is broken up in the general case into two complex-conjugate contours L_1 and L_2. The integrals along these contours are also complex conjugate, and therefore Eq. (5) reduces to the condition

$$\int_L=\int_{L_1}-\int_{L_2}=\mathrm{R}e^{i\psi}-\mathrm{R}e^{-i\psi}\sim\sin\psi=0,$$

i.e.,

$$\psi=\pi n.\tag{6}$$

Thus, to determine the roots of F(a, 1; −x) it is sufficient to find the phase of one of the integrals (for example, the integral along the contour L_2). This phase is obviously equal to the sum of the phase θ of the integrand function at the saddle point, and a certain phase $\overline{\varphi}$ of the differential dz, averaged along the contour. It can be assumed in first approximation that $\overline{\varphi}$ is approximately equal to φ_0, the phase of the differential in the most essential saddle point. To obtain the value of the phase ψ in the next approximation, we can use the asymptotic expansion of the integral obtained by the saddle-point method.

4. Let us consider first the case of sufficiently large cutoff parameters $2D/a_0$ and not too small energies ϵ, when

$$(1+1/x)^2>4a/x.\tag{7}$$

In this case the contour L_2 passes through both saddle points lying on the real axis, and consequently both points contribute to the phase ψ. To calculate the phase, it is convenient to break up the integral along the contour L_2 into two integrals, along the contours $l_1(0,\ z_2)$ and $l_2(z_2,\ +\infty)$ (Fig. 1b). The integrals along l_1 and l_2 can be respectively represented by the following asymptotic series:

$$I_1=\Phi(z_1)\left\{1+\frac{3\psi_4(z_1)\psi_2(z_1)-5\psi_3^2(z_1)}{24\psi_2^3(z_1)}+\ldots\right\}\times\left(\frac{2\pi}{-\psi_2(z_1)}\right)^{1/2},\tag{8}$$

$$I_2=\frac{\Phi(z_2)}{2}\left\{\left(\frac{2\pi}{\psi_2(z_2)}\right)^{1/2}e^{i\pi/2}-\frac{2\pi}{3}\,\frac{\psi_3(z_2)}{\psi_2^2(z_2)}+\frac{\sqrt{\pi}}{4\psi_2^3(z_2)}\left[\frac{5}{4}\left(\frac{\psi_3(z_2)}{\psi_2(z_2)}\right)^2-\frac{\psi_4(z_2)}{\psi_2(z_2)}\right]e^{i3\pi/2}+\ldots\right\},\tag{9}$$

where $\psi_k(z_{1,2})$ is the k-th derivative at the point z_1 or z_2, and $\Phi(z_1)$ and $\Phi(z_2)$ are the values of the integrand at the saddle points. The integral along the contour L_2 is then represented by the sum of the expansions (8) and (9):

$$I=I_1+I_2.\tag{10}$$

Separating the real and imaginary parts in (10), we obtain from (6) an equation for the roots of the function (5):

$$\psi = -\tan^{-1}\frac{\operatorname{Im} I}{\operatorname{Re} I} = \pi n, \tag{11}$$

which makes it possible to calculate the phase ψ with arbitrary degree of accuracy.

Let us find ψ for $x \gg a$. This condition, as will be shown below, is equivalent to the inequality $D/a_0 n^2 \gg 1$, i.e., it corresponds to a consideration of levels whose Bohr radii are much smaller than the Debye length in the absence of the perturbation.

At large cutoff radii, our solution should obviously be close to the Coulomb solution. In fact, when $x \to \infty$ the contribution to the integral I from the point z_2 will be small compared with the contribution of z_1. Neglecting the contribution of z_2, we get

$$\pi n = \psi \approx \pi a, \qquad a = \varepsilon^{-1/2} \approx n.$$

The phase introduced by the contour l_2 (by the point z_2) determines the degree of deviation of the solution under consideration from the pure Coulomb solution at large x. Retaining only the first terms of the imaginary and real parts of the expansion (10) and recognizing that $\psi_2(z_1) < 0$, and $\Phi(z_1)$ contains a phase $-\pi a$, we obtain from (11) an equation

$$a = \varepsilon^{-1/2} \approx n + \frac{e^{-x+2a}}{2\pi}\left(\frac{x}{n}\right)^{2n-1}, \tag{12}$$

in which the second term constitutes the correction to the energy levels of the isolated hydrogen atom.

We see from (12) that the levels for which the Bohr radius is much smaller than the Debye length change very little.

5\. At sufficiently small ϵ (and arbitrary $2D/a_0$), when

$$(1 + 1/x)^2 < 4a/x, \tag{13}$$

it is convenient to determine the dependence of the level energy on D by expanding the confluent hypergeometric function in a series in Bessel functions:[9]

$$F(a, \gamma + 1, x) = \Gamma(\gamma + 1)(\varkappa x)^{-\gamma/2} e^{x/2} \sum_{k=0}^{\infty} A_k\left(\varkappa, \frac{1}{2} + \frac{\gamma}{2}\right) \times \left(\frac{x}{4\varkappa}\right)^{k/2} J_{\gamma+k}(2\sqrt{\varkappa x}), \tag{14}$$

where $\kappa = 1/2 + \gamma/2 - a$ and $A_k(\kappa, \lambda)$ are the coefficients in the expansion

$$e^{2\varkappa z}(1 - z)^{\varkappa-\lambda}(1 + z)^{-\varkappa-\lambda} = \sum_{k=0}^{\infty} A_k(\varkappa, \lambda) z^k, \qquad |z| < 1.$$

For these coefficients we have the recurrence relations[9]

$$A_0(\varkappa, \lambda) = 1, \quad A_1(\varkappa, \lambda) = 0, \quad A_2(\varkappa, \lambda) = \lambda,$$

$$(k + 1)A_{k+1}(\varkappa, \lambda) = (k + 2\lambda - 1)A_{k-1}(\varkappa, \lambda) - 2\varkappa A_{k-2}(\varkappa, \lambda), \quad k = 2, 3, \ldots$$

Substituting the expansion (14) in (4), we obtain an equation for determining the energy levels adjacent to the continuum, in the form

$$\sum_{k=0}^{\infty} A_k\left(\varkappa, \frac{1}{2}\right)\left(\frac{x}{4\varkappa}\right)^{k/2} J_k(2\sqrt{\varkappa x}) = 0, \qquad \varkappa = \varepsilon^{-1/2} - \frac{1}{2}. \tag{15}$$

When $\kappa \gg 1$ the zeroes of (15) are given approximately by the expression

$$x = \frac{j_{0n}^2}{4}\left\{1 + \frac{1}{3(4\varkappa)^2}[j_{0n}^2 - 2]\right\} + O(\varkappa^{-4}), \tag{16}$$

where j_{0n} is the n-th root of the function $J_0(y)$. Neglecting in (16) terms of order κ^{-4} and above, we find that the dependence of the energy of the nS level on the Debye radius is given by

$$\frac{2D}{a_0} = \frac{1}{2}x + \frac{j_{0n}^2}{4}\left\{1 + \frac{1}{48\varkappa^2}[j_{0n}^2 - 2]\right\}. \tag{17}$$

When

$$\alpha_n^0 = 2D/a_0 = 1/4\, j_{0n}^2 \tag{18}$$

the nS level reaches the continuum.

In particular, the first level, corresponding to the ground state in our model of the hydrogen model, vanishes when $\alpha_1^0 = 1.45$, which is quite close to the value $\alpha_1^0 = 1.68$ obtained by Trubnikov and Yavlinskiĭ[10] for the potential (1). The critical values of the Debye length, which determine the moment of the transition of the levels with $l \neq 0$ to the continuous spectrum, are determined by expressions similar to (18), $a_{nl}^0 = 1/4\, j_{2l,n}^2$, which can be easily obtained from (3) by using the expansion (14) and taking the limit as $k \to 0$.

Formulas (12) and (17) determine the behavior of the energy levels as functions of the Debye radius at $2D\epsilon/a_0 \gg 1$ and $2D\epsilon/a_0 \ll 1$, respectively. In the intermediate region, the levels can be determined with arbitrary degree of accuracy from (11), by taking enough terms in the expansion for the integral along the contour L_2. In addition, there are several points $\epsilon^{-1/2} = k$ ($k = 2, 3, \ldots$) where the function $F(a, 1; -x)$ reduces to the Laguerre polynomials $L_{a-1}(x)$, the roots of which

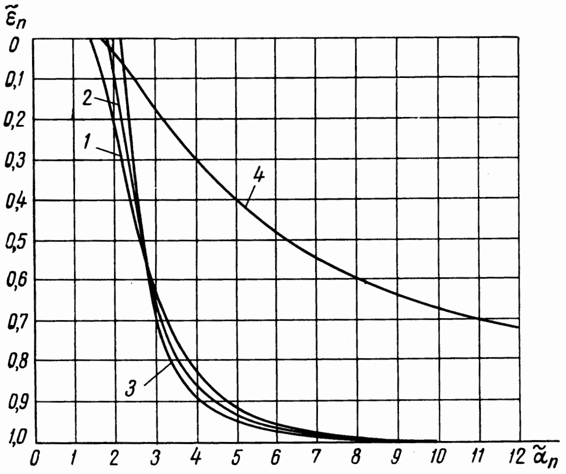

FIG. 2

have been tabulated.[11] The dependence of the first three S-levels on the Debye length is shown in Fig. 2 (curves 1, 2, and 3, respectively), where the following dimensionless quantities have been introduced:

$$\tilde{\varepsilon}_n = \frac{|E|}{me^2/2\hbar^2 n^2} = \frac{|E|}{|E_n|}, \quad \tilde{\alpha}_n = \frac{2D}{a_0 n^2}.$$

The figure shows for comparison a plot of $\tilde{\epsilon}_1 = f(\alpha_1)$ (curve 4) for the Debye potential, as obtained from the results of [4]

Comparison shows that although the corresponding levels in the Debye and in the cut-off Coulomb potentials occur at close values of the parameter α, they behave quite differently with increasing D.1) It must be noted that at small screening the hydrogen-atom level shifts calculated in [4] coincide with the results of Pargamanik,[1] which, as indicated by Kudrin and Tarasov,[2] are incorrect. According to their paper, these shifts should be much smaller, and from this point of view it can be assumed that the model of effective two-particle interaction in the form of a Coulomb potential cut off at the Debye lengths yields more correct results for the bound-state energy (compared with the Debye potential).

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1)Comparison of the same two models of interaction as applied to problems of particle scattering in a plasma x is made in[12].

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