

Screening of atoms in a plasma

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A self-consistent determination of the atom-level perturbation in a conducting medium is considered. The solution is obtained for the case of a hydrogen atom in a metal. Correct matching of the atom to the medium decreases the shifts of the atomic levels and changes the qualitative dependence of these shifts on the density of the medium. The levels approach asymptotically the continuous spectrum with increase of density. The shift of the 1s ground level of a hydrogen atom in an alkali metal is relatively small and can be calculated by an appropriate perturbation theory.

1. Knowledge of the variation of the binding energy of atomic electrons when the atoms land in a plasma medium is important for many applications. A rarefied plasma alters greatly the energies of highly excited states, and this influences the emission spectra near the limits of the series, and also the probabilities of such processes as impact-radiative recombination, dielectric recombination, and others. In dense media at both high and low temperatures (e.g., in metals under normal conditions), even the ground states are strongly perturbed, so that the existence of even one bound state remains questionable.

If a particle with charge Z is placed in a plasma medium, the total potential φ is given in the linear approximation by¹

$$\varphi = (Z/r) \exp(-r/D), \quad (1)$$

where r is the distance from the particle and D is the Debye screening radius. Here and below we use atomic units ($e^2 = m_e = \hbar = 1$) in which, for example the unit of length is the Bohr radius $a_0 = 5.29 \cdot 10^{-9}$ cm.

To determine the energy-level shift of an atom in a plasma medium one frequently uses the method of quantization in the potential (1). It is assumed that the free electrons of the plasma screen the atomic nucleus, while the bound electrons move in this screened potential. Various modifications of this method are also used and are based on similar physical premises.

The number of bound states in the potential (1) is finite and decreases with decrease of D . For a certain sufficiently small D (or sufficiently high density) there are no such states at all. The Debye radius D for a dense plasma in a metal is so small that the ground state level of, say, a hydrogen atom turns out to be close to the continuum.² It is assumed on this basis^{2,3} that a proton in a metal has apparently no bound electron. The presence or absence of a bound electron is important for the energy loss by atoms entering into metals at low velocities, $v \ll 10^8$ cm/s.

Quantization in the potential (1) to determine the energies of bound atomic electrons is in fact an illegitimate operation that leads to wrong results. The error is due to incorrect coordination of the atom with the plasma medium.

When an atom lands in a metal the parameters of the atom and the metal deviate from their unperturbed values in a coordinated manner: the perturbations of the metal and the atom depend on one another. In particular, perturbation of the metal and its reaction on the atom depend on the charge state of the atom itself. The potential (1) is established in the

plasma medium only if the charge Z has no bound electrons, and the screening is only by the metal electrons.

A correctly coordinated determination of the atomic levels should take into account the presence of the bound electrons whose energies are sought. The plasma is then perturbed by a particle that already has bound electrons. The energy levels, say, of a neutral atom should be determined under the condition that the plasma medium is perturbed by a neutral particle and not by a charged one, and this in turn decreases substantially the perturbation of the atom.

Quantization in the potential (1) is incorrect for one other reason.

The potential (1) is established in the case when a positively charged nucleus Z is screened by the charge, of equal absolute value, of the free electrons located in a sphere of radius $\sim D$. Quantization in the potential (1) means addition to this system of one more electron, so that a negatively charged system is obtained. This contradicts the principle of total screening of the charge in the conducting medium. It will be shown below, in the actual solution of the problem, that this discrepancy is eliminated by a nontrivial (for the Thomas-Fermi method) subdivision of the screening electrons into free and bound ones.

Our present task is to find the shifts of the atomic level for correct coordination of the atom with the metallic plasma medium at arbitrary value of its density and a Thomas-Fermi description of its electrons. The atomic electrons will be considered by a quantum-mechanical approach. A general analysis is carried out of the qualitative dependence of the binding energy of the atomic electrons on the plasma density, and it is shown that this dependence is different than for the potential (1). The atomic levels approach the continuum asymptotically with increase of the density of the medium, and there are no finite densities at which the levels can be pushed out into the continuum.

A quantitative solution will be given for the case of low plasma-metal densities, when the shifts of the atomic levels can be calculated by perturbation theory. Owing to correct coordination, the metal-electron densities at which perturbation theory is valid turns out to be much larger than for quantizing in the potential (1), so that perturbation theory can be used for many real metals.

2. Let us prove some general statements concerning the shift of the atomic levels, using the assumption that the charges of the medium and of the atom are additive, i.e., assuming that the total charge density Q of the combined atom + medium system is equal to the sum of the charge

densities ρ of the plasma-medium electrons and of the ρ_{qu} of the atomic electrons:

$$Q = \rho + \rho_{qu}.$$

Let us see first how serious are the constraints imposed by the assumed additivity of the charges. The electrons of the atom and of the medium interact in the combined medium both directly and by exchange, and this interaction is in general not small. It is therefore impossible to single out some electron group that can be assumed to belong only to the atom and not to the medium. The atomic electrons are continuously exchanged with the electrons of the medium. This, however, does not mean in general that the density additivity assumption breaks down. Since the electrons are indistinguishable, it is immaterial which of them are located at a given instant on atomic orbits. In the Hartree-Fock (HF) approximation, which takes the exchange into account, the total density Q of the charges of the atom + medium system is equal to the sum of the densities from individual orbitals ψ_i :

$$Q = e \sum_i^N |\psi_i|^2$$

(N is the number of orbitals filled with electrons), since the different are mutually orthogonal. It is this equality which ensures the additivity we need. A fraction of the orbitals ψ_i (and a large one at that) describes the states of the electron in the continuous spectrum of the conduction band of the metal, and constitutes the charge density of the medium. If the HF orbitals ψ_i include some that are localized around an atom, the latter must be regarded as atomic and they represent the charge density of the atomic electrons. Additivity is thus present in the HF approximation. Since the HF method describes well enough the properties of many-electron atoms, there is every reason for assuming that the charge-additivity condition is quite well met in our present problem.

Let us show that if the charges are additive, introduction of a neutral atom into a medium of any density allows all the electrons to remain bound to the atom.

The total potential φ of the electric field satisfies the Poisson equation

$$\nabla^2 \varphi = -4\pi(\rho_0 - \rho - \rho_{qu} + Z\delta(r)), \quad (2)$$

where ρ_0 is the average density of the positive charge (of the atom nuclei) of the medium, and $\delta(r)$ is the delta-function. The core of the introduced atom is at the point $r = 0$.

In a conducting medium, the positive charge Z of the introduced atomic nucleus is completely screened by the charge of the electrons. Some of these electrons can be on bound orbits, and the remainder is supplied by the conduction band, so that the neutrality condition that follows from (2) on the basis of the Gauss theorem can be written in the general case in the form

$$Z = N + \int (\rho - \rho_0) d\mathbf{r}, \quad (3)$$

where

$$N = \int \rho_{qu} d\mathbf{r} \quad (4)$$

is the number of electrons bound to the atom.

Assume that all electrons remain bound to the atom, i.e., $N = Z$. We then obtain from (3)

$$\int (\rho - \rho_0) d\mathbf{r} = 0, \quad (5)$$

meaning that the total charge supplied by the medium to the region of the atom is zero. The medium is only polarized.

From the integral neutrality condition (5) for the medium follows validity of the assumption $N = Z$ that the number of electrons bound to the atom is conserved. Indeed, the total potential φ can be written on the basis of the charge additivity in the form of the sum

$$\varphi = Z/r + \Phi_m + \Phi_{qu}, \quad (6)$$

where Φ_{qu} is the potential produced by the bound (quantum) electrons, Z/r is the potential of the introduced atomic nucleus, and Φ_m is the potential produced by the charges $\rho - \rho_0$ of the medium. From condition (5), or from the condition that the total charge of the medium be zero, it follows that at large distances from the core of the introduced atoms ($r \rightarrow \infty$) the value of Φ_m decreases more rapidly than r^{-1} . This means in turn that the potential

$$V = Z/r + \Phi_m,$$

in which the bound electrons move has, just as in the unperturbed atom, a Coulomb asymptotic $V \rightarrow Z/r$. Obviously, Z electrons can be bound in a potential well with the same asymptotic.⁴ Moreover, all the electronic excited states present in the unperturbed atom at $V \equiv Z/r$ remain bound in such a potential. (We emphasize that V is the potential acting on the entire bound-electron system as a whole.)

Thus, by assuming the equality $N = Z$, we arrive at still stronger statement: all the electrons remain bound to the atom, and furthermore not only in the ground state but also in all the excited states. This means that the condition that the number of electrons bound to the atom be preserved accords with the correct coordination of the atom with the medium.

Naturally, the system considered can be also in an ionized state if several electrons are removed from the atom by some process.

The foregoing qualitative analysis based on a consistent coordination of the medium and the atom leads for the atom's energy levels in a medium to an entirely different behavior than the method of quantization in the potential (1). There exist no finite values of the medium's density at which the atomic levels can be pushed out into the continuum. Of course, an increase of the density of the medium leads to a stronger screening of the atomic core by the electrons. More electrons of the medium penetrate into the atomic orbits. By virtue of the integral neutrality (5), however, at larger distances r there is produced an excess of positive charge of the medium, so that the potential V again approaches the Coulomb potential Z/r . The quantum orbits of the atom are located precisely in the region of space with excess positive charges.

What decreases exponentially as $r \rightarrow \infty$ is the total potential. In the case of a neutral atom, φ is equal to the sum of terms that are mutually cancelled out on the asymptote, viz., the potential Φ_{qu} of the bound (quantum) electrons,

$$\Phi_{qu} = - \int \frac{\rho_{qu}(r')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' \rightarrow - \frac{Z}{r}, \quad (7)$$

and the potential V due to the core and the medium, with an asymptotic value, as already mentioned, $+ Z/r$.

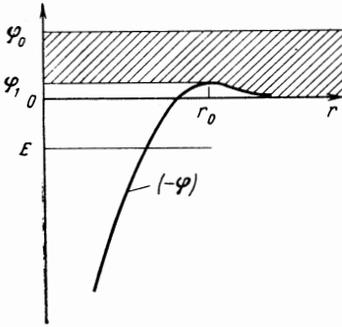


FIG. 1. Filling of energy states of the continuous spectrum in the region of the atom by TF electrons. The thick line shows the total potential for the electrons ($-\varphi$).

3. We consider specifically the energy levels of a hydrogen atom in a metal under normal conditions, when the metal temperature is much lower than the Fermi energy φ_0 . In this case the electrons of the metal can be described using the Thomas-Fermi (TF) approximation. Their density is determined by the local value of the potential φ , which is attracting for them in the region of the atom (see Fig. 1).

In the usual TF method it is assumed¹ that at any point of space the electrons fill all the states with momenta from zero to the maximum Fermi momentum. Such a filling of the momentum space is in our case unsuitable for the following reasons. We describe a bound electron of the hydrogen atom on the basis of the quantum-mechanical Schrödinger equation. If the density of the remaining electrons is expressed with the aid of the usual TF expression, it turns out that part of these electrons will have negative total energies and will be consequently bound to the atom. The number of all the electrons bound to the atom is then indeterminate. If we place a bound electron on a quantum orbit, we must see to it that all the remaining electrons be only in the continuous spectrum of the conduction band (see Fig. 1). To this end we could subtract from the usual density of the TF electrons the density of those whose energies are negative. This procedure, however, is not enough.

One more circumstance complicates somewhat the formulation of the problem, a formulation perfectly correct with respect to the number of bound electrons. In view of the integral neutrality condition (5), the total potential φ should be of alternating sign. Equality of the total charge of the medium (5) to zero requires that the density $\rho - \rho_0$ be of alternating sign as a function of distance. This means (if the electrons are described by the TF method) that if a region attracting the band electron exists near the nucleus, a region that repels them should exist far from the nucleus. The total potential for the electrons (i.e., $-\varphi$) should have a maximum. The bound electrons will then be those with energies lower than the top φ_1 of the potential barrier (see Fig. 1). It is the density of just these electrons which should be subtracted from the total density of the TF electrons. The charge density $\rho - \rho_0$ of the medium, which tends to zero at infinity (by virtue of the neutrality condition), is then equal to

$$\rho - \rho_0 = \frac{2^{7/2}}{3\pi^2} [(\varphi_0 + \varphi)^{3/2} - (\varphi_1 + \varphi)^{3/2} \theta(r_0) - \varphi_0^{3/2}], \quad (8)$$

where $\theta(r_0)$ is the step function: $\theta(r < r_0) = 1$, $\theta(r > r_0) = 0$. The first term in the square brackets of (8) is the total density of electrons with momenta from zero to the maxima

corresponding to the maximum energy of the occupied state of the band—the Fermi energy φ_0 . The second term is the density of electrons with energies lower than the top of the potential barrier φ_1 , i.e., the density of the electrons bound to the atom. The last term in (8) is the density of the positive charge of the ions of the metal, which we shall assume to be independent of the coordinates (the model of smeared ion charge) and which is not changed when an additional atom is introduced into the metal.

The equations describing the atom + metal system can now be written in the form

$$\nabla^2 \Phi_m = \frac{2^{7/2}}{3\pi} [(\varphi_0 + \varphi)^{3/2} - (\varphi_1 + \varphi)^{3/2} \theta(r_0) - \varphi_0^{3/2}], \quad (9)$$

$$\nabla^2 \psi + 2(E + Z/r + \Phi_m)\psi = 0, \quad (10)$$

where ψ and E are the wave function and energy of the atomic electron described with the aid of the quantum Schrödinger equation (10). The Poisson equation (9) for the potential Φ_m of the metal is obtained from the Poisson equation by an identity transformation, viz., by substituting in it the total potential φ in the form of the sum (6) and eliminating the potential of the core on the basis of the equality $\nabla^2(Z/r) = Z\delta(r)$ and of the potential of the quantum electron on the basis of the equalities

$$\nabla^2 \Phi_{qu} = -\nabla^2 \int |\psi|^2 d\mathbf{r}' / |\mathbf{r} - \mathbf{r}'| = -|\psi|^2 \equiv \rho_{qu}.$$

The system (9) and (10) must be solved subject to the condition that the wave function ψ be finite (this permits finding the eigenenergy E), and that the potential Φ_m be finite as $r \rightarrow 0$ and decrease as $r \rightarrow \infty$.

Under the foregoing assumptions, the wave function ψ_0 of the unperturbed atom remains spherically symmetrical also inside the metal. We can therefore seek in this case spherically symmetric solutions ψ and Φ_m of Eqs. (9) and (10). Introducing new functions, we get

$$\chi_m''(r) = \frac{2^{7/2}}{3\pi} r [(\varphi_0 + \varphi)^{3/2} - (\varphi_1 + \varphi)^{3/2} \theta(r_0) - \varphi_0^{3/2}], \quad (11)$$

$$P''(r) + 2[E + (Z + \chi_m)/r]P = 0, \quad (12)$$

$$\Phi_m \equiv \chi_m/r, \quad \psi = P(r)/r. \quad (13)$$

These sets of equations contain two unknown parameters: the height φ_1 of the potential barrier and the distance r_0 at which $\varphi(r_0) = \varphi_1$. They can be obtained from the following considerations. At the point r_0 we have a zero derivative $\varphi'(r_0) = 0$, i.e., a zero electric field. This means that the neutrality of the total charge is so to speak twofold: the total charge inside the sphere $r < r_0$ is zero, and the total charge in the outer region $r_0 \leq r < \infty$ is separately equal to zero.

4.1. We consider now the solution of the system (11), (12) in the limit of a rarefied medium, i.e., low values of ρ_0 and accordingly of φ_0 . For metals under normal conditions these parameters are small in atomic units. The atomic unit of density is $a_0^{-3} = 6.76 \cdot 10^{24} \text{ cm}^{-3}$. The densities of the quasi-free electrons of the conduction bands of metals are in the range $8 \cdot 10^{22} - 9 \cdot 10^{27} \text{ cm}^{-3}$, or $\rho_0 \approx (1.2 - 0.14) \times 10^{-2}$ in atomic units. The Fermi energy is in the range 0.3–0.06 a.u. (7–1.5 eV).

The perturbation of the atom inside a rarefied medium is small, and the total potential φ is close to the static (unperturbed) potential $\Phi_{at}^{(0)}$ of the atom:

$$\varphi \approx \Phi_{at}^{(0)} = Z/r + \Phi_{qu}^{(0)}, \quad (14)$$

which is ~ 1 in the principal region. This allows us to expand the density of the band electrons (8) in the region of the atom in terms of the small ratio $(\varphi_0/\varphi) \ll 1$ ($\theta = 1$ in this region):

$$\rho - \rho_0 \approx 2^{1/2} \pi^{-2} (\varphi_0 - \varphi_1) \varphi^{1/2} \quad (\varphi_0 \ll \varphi, \theta = 1, r \leq r_0). \quad (15)$$

Let us assess the order of magnitude of this density. In an unperturbed metal the band electron density obtained by TF method is $\rho(\infty) = (2^{1/2} \pi^{-2}) \varphi_0^{3/2}$. The density (15) is much higher than this unperturbed density. The ratio $|(\rho - \rho_0)/\rho_0| \approx (\varphi/\varphi_0)^{1/2} \gg 1$ (it will be shown below that $\varphi_1 \ll \varphi_0$ as $\varphi_0 \rightarrow 0$). Thus, a relatively large amount of electronic charge flows into the region of the atom. Its absolute value, however, remains small, since (15) is proportional to the small quantity φ_0 (two inequalities are satisfied: $\rho_0 \ll |\rho_0 - \rho| \ll 1$), and the perturbation of the atom remains weak nonetheless.

Using (14), we obtain from the Poisson equation (11) a relation for the calculation of χ_m (or Φ_m):

$$\chi_m'' \approx 2^{3/2} \pi^{-1} (\varphi_0 - \varphi_1) r [\Phi_{\text{at}}^{(0)}]^{1/2}. \quad (16)$$

The right-hand side of this relation contains no unknown function, so that χ_m is determined by double integration. The boundary condition that χ_m must satisfy at $r = 0$ should obviously be $\chi_m(0) = 0$, since $\Phi_m(0)$ should be finite by virtue of the integral neutrality (5). As $r \rightarrow \infty$ we can also put $\chi_m'(\infty) = 0$. Indeed, the expansion (15) [and hence (16)] is generally speaking incorrect as $r \rightarrow \infty$. At large distances, where the expansion (15) is not valid, the total potential tends to zero as $r \rightarrow \infty$, and becomes small, of the order of φ_0 , so that it can be set equal to zero when the principal term of the expansion of χ_m is determined. We obtain thus

$$\Phi_m \approx \frac{2^{3/2} (\varphi_0 - \varphi_1)}{\pi r} \int_0^r dy \int_y^\infty [\Phi_{\text{at}}^{(0)}(x)]^{1/2} x dx. \quad (17)$$

In first-order approximation the atomic-level shift is

$$\Delta E \equiv E - E_0 \approx \langle \psi_0 | \Phi_m | \psi_0 \rangle, \quad (18)$$

which leads, when (17) is used, to

$$\Delta E \approx \frac{2^{3/2}}{\pi} (\varphi_0 - \varphi_1) \int_0^\infty \psi_0^2 \frac{dr}{r} \int_0^r dy \int_y^\infty [\Phi_{\text{at}}^{(0)}(x)]^{1/2} x dx. \quad (19)$$

This expression is the end purpose of the calculations in the perturbation-theory approximation. It contains the unknown quantity φ_1 which we now proceed to calculate.

4.2. We shall show that $\varphi_1 \ll \varphi_0$ as $\varphi_0 \rightarrow 0$, and therefore the quantity φ_1 can be neglected in Eqs. (17) and (18) above in the case of perturbation theory. In other words, in perturbation theory the condition that there be no bound TF electrons is met if the free electrons fills an interval of positive energies $\{0, \varphi_0\}$ at any point of space.

With decrease of the density of the medium, the total potential φ should obviously approach, in an ever increasing volume around the atom, the unperturbed static potential of the atom $\varphi \sim \Phi_{\text{at}}^{(0)}$. This means that the point r_0 should in this case move farther away: $r_0 \rightarrow \infty$ as $\varphi_0 \rightarrow \infty$. We shall show below that $\varphi_1 \ll \varphi_0$ as $\varphi_0 \rightarrow 0$, so that we can use for the density (8) the linearized expression

$$\rho - \rho_0 \approx (\lambda^2/4\pi) \varphi \quad (r \geq r_0).$$

Equation (11) takes then the form

$$\chi_m'' - \lambda^2 \chi_m = \lambda^2 r \Phi_{\text{at}}^{(0)} \quad (r \geq r_0), \quad (20)$$

where

$$\lambda^{-1} \equiv D = 2^{-5/4} \pi^{1/2} \varphi_0^{-1/4} \quad (21)$$

is the Debye radius for a degenerate Fermi gas.

Equation (20) has a general solution that decreases as $r \rightarrow \infty$, viz.,

$$\chi_m = C e^{-\lambda r} - \frac{\lambda}{2} \left[e^{-\lambda r} \int_{r_0}^r e^{\lambda x} \Phi_{\text{at}}^{(0)}(x) x dx + e^{\lambda r} \int_r^\infty e^{-\lambda x} \Phi_{\text{at}}^{(0)}(x) x dx \right], \quad (22)$$

where the indeterminate constant C will be determined below from the condition $\varphi'(r_0) = 0$.

The static potential $\Phi_{\text{at}}^{(0)}$ of the atom is equal to the sum of the potentials of the core and of the atomic electrons (7). For a spherically symmetric neutral-atom wave function it can be written in the form

$$\Phi_{\text{at}}^{(0)} = \int_r^\infty (x/r-1) P_0^2(x) dx. \quad (23)$$

For a neutral hydrogen atom in the ground state we have¹

$$\Phi_{\text{H}(1s)}^{(0)} = (1+1/r) e^{-2r}.$$

In the case of a neutral atom,

$$\Phi_{\text{at}}^{(0)} \sim \exp(-2\alpha r),$$

and the integrals in (22) and (23) can be calculated by parts, by integrating the exponential and differentiating the remaining integrand. This operation corresponds to expansion in powers of $r_0^{-1} \ll 1$. Integrating once, we get

$$\chi_m \approx C e^{-\lambda r} + \lambda^2 |P_0(r)|^2 / 4\alpha^2 (4\alpha^2 - \lambda^2) r, \quad \alpha \approx (2|E_0|)^{1/2}. \quad (24)$$

We obtain similarly the asymptote of the atomic potential:

$$\Phi_{\text{at}}^{(0)}(r) \approx P_0^2(r) / 4\alpha^2 r^2. \quad (25)$$

The condition $\varphi'(r_0) = 0$ (vanishing of the charge inside the sphere $r \leq r_0$) determines C :

$$C = -e^{\lambda r_0} P_0^2(r_0) / 2\alpha \lambda r_0, \quad (26)$$

while the vanishing of the total charge outside the sphere $r = r_0$ allows us to find the value of r_0 :

$$r_0 \approx 4\alpha^2 / \lambda^3 = 4\alpha^2 D^3. \quad (27)$$

the maximum barrier height φ_1 turns out to be

$$\varphi_1 = -\varphi(r_0) = (\lambda/2\alpha)^5 P_0^2(r_0). \quad (28)$$

At low density, the Debye radius D is larger than the electron shell of the atom, so that according to (27) the point r_0 is located far outside the atom and moves farther away with decrease of φ_0 (with increase of D). It can be seen from (28) that φ_1 decreases exponentially with decrease of φ_0 . Consequently φ_1 can be neglected in the equations above.

5. We consider now quantitative results for the case of a neutral hydrogen atom. Neglecting φ_1 in (18), we write the expression for the ground-state energy shift in the form

$$\Delta E = \frac{2^{3/2}}{\pi} \varphi_0 \int_0^\infty r e^{-2r} dr \int_0^r dy \int_y^\infty x (\Phi_H)^{1/2} dx, \quad (29)$$

$$\Phi_H = (1+r^{-1})e^{-2r}. \quad (30)$$

Integrating by parts several times, we reduce this expression to the form

$$\Delta E = \frac{2^{3/2}}{\pi} \varphi_0 \left[\int_0^\infty (x^2+x)^{1/2} e^{-x} dx - \int_0^\infty (x+1) (x^2+x)^{1/2} e^{-3x} dx \right]. \quad (31)$$

Numerical calculation of the integrals yields

$$\Delta E_{H(1s)} = 1.87 \varphi_0 = 0.58/D^4. \quad (32)$$

For $\varphi_0 \approx 2$ eV (alkali metals) we obtain $\Delta E = 3.0$ eV, which is 4.5 times smaller than the initial binding energy 13.6 eV of the ground state of the hydrogen atom, so that perturbation theory can be used. For dense metals such as iron we have $\varphi_0 \sim 5$ eV and the shift increases to ~ 10 eV, so that perturbation theory cannot be used. Perturbation theory overestimates the electron density near the core of the atom, so that the exact shift should be smaller.

Applying perturbation theory to the potential (1), we obtain $\Delta E \sim D^{-1}$, which is much larger than (32) as $D \rightarrow \infty$. Thus, correct coordination leads in the perturbation-theory limit to much lower perturbations of the atom.

6. Perturbation in a dense plasma of multiply charged aluminum ions was considered in a recent paper,⁵ likewise in

the smeared-positive-charge model but using the ion-sphere approximation.⁶ The boundary condition imposed on the solution did not accord with the problem considered: it was assumed in Ref. 5 that a nonzero electric field exists only inside a sphere $r < R_0$ (the radius R_0 of this sphere was assumed equal to the average distance between the plasma particles), and outside this sphere, at $r \geq R_0$, the plasma was assumed to be not perturbed at all by the ion. Such solutions are usually considered in investigations of compressed matter or crystals, and they are continuous on the boundaries of individual atoms at $r = R_0$. In the case of an impurity atom in a solid or plasma, however, the boundary conditions must be applied as $r \rightarrow \infty$, taking into account by the same token the perturbation of the plasma by the atomic particle.

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