

Plasma approach to the theory of photoabsorption and polarizability of complex atoms

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The problem of the dynamic response of multielectron atoms is solved within the framework of the Thomas-Fermi statistical theory. The interaction between the atom and radiation is described in the local dielectric constant approximation, the dielectric constant being defined by the plasma formula. In this approach the polarizability and photoabsorption strictly satisfy the dispersion relationships and the sum rule. Photoabsorption in this case is due to transformation of the energy of the external field into Langmuir oscillations near the critical point at which the local plasma frequency of the atomic electrons is the same as that of the external field. The results are compared with the experimental data and with other theoretical approaches. An approximate treatment of the shell structure yields a description of some features of the frequency dependence of the photoabsorption cross section.

In spite of the state of perfection of the old methods of calculation of atomic structure and the development of new ones¹⁻³ and the application of the most powerful calculating techniques, the theoretical description of the properties of complex multielectron atoms still remains a problem of current interest. One of the traditional approaches to this problem is the use of the Thomas-Fermi statistical theory.

The statistical theory has been widely and successfully used to calculate the electron density^{4,5} and the polarizability⁶ of the atomic shell, and also to describe the equation of state of highly compressed and ionized matter.⁷⁻⁹ Significantly fewer papers have been dedicated to the optical properties of complex atoms (see the review in Ref. 10). In the present paper an effort is undertaken to achieve a consistent statistical description of the photoionization and the polarization of multielectron atoms. Our approach is closest to that of Lundqvist *et al.*^{11,12} However, we have succeeded in dispensing with a number of previously used approximations and in considering not only the photoabsorption cross section, but also the real part of the polarizability.

1. BASIC EQUATIONS

In the study of the interaction of multielectron atoms with an electromagnetic field it is natural to use an approach which is customary in plasma physics problems—the classical kinetic Vlasov equation with self-consistent field. If the wavelength of the incident radiation is much greater than the characteristic dimensions of the atom, $\lambda \gg a$, then the self-consistent field can be assumed to be a potential field and the system of Vlasov equations has the form (here and below we use the atomic system of units $\hbar = m = |e| = 1$):

$$\frac{\partial f}{\partial t} + \mathbf{p} \frac{\partial f}{\partial \mathbf{r}} - \nabla U \frac{\partial f}{\partial \mathbf{p}} = 0, \quad (1a)$$

$$\Delta U = 4\pi [Z\delta(\mathbf{r}) - n], \quad n = \int f d\mathbf{p}, \quad (1b)$$

where $f(\mathbf{r}, \mathbf{p}, t)$ is the electron distribution function, $U(\mathbf{r}, t)$ is the electron energy in the self-consistent field, $n(\mathbf{r}, t)$ is the electron density, and the term $Z\delta(\mathbf{r})$ takes into account the presence of the nucleus. In the absence of an external perturbation we have $f = f_0(r, p)$, $U = \varphi(r)$, $n = n_0(r)$, and Eq. (1a) has a solution in the form

$$f_0(r, p) = \frac{2}{(2\pi)^3} \theta(E_F - E), \quad E = p^2/2 + \varphi(r). \quad (2)$$

The use of this expression in Eqs. (1b) leads to the Thomas-Fermi (TF) statistical model:

$$n_0(r) = \frac{p_F^3(r)}{3\pi^2}, \quad p_F(r) = [2(E_F - \varphi(r))]^{1/2}, \quad (3)$$

$$E_F - \varphi(r) = \frac{Z}{r} \chi(r/l_{TF}), \quad l_{TF} = \frac{(3\pi)^{2/3}}{2^{1/3}} Z^{-1/3},$$

where $\chi(x)$ is the Thomas-Fermi function. Thus, in the approach under consideration the Thomas-Fermi theory arises as a model of the unperturbed state of the atom.

In order to consider small perturbations, we linearize Eqs. (1) in the small monochromatic deviations δf , $\delta U = -V$, and δn of the quantities f , U , and n from their unperturbed values:

$$-i\omega \delta f + \mathbf{p} \frac{\partial \delta f}{\partial \mathbf{r}} - \nabla \varphi(r) \frac{\partial \delta f}{\partial \mathbf{p}} = -\nabla V(\mathbf{r}) \frac{\partial f_0}{\partial \mathbf{p}}, \quad (4a)$$

$$\Delta V(\mathbf{r}) = 4\pi \delta n(\mathbf{r}), \quad \delta n(\mathbf{r}) = \int \delta f(\mathbf{r}, \mathbf{p}) d\mathbf{p}. \quad (4b)$$

It is necessary to supplement these equations with a boundary condition on the potential $V(\mathbf{r})$. In order to find the optical constants of the atom, we must solve the scattering problem for the system described by Eqs. (4). In the long-wavelength approximation $\lambda \gg a$ the corresponding boundary conditions have the form

$$V(\mathbf{r})|_{r \rightarrow \infty} = -\mathbf{e}_0 \mathbf{r} + \frac{\mathbf{d}\mathbf{r}}{r^3}, \quad \mathbf{d} = \alpha(\omega) \mathbf{e}_0, \quad (5)$$

where \mathbf{e}_0 is the amplitude of the incident wave and $\alpha(\omega)$ is the dipole dynamic polarizability of the atom.

Equations (4) with the boundary condition (5) constitute a consistent formulation of the problem of photoionization and dynamic polarizability of a TF atom. However, due to the nonlocal coupling between the quantities δn and V which follows from Eqs. (4), the solution of this problem is associated with significant calculation difficulties, and up until now has not been considered.¹⁾

In the two limiting cases $\omega = 0$ and $\omega \rightarrow \infty$ the situation simplifies considerably. Setting $\omega = 0$ in Eqs. (4), we easily

obtain

$$\delta f = \frac{2}{(2\pi)^3} V(\mathbf{r}) \delta(E_F - E), \quad \delta n = \frac{p_F(r)}{\pi^2} V(\mathbf{r}); \quad \omega=0, \quad (6)$$

and the equation for the function $V(\mathbf{r})$ takes the form

$$\Delta V(\mathbf{r}) = \frac{4}{\pi} p_F(r) V(\mathbf{r}). \quad (7)$$

This equation was obtained in Ref. 14 by direct linearization of the TF equation. The method of calculating the statistical polarizability of the atom based on it was developed in Refs. 15 and 16, and for multielectron atoms and ions in many cases it gives very satisfactory agreement with experiment.

Below we will consider the opposite limiting case $\omega \rightarrow \infty$. As for $\omega = 0$, in this case the coupling between the quantities turns out to be local, and it can be derived from Eqs. (4). However, the correct result can be obtained more simply from the following considerations: it is well known that in the long-wavelength approximation $\lambda \gg a$ the scattering of the electromagnetic wave by a particle is described by the equation^{17,18}

$$\operatorname{div}[\varepsilon(\mathbf{r}, \omega) \nabla V(\mathbf{r})] = 0 \quad (8)$$

with boundary condition (5). Substituting the well-known high-frequency approximation for the dielectric constant

$$\varepsilon(\mathbf{r}, \omega) \Big|_{\omega \rightarrow \infty} = 1 - \frac{\omega_p^2(\mathbf{r})}{\omega^2}, \quad \omega_p^2(\mathbf{r}) = 4\pi n(\mathbf{r}), \quad (9)$$

into Eq. (8), we obtain an equation for the dynamic polarizability of the TF atom which is equivalent to Eqs. (4) in the limit $\omega \rightarrow \infty$.

Note that there is no contradiction in the simultaneous use of the long-wavelength approximation (8), (5) to the scattering problem in the high-frequency limit (9). The condition $\lambda \gg a$ for the atom actually means $\omega < \omega_a \sim 10$ keV while the region of applicability of relation (9) is determined by the condition $\omega > I_0$ where $I_0 \gtrsim 10$ eV—the ionization potential of the electron shell that gives the main contribution to the absorption cross section. For a consistent (within the framework of TF theory) consideration of the entire frequency interval $I_0 < \omega < \omega_0$, it is necessary to base the derivation directly on Eqs. (4). However, as will become clear in what follows, even the simple approximation (8), (9) leads to interesting physical results.

2. POLARIZABILITY OF THE THOMAS-FERMI ATOM

2.1. General properties of the polarizability

Making use of the spherical symmetry of expression (9), we separate out the angular variables in Eqs. (5) and (8):

$$V(\mathbf{r}) = V(r) \cos \theta, \quad (10)$$

where θ is the angle between \mathbf{r} and \mathbf{e}_0 .

We then obtain for the function $V(r)$ the equation

$$V''(r) + \left[\frac{2}{r} + \frac{\varepsilon'(r, \omega)}{\varepsilon(r, \omega)} \right] V'(r) - \frac{2}{r^2} V(r) = 0, \quad (11)$$

$$V|_{r \rightarrow \infty} = -e_0 r [1 - \alpha(\omega)] / r^3.$$

Here the prime denotes differentiation with respect to r .

For $\operatorname{Im} \varepsilon(r, \omega) \equiv 0$ Eq. (11) has a singularity associated with the possibility of the vanishing of the function $\varepsilon(r, \omega)$ at

some point $r = r_0$. This singularity gives rise to an imaginary part of the polarizability $\alpha(\omega)$, and therefore of the photoabsorption cross section:

$$\sigma(\omega) = \frac{4\pi\omega}{c} \operatorname{Im} \alpha(\omega). \quad (12)$$

From the physical point of view, the condition $\varepsilon(r_0, \omega) = 0$ implies in the neighborhood of the radius $r = r_0$ plasma oscillations of the electron shell of the atom, analogous to the plasma oscillations of a homogeneous electron gas, can be resonantly excited. The transformation of the energy of the external field into these oscillations also leads to photoabsorption. This classical mechanism of photoabsorption in atoms was first discussed in Ref. 11; however, a consistent quantitative consideration of this question on the basis of Eq. (11) has up till now not been carried out.

In Ref. 19 the general properties of Eq. (11) were investigated, and an analytic solution of the problem for $\varepsilon(r, \omega)$ in the form of Eq. (9) was also obtained in the model case in which the electron density depends linearly on r . As was shown in Ref. 19, if the function $\varepsilon(r, \omega)$ is a sufficiently smooth function of r and possesses the usual analytic properties in the variable ω (see Ref. 20), then the polarizability $\alpha(\omega)$ defined in Eq. (11) satisfies the Kramers-Kronig relations, and the photoabsorption cross section (12) satisfies the dipole sum rule. Further, the following formula was derived from $\operatorname{Im} \alpha(\omega)$ in Ref. 19:

$$\operatorname{Im} \alpha(\omega) = \frac{\pi}{3} \left[\frac{r^2}{|\varepsilon'(r, \omega)|} \left| \frac{\varepsilon(r, \omega) V'(r)}{e_0} \right|^2 \right]_{r=r_0}, \quad (13)$$

where r_0 is a function of the frequency and is defined by the equation $\varepsilon(r_0, \omega) = 0$ (it is assumed that this equation has a unique solution). Note that the potential $V(r)$ diverges logarithmically at the singular point $r = r_0$, and the quantity $\varepsilon V'$, which coincides with the radial component of the induction vector to within a factor of $\cos \theta$, is finite at $r = r_0$.

The polarizability $\alpha(\omega)$ has no singularities for real ω , nor for any continuous distribution $\varepsilon(r, \omega)$. The presence of singularities would imply the existence of undamped free oscillations of the homogeneous dielectric particle, which are described by Eq. (11) with null boundary conditions. Such oscillations were discussed in Refs. 21 and 22 (see also Ref. 10). Indeed, they are possible only in the case of homogeneous particles (for a more detailed discussion, see Ref. 19). For $\varepsilon(r, \omega)$ of the form of Eq. (9) the photoabsorption has a continuous spectrum and is obviously nonzero for all frequencies $\omega < \omega_{\max}$, where $\omega_{\max} = (4\pi n_{\max})^{1/2}$, i.e., it is defined by the maximum value of the electron density in the atom.

2.2. Numerical results in the TF mode; discussion of the experiment

Let us pass on now to the calculation of the dipole dynamic polarizability of the TF atom. According to the previous subsection this quantity is defined by Eq. (11), where the dielectric constant is given by Eq. (9), and for $n(\mathbf{r})$ it is necessary to use the electron density in the TF atom. In the TF theory the structure of the atom (ion) is prescribed by two parameters—the charge of the nucleus Z and the degree of ionization $q = (Z - N)/Z$. Transforming to dimensionless coordinates $r = x/l_{\text{TF}}$ [see Eqs. (3)], it can be easily shown that the dependence of α on these quantities has the

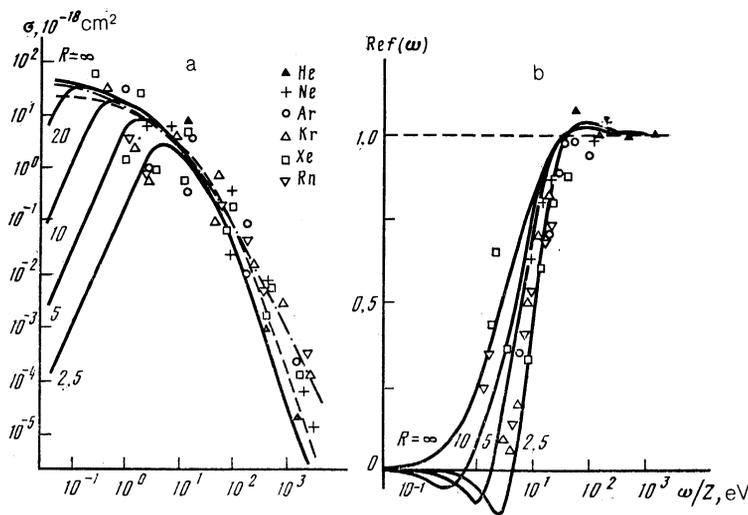


FIG. 1. The solid curves represent (a) the photoabsorption cross section and (b) the real part of the modified scattering factor [see Eq. (15)], calculated for a neutral atom ($R = \infty$) and ions in the TF model. The values $R = 2.5, 5, 10,$ and 20 (the numbers are given alongside the curves) correspond to the degrees of ionization $q = 56, 30, 12,$ and 3% . In Fig. 1a are also plotted experimental data²⁵ on the photoabsorption of the rare gases. The dashed and dash-dot curves are respectively the calculated results of the authors of Ref. 11 and Ref. 26. Figure 1b also shows the calculated values of $\text{Re } f(\omega)$ for the rare gases from the tables in Ref. 24. The plotting symbols for the different elements are the same in both figures.

form

$$\alpha(\omega, Z, q) = \frac{1}{Z} \alpha_R \left(\frac{\omega}{Z} \right). \quad (14)$$

Here α_R is a general function for all ions of the same degree of ionization, and R is the dimensionless radius of the ion, which is uniquely connected with q (see Ref. 23). In order to conserve the scaling properties of TF theory, it is more convenient to consider the photoabsorption cross section (12) and the modified scattering factor (this quantity differs by the factor N from the commonly used scattering factor—see, e.g., Ref. 24):

$$f(\omega) = \alpha(\omega) / \alpha_\infty, \quad \alpha_\infty = -N / \omega^2, \quad (15)$$

where $\alpha_\infty = \alpha(\omega) |_{\omega \rightarrow \infty}$ is the polarizability of a swarm of N free electrons. As can be seen from Eq. (14), the quantities σ and f depend on ω and Z only through the combination ω/Z , and therefore these dependences are general for all ions of given degree of ionization q .

Results of the numerical solution of Eq. (11) are presented in Figs. 1a and b. The families of curves depicted there correspond to different values of R , so that $R = \infty$ corresponds to the neutral atom in the TF model. As $\omega \rightarrow \infty$, the absorption cross section falls off as $(\omega/Z)^{7/3}$ for the ion and falls to a constant value for the neutral atom, and as $\omega \rightarrow 0$, it has the value $\sigma \propto (Z/\omega)^3$. Note however that these limiting forms have a bounded region of applicability since they are determined by the behavior of the electron density at the boundary (in the case $\omega \rightarrow 0$) and in the center (in the case $\omega \rightarrow \infty$) of the atom, where the TF model is inapplicable. For $\omega \gtrsim 100Z$ eV the real part of the polarizability falls to its own asymptotic limit α_∞ (see Fig. 1b), which corresponds to the free electron model.

It is interesting to observe that the frequency dependences of $\text{Re } \alpha(\omega)$ and $\text{Im } \alpha(\omega)$ have the typical dispersion form (see Fig. 2), as if we were dealing with an absorption "line." This has to do not so much with the specifics of the TF model as with the general properties of Eq. (11), which, as has been pointed out, ensure that the dispersion relations are fulfilled for $\alpha(\omega)$ independently of the form of the electron density distribution $n(r)$. In the vicinity of the absorption maximum according to the Kramers-Kronig relations $\text{Re } \alpha(\omega)$ passes through zero and there is a region of negative

dispersion (i.e., $d \text{Re } \alpha(\omega) / d\omega < 0$).

In Fig. 1a the experimental values of the photoabsorption cross sections of atoms of the rare gases He, Ne, ..., Rn are plotted based on the data in the tables in Ref. 25. The experimental points were chosen so as to demonstrate the maximum deviations of the experimental data from the photoabsorption curve of the neutral TF atom. The main sources of these deviations are the jumps in the photoabsorption at the ionization thresholds of the inner shells, which, naturally, are not described by the classical model, and also the nonmonotonic behavior of the experimental curves in the region $\omega \lesssim 10Z$ eV. Although the numerical values in some cases differ by an order of magnitude, overall, as can be seen from Fig. 1a, the statistical model describes the general behavior of the photoabsorption curves fairly well over a wide frequency interval.

In contrast with the photoabsorption, there are practically no experimental data for the real part of the dynamic polarizability of the atoms in the frequency interval under consideration, $I_0 < \omega < \omega_0$. Direct calculations of this quantity by the usual quantum-mechanical methods are quite laborious and few in number. In principle, the quantity $\text{Re } \alpha(\omega)$ can be reconstructed from known experimental values of $\sigma(\omega)$ with the help of formula (12) and Kramers-Kronig

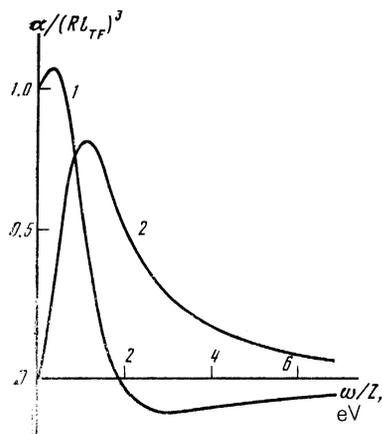


FIG. 2. The real (1) and imaginary (2) parts of the dynamic polarizability of the TF ion. The curves have the typical dispersion form with resonant frequency $\sim 1.5Z$ eV; $R = 5, q = 30\%$.

relations. Such calculations were carried out in Ref. 24, and the results of these calculations are depicted in Fig. 1b. This figure does not show values of $\text{Re} f(\omega)$ in the narrow regions near the absorption regions, where $\text{Re} f(\omega)$ diverges logarithmically, and our approach, obviously, becomes inapplicable. With the exception of these regions, the data of Ref. 24, as can be seen from Fig. 1b, are in fairly good agreement with our results, and better agreement is achieved for the curves with $R = 2.5-5$.

The collective levels of the TF atom, found theoretically in Ref. 13, have energies $\omega_1 = 13.7Z$ eV and $\omega_2 = 36Z$ eV and fall in the interval depicted in Fig. 1a. However, as can be seen from the figure, the photoabsorption cross section and polarizability in this frequency interval, which we have considered on the basis of Eq. (11), are smooth functions of ω . Only a numerical solution of Eqs. (4) with the boundary conditions (5) can give a final answer to the question whether the collective levels found in Ref. 13 correspond to any resonances in the dynamic response of the TF atom.

2.3. Comparison with the results of Refs. 11 and 12

To conclude this subsection, let us briefly compare our results with the results of other approaches, also based on the use of the statistical theory of the atom. As was already mentioned, this mechanism of photoabsorption in multielectron atoms—its classical, collective character—was first discussed in a paper by Brandt and Lundqvist.¹¹ The quasihomogeneous approach which these authors used to calculate the polarizability leads to the expression

$$\alpha^{BL}(\omega) = \int_0^{\infty} \frac{\varepsilon(r, \omega) - 1}{\varepsilon(r, \omega)} r^2 dr. \quad (16)$$

This formula links the photoabsorption in a qualitatively valid way with the condition $\varepsilon = 0$; it also satisfies the Kramers-Kronig relations. From Eq. (16) expressions for the imaginary part of the polarizability and for the photoabsorption cross section follow immediately:

$$\text{Im} \alpha^{BL}(\omega) = \pi \frac{r^2}{|\varepsilon'(r, \omega)|} \Big|_{r=r_0}, \quad (17)$$

$$\sigma^{BL}(\omega) = \frac{8\pi^{3/2}}{c} \frac{n^{3/2}(r)r^2}{|n'(r)|} \Big|_{r=r_0}. \quad (18)$$

An important difference between formula (17) and the exact relation (13) consists in its locality—the photoabsorption cross section (18) is determined here by the local characteristics of the electron density distribution $n(r)$ at the resonant point. In our approach Eqs. (16)–(18) can be obtained from Eq. (11) if the term $\propto \varepsilon'/\varepsilon$ in it is considered by means of perturbation theory (or, equivalently, the quasihomogeneous approximation). This destroys the self-consistency of the problem; in addition, due to the presence of the singularity in the term $\propto \varepsilon'/\varepsilon$ such a perturbation theory is invalid. The photoabsorption cross section of the TF atom, calculated according to Eq. (18), is shown in Fig. 1a (Ref. 11). Numerically, these results differ from ours by a factor of ~ 0.3 as $\omega \rightarrow 0$ and a factor of ~ 5 and $\omega \rightarrow \infty$.

We emphasize, in closing, the physical difference of our approach from that of Refs. 11 and 12. In Refs. 11 and 12 allowing for self-consistency reduces to using the TF density in Eq. (18), which, naturally, is the solution of the self-con-

sistent equations (1) in the absence of an external field. At the same time, as was shown in Sec. 1, a consistent electrodynamic treatment of the atomic polarizability leads to the self-consistent equations also for an induced potential due to an external field [see Eq. (8)].

For completeness of presentation, Fig. 1a also shows the results of the calculation of the photoabsorption cross section obtained by consideration of the hydrodynamic oscillations of the TF atom.²⁶

3. ACCOUNT OF THE SHELL STRUCTURE OF THE ATOM

Equation (8) and expression (9) were obtained in Sec. 1 as the high-frequency approximation to Eqs. (4). Here in the consistent, self-consistent approach the electron density $n(r)$ in Eq. (9) is defined by the formulas of TF theory (3). It would be interesting to try to use the actual electron density of the atom $n(r)$ in place of $n_0(r)$ in Eq. (9). This destroys the self-consistency in the description of the unperturbed ground state, but allows us to treat the influence of the shell structure of the atom, which, as is well known, is not described by the TF model.

In the quantum-mechanical description the electron density is expressed in terms of the radial wave functions

$$n(r) = \frac{n_r(r)}{4\pi r^2}, \quad n_r(r) = \sum_{\gamma} N_{\gamma} |P_{\gamma}(r)|^2, \quad (19)$$

where N_{γ} is the number of equivalent electrons in the shell γ . As P_{γ} we use the nodeless Slater functions of the form

$$P(r) = Cr^{\mu} e^{-\beta r}. \quad (20)$$

The values of the parameters C , μ , and β for each shell are given in Ref. 27. Formulas (19) and (20) reproduce the shell structure of the radial density $n_r(r)$ (note that here as before $n(r)$ a monotonic function) and are in good agreement with the results of calculations based on the Hartree-Fock method. For example, for Ar the difference in the interval $r \leq 2.5$ is less than 10% (see Fig. 3).

The results of the calculation of the optical characteristics of the Ar atom using expressions (19) and (20) are shown in Fig. 4. Their main peculiarity in comparison with

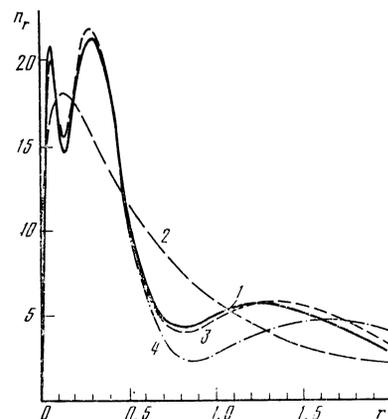


FIG. 3. Distribution of the radial electron density in the argon atom. Curve 1 is the Hartree-Fock approximation, 2 is the Thomas-Fermi model. Curves 3 and 4 are calculated according to the Slater formulas (19) and (20) with the value of β for the 3(sp) shell equal to 2.25 (3) and 1.87 (4) (see text).

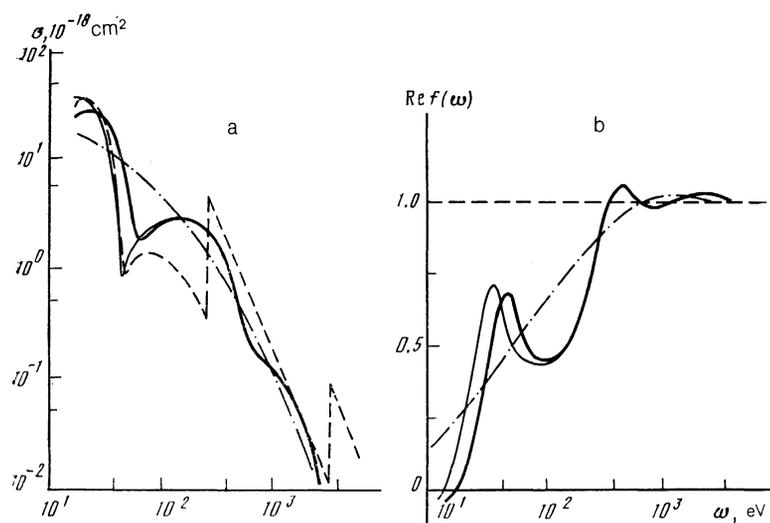


FIG. 4. The photoabsorption cross section (a) and the real part of the modified scattering factor [b, see Eq. (15)] for argon. The dash-dot curves correspond to the result of calculations using the electron density in the TF model; the solid curves correspond to the results of calculations using the Slater formulas (19) and (20) with the value β for the 3(*sp*) shell equal to 2.25 (thick lines) and 1.87 (thin lines). Figure 4a also shows the experimental photoabsorption curves of argon (dashed line).

the results in the TF model is the nonmonotonic behavior of the curves $\sigma(\omega)$ and $\text{Re } f(\omega)$ and, in particular, the appearance of a minimum of the photoabsorption, which is observed experimentally and has received the name of the Cooper minimum.²⁸ In the quantum-mechanical treatment the appearance of this minimum has no simple physical interpretation and is usually associated with the vanishing of the matrix element of the bound-free transition, which gives the main contribution to the absorption cross section.²⁹ In the plasma approach, which we have taken, the photoabsorption cross section is uniquely determined by the electron density of the atom, and not by the wave functions, as in quantum mechanics. This is especially easy to visualize in the theory of Lundqvist, in which the photoabsorption cross section is expressed in terms of the electron density and its derivative at the resonant point, which is determined by the condition $4\pi n(r_0) = \omega^2$ [see Eq. (18)]. Indeed, as follows from Sec. 2, the relation between $\sigma(\omega)$ and the electron density is nonlocal, and according to expression (12) and Eq. (11), is determined by the entire course of the distribution $n(r)$.

The character of the dependence of the photoabsorption on the electron density $n(r)$ is illustrated by Fig. 4a. It can be seen from it that the agreement with experiment in the region $\omega \leq 50$ eV improves ($\sim 10\%$) if for the outer 3(*sp*) shell in place of the value $\beta = 2.25$ recommended in Ref. 27 one takes $\beta^* = 1.87$. Note that this value is closer to the experimental value $\beta_{\text{expt}} = 1.08$, determined by the ionization potential of argon. As can be seen from Fig. 3, making this change in β shifts the maximum of the radial density of the 3(*sp*) shell away from the nucleus, its value remains practically unchanged. The results of calculation for the other rare gases lead to an analogous picture.

Thus, the approach that we have taken here gives a valid qualitative description of the peculiarities of the photoabsorption cross section of various atoms in the low-frequency part of the spectrum, including the nonmonotonic dependence of the cross section on energy. Unfortunately, an analogous systematic comparison of theory with experiment for the real part of the polarizability is still impossible due to the absence of detailed experimental data.

4. CONCLUSION

In this paper we have developed a statistical theory of the dynamic polarizability of complex atoms. As in Refs. 11

and 12, the photoabsorption turns out to be connected with the resonant excitation of plasma oscillations of the atomic electrons. We have shown that even an elementary account of the shell structure of the atom leads to satisfactory agreement with experiment outside the photoabsorption regions. In spite of its limited accuracy, the theory can be used as a universal method to calculate the optical characteristics (the real and imaginary parts of the dielectric constant) of materials in the vacuum ultraviolet and soft x-ray regions of the spectrum.

The photoabsorption cross sections can be found by the proposed method in the region $\omega < \omega_{\text{max}}$, i.e., when the frequency of the incident radiation is less than the maximum plasma frequency of the atom. For $\omega > \omega_{\text{max}}$ the cross section is identically equal to zero, which is a consequence of the implemented approximations. To consider the photoabsorption in the region $\omega < \omega_{\text{max}}$ on the basis of system of equations (4), a more accurate account of single-particle effects is necessary.

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¹⁾ Equations (4) were used in Ref. 13 to describe the atom, but the authors of this article restricted themselves to a consideration of the free oscillations of the electron shell, i.e., to the problem with null boundary conditions.

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