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Thomas-Fermi atom in a static homogeneous electric field

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The Thomas-Fermi (TF) atom in an external homogeneous electric field has been discussed. We introduce the appropriate TF equation and the boundary conditions. The TF equation for this problem has no spherical symmetry. We approximate the partial differential TF equation by the set of simple ordinary differential equations. Our approximation is valid for "very large" electric field values (much larger than those for which the perturbation theory is justified). We found the TF solutions for various values of the electric field and various numbers of bounded electrons. The external electric field ionizes and polarizes the atom. We have shown that ionization of a multielectron atom is substantial even when the external field is significantly smaller than the atomic one.

I. INTRODUCTION

The purpose of this paper is to solve the standard Thomas-Fermi (TF) model for an atom placed in an external electric field. This problem seems to be of a great importance. Atoms in an external electric field are discussed in any quantum-mechanics text book. This analysis is usually limited to weak fields, when a perturbation theory is valid. On the other hand, strong field-atom interactions are extensively investigated in the framework of quantum optics. However, in this case, fields are usually in a resonance with one atomic transition and only one electron is involved in the process under investigation. The TF model allows one to obtain the self-consistent potential and the electron-density distribution function of the multielectron atom. In spite of the long history and large-scale applications of the TF model in various contexts, only spherically symmetric solutions of this model are known. Nevertheless, nonspherical solutions of the TF model could be as useful in a theoretical modeling of a different phenomenon as the spherically symmetric solutions have been so far.

Recent experiments[1,2] on the multiple ionization of atoms by strong laser pulses can serve us as an example of such a phenomenon. As a result of the interaction of the highly intense laser light with an atomic beam the multiply charged ions are produced. Although this interaction has no resonance character, the external field is so large that it cannot be treated as a perturbation. Detailed quantum-mechanical analysis of a strong-field–multielectron-atom interaction can be described by the time-dependent Hartree-Fock model (TDHF). Kulander[3] made some attempts to solve the TDHF equations; however, the solution requires an extremely powerful computer even in a case of helium atoms. The "classical" approximation to the Hartree-Fock model is the Thomas-Fermi or the Thomas-Fermi-Dirac (TFD) equations. In the low-frequency limit of an external field the static TF description of an atom in the electric field can successfully explain[4] some of the results of the experiment of Yargeau *et al.*[2] on the multiple ionization of atoms performed in the infrared regime of the light spectrum. The multiple ionization begins at the laser intensities close to the 10^{14} W/cm^2, which corresponds to the electric field strength of about $E \approx 10^{-2} E_{\rm at}$, where $E_{\rm at} = e/a_0^2$ is the atomic field (a_0 is the Bohr radius). One can ask here the immediate question: Can the multiply charged ions be produced in the nondynamical process as a result of the interaction of atoms with such a weak, in the atomic scale, static external field? The simple estimation of an atomic hydrogen gives a positive answer. The barrier of the hydrogen potential is lowered by the electric field (Fig. 1). One can easily compute the strength of the electric field that lowers the potential barrier significantly, so that the electron bounded as tightly as in the ground state of the hydrogen atom is ionized. The appropriate equations are as follows:

$$e^2/r_0^2 = Ee \ , \tag{1.1a}$$

$$-e^2/r_0 - r_0 eE = \tfrac{1}{2} a_0 e E_{\rm at} \tag{1.1b}$$

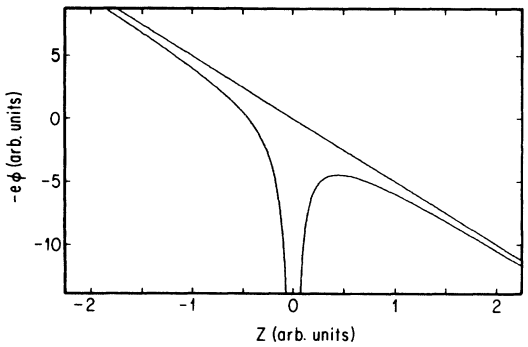

FIG. 1. Potential energy of the electron in a hydrogen atom placed in an external homogeneous electric field as a function of the distance to the nucleus. The energy is plotted along the external field direction (z is the Cartesian coordinate). The straight line represents the energy of the interaction with the external field.

(r_0 is the distance from the nucleus to the maximum of the potential barrier). Equation (1.1a) is just the condition determining the position of the potential barrier, while (1.1b) expresses an electron energy. As follows from (1.1), the required external field has the value $E=\frac{1}{16}E_{\rm at}$, which corresponds to the laser intensities $I=\frac{1}{256}$, $I_{\rm at}\approx 10^{14}$ W/cm^2. This is just the intensity for which the multiple striping of atoms is observed. The above estimation clearly shows that if the external static electric field is applied to an atom (even if this field is considerably weaker than the atomic one), the effect of lowering the potential barrier is significant and may cause the essential ionization of the atom.

Up to now, the TF model of an atom in a static homogeneous electric field has not been solved properly. Bruch and Lehnen[5] calculated the electric polarizability of atoms with the help of the TFD model. They conclude that within the approximation they have made, the TF model for an atom in the external field does not have any solution. This is due to the fact that they neglected the ionization of the atom by the electric field and therefore the TF function in infinity cannot fulfill required boundary conditions. On the other hand, Krainov and Manykin[6] mentioned the possibility of the application of the TF model to the description of the strong-field ionization phenomenon. However, in order to estimate the ionization degree they use the spherically symmetric solution of the TF equation. A proper description of the TF atom in an external electric field does not allow for a separation of the polarization and the ionization phenomena.

In our paper we introduce the approximate equations describing the TF atom in a static external electric field. With the help of these equations we discuss the various characteristics of the multielectron atom, particularly the ionization degree as a function of the electric field. We begin our paper, presenting, in Sec. II the TF model and the way of reducing its partial differential TF equation to a set of ordinary equations. The validity of our approximations and a detailed analysis of solutions of the TF equation are discussed in Sec. III. We give the TF function and the TF potential for various values of the electric field and ionization degree. Our calculations show that the electric field can ionize and polarize the atom. The neutral TF atom does not exist if an external electric field is present. For each value of the field there exists an ion of the minimal ionization degree. Solutions of the TF equation correspond to ions of all possible ionization degrees up to a certain minimal value (for a given electric field). Particular attention has been given to the ions of the minimal ionization degree. We calculated the ionization degree, Fermi energy, and induced dipole moment as a function of the electric field for the minimally ionized atoms. Conclusions and final remarks are presented in Sec. IV.

II. MODEL AND APPROXIMATE METHODS OF ITS SOLUTION

A. Thomas-Fermi model

The Thomas-Fermi equation was introduced in the mid 1920's by Thomas and independently by Fermi[7] in order to describe the self-consistent potential of multielectron atoms. The TF model is based on statistical mechanics. It assumes the thermal equilibrium of the electron gas. The electron-electron interaction is included through the mean field. The Pauli exclusion principle is the only quantum feature of this model. Nevertheless, the TF model is in qualitative agreement with experimental data. The advantage of the TF model is in its simplicity and universality (atoms of different Z differs by the scaling units only). If one is interested in a qualitative understanding of some physical processes, the TF model can be very useful.

The standard TF equation is based on the Poisson equation for the potential generated by a nucleus and surrounding electron cloud. However, in a self-consistent model this potential is related to the charge-density distribution function. The relationship between potential and electron distribution function can be obtained by minimizing the following TF energy functional:[8]

$$E_{\rm TF}[\rho]=\int d^3r\left[\tfrac{3}{10}(3\pi^2)^{2/3}(\hbar^2/m)\rho(\mathbf{r})^{5/3}+\rho(\mathbf{r})e\left[\tfrac{1}{2}\int d^3r'\rho(\mathbf{r}')e/|\mathbf{r}-\mathbf{r}'|-[\phi_{\rm ex}(\mathbf{r})+Ze/r]\right]\right], \tag{2.1}$$

where $\rho(\mathbf{r})$ is the electron number density at position $\mathbf{r}$ to the nucleus. The first term represents the electron kinetic energy and the second one the potential energy of the system, i.e., the electron-electron interaction (the self-energy also), the interaction with an external field $\phi_{\rm ex}(\mathbf{r})$ (if such exists), and the interaction with the nucleus. This energy expression, together with the Poisson equation, leads to the TF equation for the self-consistent potential $\phi(\mathbf{r})$:

$$\Delta\phi(\mathbf{r})=\begin{cases}\dfrac{32\pi^2}{3(2\pi\hbar)^3}\{2me[\phi(\mathbf{r})-\phi_0]\}^{3/2} & \text{if } r(\theta,\Phi)\le r_0(\theta,\Phi)\ ,\\ 0 \quad \text{otherwise}\ ,\end{cases} \tag{2.2}$$

where $-e$ is an electron charge and $\mathbf{r}_0$ is the radius of electron cloud. Since Eq. (2.1) should be subject to the normalization condition on ρ we have introduced the Lagrange multiplier ϕ_0, which means the potential at the surface where the electron density vanishes. Therefore ϕ_0 is related to the electron Fermi energy; i.e., the maximum energy of bounded electrons is $E_F=-e\phi_0$.

The TF self-consistent potential $\phi(\mathbf{r})$ is defined as

$$\phi(\mathbf{r})=-e\int d^2r'\rho(\mathbf{r}')/|\mathbf{r}-\mathbf{r}'|+[\phi_{ex}(\mathbf{r})+Ze/r]\ . \tag{2.3}$$

With the above definition, the nucleus and external field potentials do not enter explicitly the TF equation (2.2). Nevertheless, solutions of (2.2) depend on these potentials through the boundary conditions. From now on, we assume that the ϕ_{ex} corresponds to a potential of the homogeneous electric field, $\phi_{ex}=-zE$ (z is the Cartesian coordinate along the electric field E direction). Introducing the standard TF units and restricting our interest to the axially symmetric solutions only, we can rewrite Eq. (2.2) in a following way:

$$\left[\frac{1}{\xi}\frac{\partial^2}{\partial\xi^2}+\frac{1}{\xi^3}\frac{\partial}{\partial w}(1-w^2)\frac{\partial}{\partial w}\right]\chi(\xi,w)=\begin{cases}[\chi(\xi,w)/\xi]^{3/2} & \text{if } \xi(w)_0<\xi(w)\\ 0 \quad \text{otherwise}\ ,\end{cases} \tag{2.4}$$

where the standard TF function $\chi(\xi,w)$ is defined:

$$\chi(\xi,w)=\xi(\varphi(\xi,w)-\varphi_0)\ , \tag{2.5}$$

and

$$r=a\xi\ , \tag{2.6a}$$

$$w=\cos(\theta)\ ,\quad 0<\theta<\pi\ , \tag{2.6b}$$

$$\varphi(\xi,w)=(a/Ze)\phi(\xi,w)\ , \tag{2.6c}$$

$$\varphi_0=(a/Ze)\phi_0\ , \tag{2.6d}$$

and

$$a=Z^{-1/3}(3\pi/4)^{2/3}\frac{\hbar^2}{2me^2}\ . \tag{2.6e}$$

If there is no external field applied to the system, the TF function χ dies not depend on the direction w. In such a case, Eq. (2.4) simplifies to the ordinary, well-known TF equation.

Writing Eqs. (2.2) and (2.4) we do not assume that the electron cloud extends to the infinity. However, we do not exclude such a situation—then $r_0(\theta)$, or equivalently, $\xi_0(w)$ are infinite. Nevertheless, having in mind the $E=0$ case, we expect that if the atom is ionized, the electron-density distribution function vanishes at finite distances at the surface $\xi_0(w)$, which determines the shape of the atom. At this surface the TF function is equal to zero, $\chi(\xi_0,w)=0$, or equivalently, $\varphi(\xi_0,w)=\varphi_0$. This condition allows one to determine the electron cloud edge $\chi_0(w)$.

In order to complete the model, the boundary conditions have to be specified. We get immediately from (2.3) and (2.5) that inside the electron cloud, in proximity to the nucleus the TF function is dominated by the term

$$\chi(\xi\to 0)\to 1\ . \tag{2.7a}$$

On the other hand, if ξ goes to infinity, the behavior of the TF function is determined by the external potential

$$\chi(\xi\to\infty)\to-\xi^2wE\ . \tag{2.7b}$$

Somewhere in between, at the electron-cloud edge the TF function is equal to zero (if ξ_0 is finite). Then one has to glue the TF solution inside the electron cloud with the general solution of the Laplace equation in the free of charge space with the static homogeneous electric field existing in infinity:

$$\chi(\xi,w)=\xi(\varphi-\varphi_0)=\xi\left[-E\xi P_1(w)+\sum_{l=0}^{\infty}\frac{A_l}{\xi^{l+1}}P_l(w)-\varphi_0\right]\ . \tag{2.8}$$

$P_l(w)$ is the Legendre polynomial and A_l is the multiple moments of the charge distribution (written in dimensionless units). These moments are induced by the external electric field and could be calculated from the definition with help of the charge-density distribution function. Particularly, A_0 is the total charge of the system, i.e., the ionization degree:

$$A_0\equiv\frac{Z-N}{Z}=1-\tfrac{1}{2}\int_{-1}^{1}dw\int_0^{\xi_0(w)}d\xi\,\xi^2\left[\frac{\chi(\xi,w)}{\xi}\right]^{3/2}\ , \tag{2.9a}$$

and A_1 is the dipole moment:

$$A_1\equiv P=-\tfrac{1}{2}\int_{-1}^{1}dw\,P_1(w)\int_0^{\xi_0(w)}d\xi\,\xi^3\left[\frac{\chi(\xi,w)}{\xi}\right]^{3/2}\ . \tag{2.9b}$$

In the $E=0$ case the TF function has radial symmetry and the total charge A_0 is the only nonvanishing moment of the charge distribution. As it indicates from (2.8) and the definition of ξ_0, the Fermi energy is, in this case, related to the total charge of the system: $-\varphi_0=[(Z-N)/Z]/\xi_0$. The total charge (or, equivalently, the Fermi energy) is the only parameter classifying the solutions. Radially symmetric solutions describe a neutral atom or positively charged ions, depending on the value of φ_0. In the neutral atom case $Z=N$ and the Fer-

mi energy is equal to zero, $\varphi_0=0$. The radius of the atom is infinite ($\xi_0=\infty$). The solutions for smaller Fermi energies $-\varphi_0$ correspond to positive ions with finite radius $\xi_0<\infty$. When a TF atom is placed in an homogeneous external electric field an extra parameter (except a total charge) is needed in order to uniquely classify the solutions. This is, of course, the value of the external electric field.

B. Approximate equations

The TF equation, even in the radial symmetry, has to be solved numerically. In an axial case a numerical solution of Eq. (2.4) for $\xi(w)<\xi_0(w)$ is complicated. The TF equation (2.4) is of the elliptical type with the Dirichlet boundary conditions. But in the problem of the type we are dealing with, the boundary has to be determined, in a self-consistent way, from the solution we are just looking for. Therefore it is more convenient, for numerical reasons, to deal with the Cauchy problem when the function and its derivatives at one of the borders are known. The problem is how to properly specify the derivatives in order to fulfill required conditions on the second boundary. Fortunately, one can easily find a general solution of the TF equation for $\xi \ll 1$ and all w. Taking into account the condition (2.7a), the TF function can be expanded into a power series of $\xi^{1/2}$ and the Legendre polynomials of w (in a radial case a similar expansion can be found in the paper of Feynman *et al.*[9]):

$$\chi(\xi,w)=1+\sum_{l=0}^{\infty} P_l(w) \sum_{k=2} a_{kl}\xi^{k/2} . \tag{2.10}$$

Substituting this expansion into Eq. (2.4) we can obtain the coefficients a_{kl}, which determine the TF function in the proximity of the nucleus. In the Table I we have listed some first nonvanishing coefficients a_{kl}. Only coefficients from the first row of Table I are independent. All others are functions of those few. Solutions of (2.4) could be classified according to the values of the coefficients $\{a\}=a_{20},a_{41},a_{62},a_{83},\ldots$. The spherically symmetric TF solution can be obtained by putting $a_{20}\neq 0$, $a_{41}=a_{62}=\cdots=0$. The terms proportional to the remaining coefficients break the spherical symmetry. For instance, terms proportional to a_{41} have a dipole shape; to a_{62}, a quadrupole; and to a_{83}, an octupole shape. The parameters $\{a\}$ have no direct physical interpretation. Nevertheless, they are strictly related to the physical quantities, since for a given Fermi energy and external field the solution is unique.

The usual way of integrating the radially symmetric TF equation is to start with the given derivative a_{20} at the point $\xi=0$. The total charge of the system, the Fermi energy, and the TF function outside the electron cloud could be calculated if the electron-density distribution function were known. We have checked numerically that if the homogeneous electric field is applied to the system, only a_{20} and a_{41} should differ from zero. This fact is not surprising, since terms proportional to a_{41} have the symmetry of the external field type. Moreover, if $a_{41}=0$ then $E=0$, and we can suppose that a_{41} is in some sense "responsible" for the electric field value. If the field in infinity has quadrupole or octupole symmetry, the coefficients a_{62} or a_{83}, respectively, should be different from zero. Specifying the values of a_{20} and a_{41} at the surface $\xi(w)=0$, we can continue integration outward. The situation is now similar to a spherical case. The surface $\xi_0(w)$, where the electron density vanishes, can be determined during the numerical integration using the condition $\chi(\xi_0(w))=0$. Outside the electron cloud the solution is given by the formula (2.8). Matching the TF function from outside the electron cloud to the numerical solution, the electric field value E and the Fermi energy $-\varphi_0$ could be obtained. At the electron-cloud edge $\xi_0(w)$ the equation (2.8) reads

$$\varphi_0+E\xi_0 P_1(w)-\sum_{l=0}^{\infty}\frac{A_l}{\xi_0(w)^{l+1}}P_l(w)=0 . \tag{2.11}$$

Expanding the left-hand side of (2.11) into the Legendre polynomials of w and neglecting (as small corrections) all terms proportional to the polynomials $P_2(w),P_3(w),\ldots,$ we get the set of two algebraic equations for E and φ_0.

Even knowing how to change the Dirichlet boundary conditions into the Cauchy problem, the numerical solution of the TF equation meets with some difficulties. Namely, the right-hand side of the TF equation (2.4) is singular at the origin of the coordinate system, which makes two-dimensional integration unstable. We can avoid this difficulty by changing our Eq. (2.4) to the set of second-order ordinary equations and restricting our in-

TABLE I. Coefficients a_{kl} of expansion of the TF function in the proximity of the nucleus $\xi \ll 1$.

a_{k0}	a_{k1}	a_{k2}	a_{k3}
a_{20}	a_{41}	a_{62}	a_{83}
$a_{30}=\frac{4}{3}$	$a_{71}=\frac{2}{9}a_{41}$	$a_{92}=\frac{2}{13}a_{62}$	$a_{113}=\frac{2}{17}(a_{83})^3$
$a_{50}=\frac{2}{5}a_{20}$	$a_{91}=\frac{3}{55}a_{20}a_{41}$	$a_{112}=\frac{1}{25}a_{20}a_{62}+\frac{1}{75}(a_{41})^2$	
$a_{60}=\frac{1}{3}$	$a_{101}=\frac{2}{27}a_{41}$		
$a_{70}=\frac{3}{70}(a_{20})^2$	$a_{111}=\frac{9}{364}(a_{20})^2a_{41}$		
$a_{80}=\frac{2}{15}a_{20}$			
$a_{90}=\frac{2}{27}-\frac{1}{252}(a_{20})^3$			
$a_{100}=\frac{1}{175}(a_{20})^2$			
$a_{110}=\frac{31}{1485}a_{20}+\frac{1}{1056}(a_{20})^4+\frac{1}{198}(a_{41})^2$			

terest to, in some sense, "weak" fields only. Expanding into the power series the TF function $\chi(\xi,w)$ in the proximity of the arbitrary direction w_0 ($\Delta w = w - w_0 \ll 1$ is a small quantity),

$$\chi(\xi,w)=\chi(\xi,w_0)+\chi_1(\xi,w_0)\Delta w+\tfrac{1}{2}\chi_2(\xi,w_0)\Delta w^2+\cdots , \tag{2.12}$$

where

$$\chi_1(\xi,w_0)=\left.\frac{\partial\chi(\xi,w)}{\partial w}\right|_{w=-w_0} , \tag{2.13a}$$

$$\chi_2(\xi,w_0)=\left.\frac{\partial^2\chi(\xi,w)}{\partial w^2}\right|_{w=w_0} , \tag{2.13b}$$

and substituting expansion (2.12) into Eq. (2.4) we obtain the following set of ordinary equations:

$$\begin{aligned}
\xi^{1/2}\frac{d^2\chi}{d\xi^2}&=\chi^{3/2}+\xi^{-3/2}[2w_0\chi_1-(1-w_0^2)\chi] ,\\
\xi^{1/2}\frac{d^2\chi_1}{d\xi^2}&=\tfrac{3}{2}\chi^{1/2}\chi_1+2\xi^{-3/2}(\chi_1+2w_0\chi_2)+\cdots ,\\
\xi^{1/2}\frac{d^2\chi_2}{d\xi^2}&=\tfrac{3}{2}\chi^{1/2}\chi_2+\tfrac{3}{4}\chi^{-1/2}\chi_1^2+6\xi^{-3/2}\chi_2+\cdots .
\end{aligned} \tag{2.14}$$

This infinite set of equations is as accurate as Eq. (2.4) and no assumption about the strength of the electric field is necessary. But it is useless to consider the infinite set (2.14) instead of Eq. (2.4). As it will be shown later, this set of equations can be truncated by a few first ones if the external field is weak, i.e., $E<e/a^2\approx E_{\rm at}Z^{2/3}$. We want to stress that independently, on the order of expansion, the first equation of our hierarchy (2.14) does not depend on the χ_2, the second on the χ_3, and so on. Therefore, if the order of the expansion is increased, it does not affect some number of the first equations.

In the proximity of the point $\xi(w)=0$, the functions χ, χ_1, and χ_2 are

$$\begin{aligned}
\chi(\xi\to 0,w)&=1+a_{20}\xi+\tfrac{4}{3}\xi^{3/2}+a_{41}w\xi^2+\cdots ,\\
\chi_1(\xi\to 0,w)&=a_{41}\xi^2+\cdots ,\\
\chi_2(\xi\to 0,w)&=\tfrac{1}{25}a_{41}^2\xi^{11/2}+\cdots .
\end{aligned} \tag{2.15}$$

For a given a_{41}, if ξ is sufficiently small, the following inequality is fulfilled:

$$\chi_1(\xi,w_0)\gg\chi_2(\xi,w_0) , \tag{2.16}$$

which means that the leading angular dependence of the TF function comes from χ_1. We expect that if the external field is "weak," the TF function $\chi(\xi,w)$ depends on the direction "very weakly almost everywhere." Only the electrons far from the nucleus are sensitive to the external field. Let us assume that the condition (2.16) is fulfilled inside the whole electric charge cloud and for all directions, i.e., for $\xi(w)<\xi_0(w)$. With the help of this assumption we can truncate the infinite set of equations (2.14) by the first two:

$$\xi^{1/2}\frac{d^2\chi(\xi,w_0)}{d\xi^2}=\chi(\xi,w_0)^{3/2}+2w_0\xi^{-3/2}\chi_1(\xi,w_0) , \tag{2.17a}$$

$$\xi^{1/2}\frac{d^2\chi_1(\xi,w_0)}{d\xi^2}=\tfrac{3}{2}\chi(\xi,w_0)^{1/2}\chi_1(\xi,w_0)+2\xi^{-3/2}\chi_1(\xi,w_0) . \tag{2.17b}$$

In a spherically symmetric case χ_1 is equal to zero, and from (2.17) we get the standard textbook TF equation at once. Equations (2.17) are approximate TF equations for the atom in the external homogeneous electric field. They have been derived under the condition (2.16), which we have justified properly for the innermost regions of atom only. In order to check the influence of the higher corrections χ_2 and χ_3, we have integrated Eqs. (2.17) and the three lowest equations of the set (2.14) for various values of initial parameters a_{20} and a_{41} and various directions w_0. As we could expect, the transformation $a_{41}\to -a_{41}$ leads simply to the change in direction of the electric field. From now on we restrict our analysis to positive a_{41} only. In Fig. 2, the typical TF function along the field direction is presented. The electron cloud is extended along the OZ axis:

$$\xi_0(w=1)>\xi_0(w_0)>\xi_0\ (w=-1)\quad\text{for}\quad -1<w_0<1 \tag{2.18}$$

(the electric field is directed to the negative part of the OZ axis). Near the nucleus the Coulombic field is very strong; therefore only the electrons for which $\xi\approx\xi_0$ ($w=1$) are affected by the external field. Therefore this region is expected to be the most dangerous one for the validity of the assumption (2.16). In Fig. 3 the functions χ, χ_1, and χ_2 are plotted for various directions and ionization degrees. Our calculations show that for $\xi\gg 1$ and $w\approx 1$, the inequality (2.16) is no longer valid. Nevertheless, as it is shown in Fig. 3, χ_2 is large for an almost neutral atom in a small range of angles, close to $\theta=0$ only. We have checked numerically that for a "small" a_{41} the influence of higher derivatives χ_2 and χ_3 on the TF function is negligible, even when these derivatives are

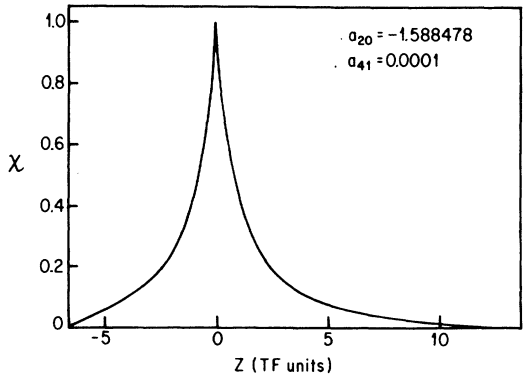

FIG. 2. Typical TF function along the direction of the external electric field.

comparatively large. Equations (2.17) are a good approximation of the TF equation (2.4) for the "not-too-large" coefficient a_{41} (i.e., the not-too-large electric fields). Our assumption is valid even if the value of a_{41} is of the order of 1, which corresponds to the strength of the electric field close to the atomic field $E < E_{at} Z^{2/3}$. The advantage of Eqs. (2.17) in comparison to (2.4) is obvious. Instead of partial differential equations of the second order, one has to deal with the set of two ordinary differential equations for each direction. The numerical solution of the set (2.4) is as easy as the integration of the standard ($E=0$) TF equation.

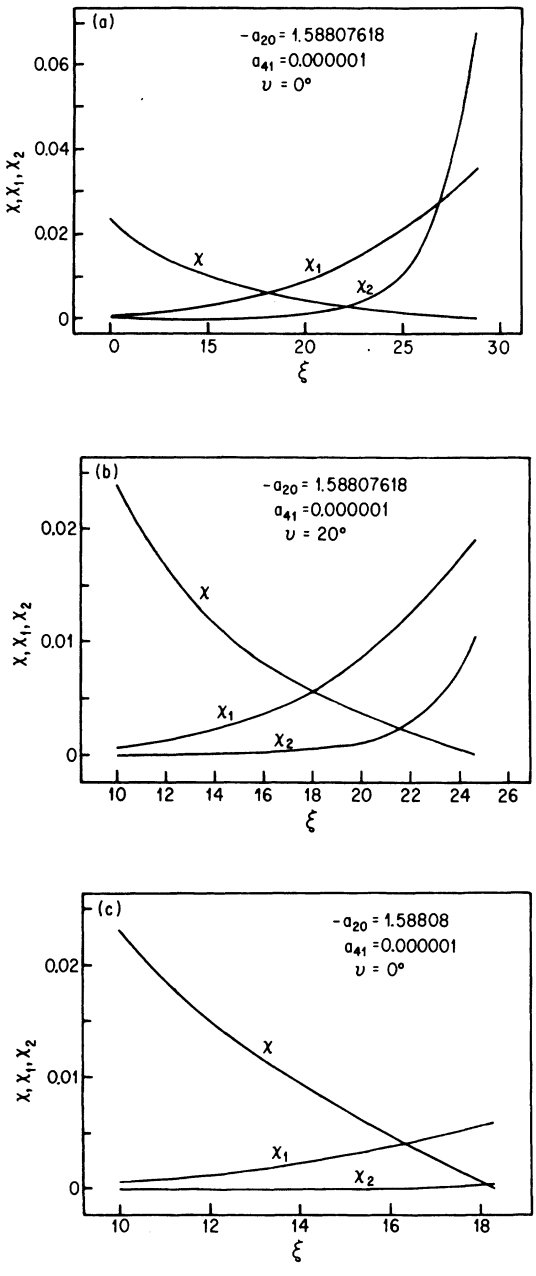

FIG. 3. Function χ, χ_1, and χ_2 in regions where our assumption $\chi_1 > \chi_2$ is not valid. (a) and (b) Small ionization degree; (c) large ionization degree.

III. FEATURES OF THE TF ATOM IN THE EXTERNAL ELECTRIC FIELD

Integrating Eqs. (2.17) for different values of parameters a_{20} and a_{41}, all the possible solutions for the TF atom in the external electric field could be obtained. But as we know from the $E=0$ case, not all values of a_{20} are allowed in the free space for a system of a nucleus and bounded electron cloud. The neutral atom is characterized by $a_{20} \approx -1.588$ ($a_{41}=0$). Smaller a_{20} correspond to positive ions. Similarly, when $E \neq 0$ (i.e., $a_{41} \neq 0$) the maximal limiting value of the first derivative, $a_{2\,\mathrm{lim}}(a_{41})$, does exist. Only $a_{20} < a_{2\,\mathrm{lim}}(a_{41})$ are allowed. For a_{20} larger than $a_{2\,\mathrm{lim}}(a_{41})$ the TF function can never reach zero value and we cannot fulfill the boundary conditions. The solution describing a neutral atom exists only for $E=0$. Other solutions correspond to positive ions of different ionization degrees: from the naked nucleus up to the maximal possible number of bounded electrons. This maximal number of bounded electrons depends on the value of the external field. The electric field ionizes the atom. Let us consider a situation when an initially neutral atom is placed in the space where the homogeneous external electric field is switched on adiabatically. If the electric field grows from its zero value, only electrons of energy exceeding the Fermi one escape from the system. The remaining part of the electron cloud is all the time in the temporal equilibrium. These electrons fill all the energy states up to the Fermi energy. During adiabatic growth of the electric field the ion of the minimal ionization degree (corresponding to the temporal value of the external field) is produced. If the field is decreased adiabatically the potential barrier grows. Only the dipole moment of an ion is changed, while the ionization degree remains constant. Ions of the minimal ionization degree for a given value of the external electric field are of special importance from the ionization process point of view. These ions correspond to the solutions for which $a_{20} = a_{2\,\mathrm{lim}}(a_{41})$.

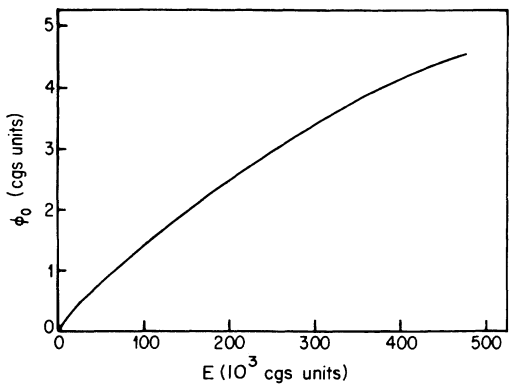

FIG. 4. Potential corresponding to the Fermi energy of the minimally ionized atoms against the electric field.

The influence of the external electric field on the multielectron atom can be described not only qualitatively, but also quantitatively, in the framework of the TF model. The minimal ionization degree, the peak of the potential barrier $-\varphi_0$, the induced dipole moment, and even the geometrical shape of the atom as functions of an external field could be easily calculated. In Fig. 4 the Fermi energy φ_0 of the minimally ionized atom as a function of external field is presented. The Fermi energy diminishes with the electric field (φ_0 grows since $E_F \approx -e\varphi_0$); the external electric field lowers the potential barrier. As the potential barrier is lowered the excess of electrons escape from the atom. The degree of ionization grows, see Fig. 5. Initially, for larger electric field, the ionization degree is larger but later begins to saturate. More interesting is the behavior of the induced dipole moment, Fig. 6. The electric field of the value $E \approx 10^{-4} Ze/a^2$ produces the ion of the maximal dipole moment (ionization degree is about 17%). This maximum is an effect of the two competitive processes. As the electric field starts to grow from its zero value the atom begins to polarize and ionize. The field is too weak to ionize an atom significantly, but is strong enough to polarize the electron cloud. The dipole moment grows. If the electric field is large, the atom is strongly ionized. Only the electrons in the neighborhood of the nucleus are left. Therefore the dipole moment goes to zero. The above result clearly shows that studying the ionization of an atom by fields of magnitude as large as $10^{-2} E_{\text{at}}$, one has to take into account the escape of electrons above the lowered potential barrier. This mechanism of ionization can be very important, not only for a static electric fields, but also in a case of optically varying ones. Such a physically simple intuitive picture of the ionization of multielectron atoms in a slowly varying electric field has been successfully proposed by us[4] in order to explain some quantitative results of the strong-field ionization phenonemon.

The formalism presented here allows one to calculate the electric polarizability α of the TF atom:

$$P = \alpha E \ , \tag{3.1}$$

where P is an induced atom dipole moment and E is an external field. However, there is no solution of the TF model corresponding to the neutral atom in the electric field; the initial slope (at $E=0$) of the function $P(E)$ presented in Fig. 6(b) can be interpreted as the polarizability of the TF atom. The quantity obtained in this way is infinite. This result is in agreement with an earlier paper.[6] The TF model does not correctly describe the ionization and polarization processes. The reason is quite obvious. The TF atom has an infinite radius. The electron density tends to zero too slowly. The TF model allows a substantial number of electrons to be far from the nucleus. These electrons are very weakly bounded. But these electrons are mainly involved in the ionization and polarization processes. Therefore it is very easy to ionize and polarize the TF atom. The ionization degree and the electron polarizability calculated from the TF model can be overestimated.

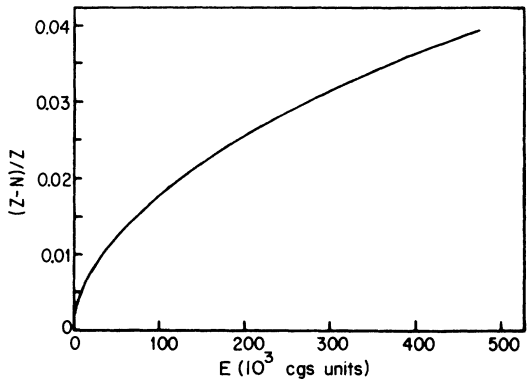

FIG. 5. Minimal ionization degree for a given value of the external field.

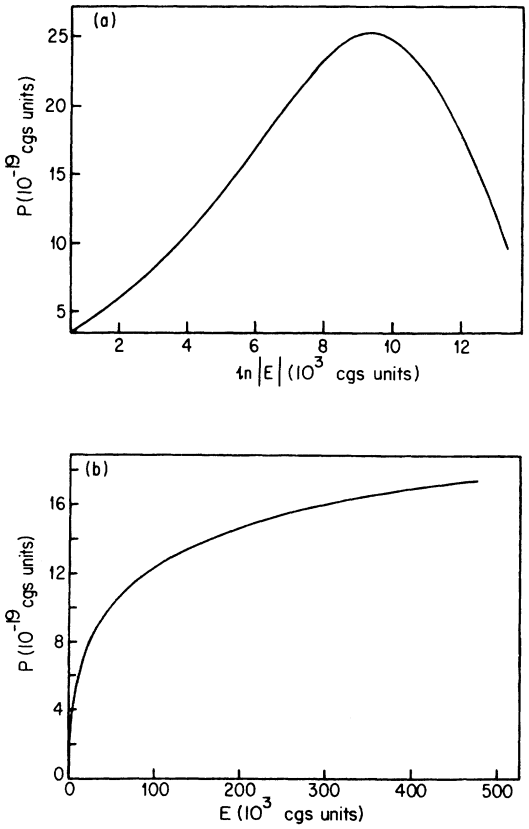

FIG. 6. Induced dipole moment of minimally ionized atoms against the external field. (a) Logarithmic scale; (b) for small electric fields $E \approx 0$.

In Fig. 7 the density of the electron cloud is presented. We do not plot the lines of constant density in the small neighborhood of the nucleus because the density is infinite at $\xi = 0$, where the nucleus is placed. Figure 7 can also be interpreted as equipotential lines for the TF atom in the external electric field. This figure visualizes the extended shape of the ions—the effect of polarization by

the electric field. The cusp in Fig. 7(a) is characteristic for all ions of the minimal ionization degree at a given electric field. This cusp is a feature of the TF model. We can better understand its origin looking at Figs. 8 and 9. These figures present a typical self-consistent TF potential—also outside the electron cloud. Far from the nucleus the potential tends to the homogeneous electric field potential. Close to the nucleus the potential is Coulombic. At some distance from the nucleus, on the OZ axis, the TF potential has a saddle point (the potential $V=1/r+Er\cos\theta$) has a similar saddle point). The equipotential line passing through this point makes a characteristic loop (Fig. 9). The potential value along this line is associated with the Fermi energy of the electrons. Electrons of larger energy go to infinity. If the electrons fill all states up to the saddle point, the minimally ionized ion will be obtained. Therefore in the TF model, ions with the maximal number of bounded electrons have a shape with a characteristic cusp—the result of the potential saddle point. Ions of a larger ionization degree have an "egglike" shape [Fig. 7(b)] without the cusp.

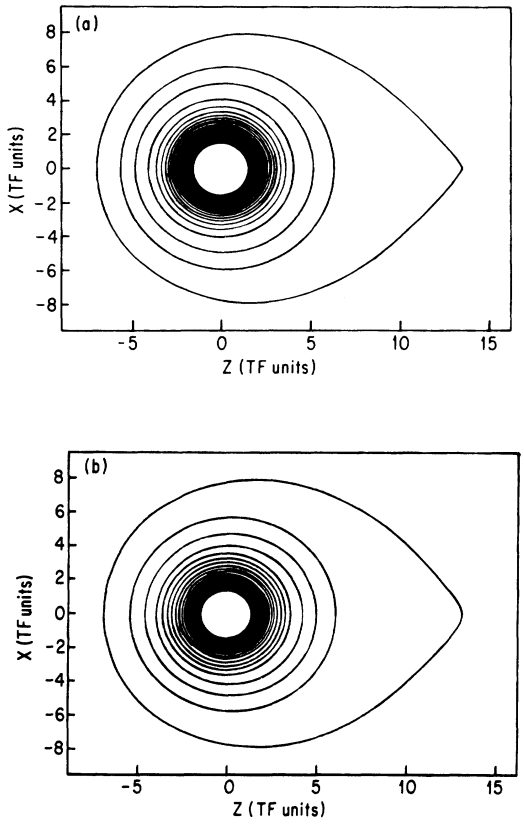

FIG. 7. Typical electron number density function—lines of a constant density. In the proximity of the nucleus the density becomes infinite—the lines of constant density are getting closer forming a black ring in a figure. (a) Minimally ionized atom; (b) larger ionization degree.

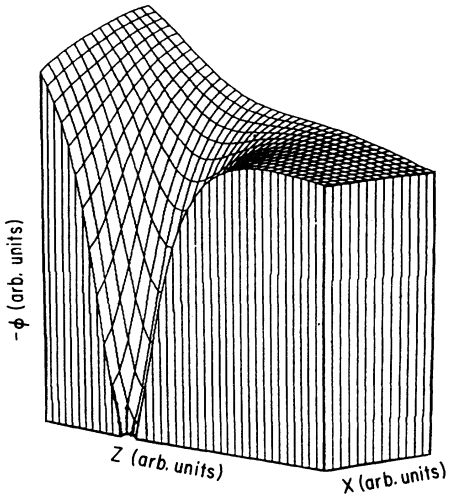

FIG. 8. Typical three-dimensional plot of the TF potential energy $-\varphi$.

IV. FINAL REMARKS

In our paper we have introduced and solved the TF equation for the atom placed in the external electric field. We have made an approximation that reduces the second-order partial differential equation to the set of ordinary equations. This approximation is valid if the electric fields are not too large. However, those fields are small in the atomic scale and very large in the laboratory scale. Such fields ionize the atom significantly.

We have obtained the TF function and the TF self-consistent potential. These quantities allow one to calculate many physical properties of the atom in an external electric field. Particularly, the induced dipole moment and ionization degree as functions of the electric field have been obtained. These quantities are very sensitive to the long-distance behavior of the TF potential. But as is well known, in this region the TF equation breaks down. Therefore we cannot expect out results to fit the experi-

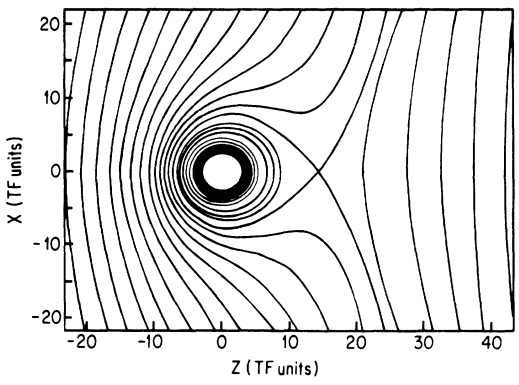

FIG. 9. TF equipotential lines.

mental data. The presented model has a very intuitive physical meaning. Although the results are qualitative rather then quantitative, the method remains valid for a different statistical model of atom based on the TF equation; for instance, to the Thomas-Fermi-Dirac equation. Including long-distance corrections to the TF equation, one can obtain more realistic models of the multielectron atom in an external electric field. "Improved" in such a way, the TF model of an atom in the external homogeneous electric field has been applied by us[4] in order to explain the recent experiments of the multielectron ionization of atoms by strong laser pulses. Contrary to the various existing theoretical attempts at an explanation of these phenomena, the TF model gives not only the simple physical picture of the ionization, but also allows one to obtain (without any fit) the quantitative results that are in very good agreement with the experimental data.

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