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# A study of density effects in plasmas using analytical approximations for the self-consistent potential

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ABSTRACT

Density effects in ionized matter require particular attention since they modify energies, wavefunctions and transition rates with respect to the isolated-ion situation. The approach chosen in this paper is based on the ion-sphere model involving a Thomas-Fermi-like description for free electrons, the bound electrons being described by a full quantum mechanical formalism. This permits to deal with plasmas out of thermal local equilibrium, assuming only a Maxwell distribution for free electrons. For H-like ions, such a theory provides simple and rather accurate analytical approximations for the potential created by free electrons. Emphasis is put on the plasma potential rather than on the electron density, since the energies and wavefunctions depend directly on this potential. Beyond the uniform electron gas model, temperature effects may be analyzed. In the case of H-like ions, this formalism provides analytical perturbative expressions for the energies, wavefunctions and transition rates. Explicit expressions are given in the case of maximum orbital quantum number, and compare satisfactorily with results from a direct integration of the radial Schrödinger equation. Some formulas for lower orbital quantum numbers are also proposed.



## 1. Introduction

Since the first studies in a stellar atmosphere context [1], the analysis of density effects in ionized matter has attracted considerable attention. This interest has been revived recently by the availability of lineshift measurements in dense plasma emission [2,3]. The description of such effects is complex since it implies the elaboration of a quantum theory of a very large system. Setting aside the molecular dynamics approaches (e.g., Ref. [4]), as stated by several authors [5,6], the various approaches used to describe these phenomena may be categorized as ion-correlation and ion-sphere models. Such approaches are usually qualified as density-functional theories. On the one hand, ion-correlation theories consider the plasma as an infinite polarizable medium, with asymptotic cancellation of free-electron and ion densities. The Debye-Hückel theory may be considered as a high-temperature limit of this formalism, which has been since developed by various authors [6–10]. On the other hand, ion-sphere [11,12] theories assume that environment effects arise from an appropriate description of the free-electron density, with no account for correlations in ion positions. Following Liberman [11], the ion-sphere theories assume that the Wigner sphere is globally neutral. Beyond the Wigner radius, the free-electron density is canceled by the other-ion density while inside the Wigner sphere, this density is obtained through various hypotheses, e.g., through a self-consistent approach such as Thomas-Fermi (TF). Such models have been widely used to get energies and transition rates for ions in a plasma as, e.g., in Refs. [13,14], and their infinite-temperature limit is the well-known uniform electron gas model (UEGM) [15].

When dealing with environment effects in plasmas, a compromise must be found between the accuracy and/or internal consistency of the model, and its tractability. For instance describing plasmas out of local thermodynamic equilibrium requires the computation of a very large set of energies, transition probabilities and collisional cross-sections. A widely used plasma model, belonging to the ion-sphere category, is the uniform electron gas model that assumes constant electron density inside the Wigner sphere and cancellation of free-electron and other ion density outside it. It allows one to get very simple analytical energies for H-like ions. And recently, we have also shown that analytical perturbed wavefunctions and transition rates may be obtained [16]. However, this appears as an infinite temperature limit, since the

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polarization of the electron density by the ion is not accounted for. A more realistic model, accounting for this polarization, is the Thomas-Fermi approximation for free electrons. In its standard form, this semi-classical theory also accounts for the Pauli principle. However this theory remains purely numerical, making, e.g., analytical computations not possible. In this work, we intend to show that simple analytical approximations can be found for this potential, at the same time keeping the accuracy of the description — not too different from Thomas-Fermi description — and its tractability since it relies on a polynomial from of the potential.

A preliminary account of the method for obtaining an analytical plasma potential has been already published [17]. We present first the details for the derivation of the analytical approximation, and then focus on some applications in hydrogen-like ions. In particular, we provide analytical expressions for energies, wavefunctions and dipole matrix elements for the higher values of the orbital quantum number.

## 2. Analytical approximation for the plasma potential

The present formalism relies on a Thomas-Fermi analysis of the electron density, that has been widely used to describe warm dense matter [12,13,18,19]. More precisely, we derive a semi-classical self-consistent density for free electrons, while bound electrons are treated in a full quantum-mechanical way. A similar hypothesis is assumed in several works, e.g., in models for density effects in H-like ions [13] or in the CASSANDRA average-atom theory [20]. Furthermore we have shown previously [17] that the use of Fermi-Dirac statistics is usually not required for not too low temperatures and moderate densities.

### 2.1. Method

Contrary to what has been mostly done elsewhere (see, e.g., Ref. [14]), we focus here the attention on approximate analytical expressions for the plasma potential $V_{\rm pl}(r)$ — linked to the local free-electron density through Poisson equation — and not for the free-electron density $n_e(r)$. The reason for that is two-fold. First, the physical quantities such as wavefunctions, energies, rate coefficients and collision cross-sections directly depend on the potential and not on the density. Second, it turned out that simple and accurate polynomial approximations are available for the radial dependence of the potential, while the free-electron density has a non-rational $r^{-1/2}$ behavior close to the nucleus that would require a less convenient non-polynomial fit formula.

The procedure chosen to obtain an analytical form of the plasma potential whatever the plasma temperature $T_e$, spatially averaged free-electron density $N_e$, and average free-electron number per ion $Z_f$ involves a three-step numerical fit, each step being individually usable to provide a polynomial approximation.

In the first step, the reduced plasma potential $v_{\rm pl}^{(1)}(r) = R_0 V_{\rm pl}^{(1)}(r)/Z_f$ — in Ref. [17] we have shown that this quantity obeys simpler scaling laws than $V_{\rm pl}^{(1)}(r)$ — is fit to the form

$$v_{\rm pl}^{(1)}(r) = 2 - r/R_0 + \sum_{i=1}^{n_c} a_i(1)(1 - r/R_0)^{i+1} \tag{2.1}$$

where $R_0$ is the Wigner radius defined by $4\pi R_0^3/3N_e = Z_f$. Atomic units are used throughout, unless explicitly mentioned. Here the coefficients $a_i(1)$ are numerically computed by least-square procedure, and depend on atomic potential, plasma temperature $T_e$ and free-electron average density $N_e$. Whatever the number $n_c$ of fit coefficients, this expression ensures that the potential is continuous at $r = R_0$ and that the electric field has the correct value on the Wigner-sphere surface $dV/dr(R_0) = -Z_f/R_0^2$, in agreement with Gauss theorem and electric neutrality condition.

It turns out that the value $n_c = 3$ provides a good compromise between accuracy of the fit and simplicity of the analytical expression. Furthermore, we have shown analytically in hydrogen-like ions [17] that the first correction to the infinite-temperature limit involves indeed a three-coefficient polynomial. As can be proved using scaling properties [17], the coefficients $a_i(1)$ obtained in this first step are not independent functions of $N_e$ and $T_e$ but of the dimensionless parameter

$$\rho = R_1/R_0 = \frac{Z_f}{\pi k T_e R_0} \tag{2.2}$$

hereafter referred as the "coupling parameter", though it differs by a factor $1/Z_f\pi$ from the usual one [15]. They are also functions of the average ionization $Z_f$ and of the potential created by the nucleus and the bound electrons. In the hydrogen-like case $Z_f = Z-1$, $Z$ being the nucleus charge, these coefficients depend simply on $\rho$ and on $Z_f/Z$.

As a second step of the fitting procedure, the high-$T_e$ analytical development provided by Eq. (15b) of Ref. [17] and a direct inspection of the numerical results presented in Appendix A suggests that these elements are correctly represented by a harmonic form

$$a_j(2) = -\frac{\delta_{j1}}{2} + \frac{\rho}{M_j\rho + P_j} \tag{2.3}$$

where $\delta_{ij}$ is the Kronecker symbol. The $M_j$ coefficients are determined by linear regression, looking at the dependence of $\rho/\left(a_j + \frac{\delta_{j1}}{2}\right)$ versus $\rho$. The $P_j$ coefficients might be derived from this linear regression. However, it appeared that the numerical accuracy obtained on the $P_j$ coefficient by this method was very poor, that is why we decided to derive these coefficients from the low-density or high-temperature form. Therefore, as mentioned in our previous work [17], we have chosen $n_c = 3$ and

$$P_1 = \frac{10/3\pi}{5Z/2Z_f - 1}, \quad P_2 = \frac{10}{3\pi}, \quad P_3 = -\frac{40}{3\pi}. \tag{2.4}$$

Examples of fit are given in Table 1 for several elements ranging from helium ($Z_f = 1$), to thallium ($Z_f = 80$).

As a third step, one may give an analytical form fitting the coefficients $M_j$ themselves as function of $Z/Z_f$. Once again a series of tests lead us to state that a harmonic dependence

$$M_j = \frac{A_j Z_f + B_j}{C_j Z_f + 1} \tag{2.5}$$

provides an acceptable estimate of the numerically derived $M_j$ coefficients. The atomic number $Z$ is implicit in this formula since one only deals here with hydrogenic ions for which $Z = Z_f+1$. These

**Table 1**
Coefficient for fitting the plasma potential in various H-like elements. The coefficients $M_j$ define the temperature and density dependence of the plasma potential according to Eqs. (2.1), (2.3). The uncertainty $\Delta M_j$ is derived from the performed linear regression.

| Element | $Z_f$ | $M_1$ | $\Delta M_1$ | $M_2$ | $\Delta M_2$ | $M_3$ | $\Delta M_3$ |
|---|---|---|---|---|---|---|---|
| He | 1 | 3.45091 | $7\times10^{-5}$ | 6.44652 | $2\times10^{-4}$ | −4.9386 | $6\times10^{-4}$ |
| Al | 12 | 1.66693 | $2\times10^{-4}$ | 2.34249 | $6\times10^{-5}$ | −1.9564 | $5\times10^{-4}$ |
| Mn | 24 | 1.37079 | $2\times10^{-4}$ | 1.97192 | $5\times10^{-5}$ | −1.6218 | $5\times10^{-4}$ |
| In | 48 | 1.16900 | $2\times10^{-4}$ | 1.70423 | $8\times10^{-5}$ | −1.3907 | $2\times10^{-4}$ |
| Tl | 80 | 1.06480 | $4\times10^{-4}$ | 1.54493 | $8\times10^{-4}$ | −1.2628 | $4\times10^{-4}$ |