High Energy Density Physics 10 (2014) 16–26

Contents lists available at ScienceDirect

High Energy Density Physics

journal homepage: www.elsevier.com/locate/hedp

Equation of state calculations based on the self-consistent ion-sphere and ion-correlation average atom models

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A R T I C L E I N F O

Article history:
Received 29 July 2013
Received in revised form
26 October 2013
Accepted 1 November 2013
Available online 9 November 2013

Keywords:
Dense plasma
Hugoniot
Equation of state

A B S T R A C T

We compare the predictions of two self-consistent average atom (SCAA) models. One is based on the ion-sphere (IS) and the other ion-correlation (IC) model applied to the representative plasma ion. We present shock-Hugoniot calculations for aluminum and molybdenum from zero up to high temperatures and pressures when relativistic effects are important. We also compare the form factors relevant to elastic photon scattering and we also present calculations for the emissivity and photoabsorption in hot aluminum plasma.

1. Introduction

The application of modern quantum theory in the modeling of the physics of high temperature plasmas has been around for at least six decades. First, the Thomas–Fermi (TF) and Thomas–Fermi–Dirac (TFD) models were extended to finite temperatures [1,2] by assuming that the occupation of the phase cells is determined by the Fermi–Dirac statistics. This assumption is maintained in the computation of the shell structures predicted by the TFD potential and this model is appropriately called the Thomas–Fermi–Dirac Shell model (TFDS) [3]. At a finite temperature the Fermi–Dirac statistics yields non-integer occupancies for the upper shells, therefore the model is not real and it represents only a statistical average, thus the model is appropriately labeled as an "average atom" (AA model). The temperature–density dependent AA model was extended to a full self-consistent model analogous to a zero temperature Hartree–Slater or Dirac–Slater model by the author in 1972 [4] and subsequently a somewhat modified version was presented in 1979 by Liberman [5]. Since then a number of papers have investigated the mathematical details of the AA model and its applications and the research is still ongoing, we just give two important references [6,7]. It should be noted at the onset, that although the AA model is widely used to calculate Equation-of-State (EOS) properties, but care has to be exercised to extend the AA model for the calculation of photoabsorption or emission in hot plasmas. In the case of high density plasmas the various broadening mechanisms render the quantum states of the AA model applicable for the computation of spectral lines and photoionization. However, for low density plasmas when the spectral lines are narrow this is no longer valid. In fact, it is known that for low density astrophysical plasma spectra the AA model is insufficient and one must apply "detailed configuration accounting" (DCA) which is more realistic with regard to the many-electron configurations. In this paper we are concerned only about the EOS and some radiative properties of high density plasmas as predicted by the AA model.

We will consider two distinct physical models within the AA approach. One is the so called "ion-sphere" (IS) model which assumes that the representative plasma ion is enclosed in a spherical cell whose radius is determined by the ion density. The representative plasma ion is neutral within the ion-sphere, all electrons, bound and free, are contained in the cell. Density effects in the IS model are governed by the Fermi level of the plasma electrons and also by boundary conditions imposed on the bound states at the ion-sphere radius In most published EOS AA papers that the author is aware of, the IS assumption, or as sometimes called, the Wigner–Seitz cell assumption is used. The other, much less used AA model is the "ion-correlation" (IC) model where allowance is made for the penetration of neighboring ions into the ion-sphere, thus modifying the electron potential compared to the IS model. Clearly, the region of interest in the IC model extends from zero to infinity and the requirement of charge neutrality for the plasma as a whole is set at infinity from the central ion. Since the perturbation of the central ion by the neighbors is a realistic assumption, one would think the IC model is more

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http://dx.doi.org/10.1016/j.hedp.2013.11.001

appropriate to account for the physics of hot plasmas. In an earlier paper [8] the author did make a brief comparison of photoionization based on the IS and IC models, but no detailed EOS properties were investigated. A critical discussion of the IC versus IS models was given in a paper by Starret and Saumon [9] in 2012 followed by a subsequent paper [10] where computed results were presented for the self-consistent pair distribution functions. The purpose of this paper is to present quantitative comparisons between the predictions of the IS and IC AA models.

We present comparisons of the computed shock Hugoniots based on the two models for aluminum and molybdenum. We also present calculated form factors relevant to elastic photon scattering and some calculations for photoemission from hot aluminum plasma. In the next section we present the rudiments of the underlying models and in Section III we present computed data. We do not wish to overwhelm the reader with a large set of detailed graphs, so we will present only those data which reflect the essential difference between the two models. For the shock Hugoniots we cover temperatures high enough for relativistic features to appear and for this reason in Appendix we give a brief discussion of the relativistic virial theorem and the relativistic TFD model.

2. Theoretical background

A complete set of self-consistent equations for the IS AA model was given in Ref. [4] long time ago and it was also discussed in detail in a more recent paper by the author [11] in conjunction with shock Hugoniot calculations. Here we recapitulate the basics and we treat the IS and IC models in a parallel fashion. The bound and free electron states satisfy a one-particle equation derivable from a self-consistent Hartree–Slater or Dirac–Slater model.

$$H\psi_{\mathrm{nljm}} = \varepsilon_{\mathrm{nljm}}\psi_{\mathrm{nljm}} \tag{1}$$

Relativistic effects appear in the high energy continuum states and also in the deeply bound states in medium Z to high Z elements. The Hamiltonian in Eq. (1) is a Dirac Hamiltonian for the two component wave function and the AA occupancies of the one-electron states (bound or free) are given by the Fermi statistics determined by the temperature and Fermi level of the plasma electrons. The cardinal element is the self-consistent potential (in a.u.-s) in which the electrons move and is given by

$$V(r) = -Z/r + V_{\mathrm{e}}(r) + V_{\mathrm{x}}(r) + V_{+}(r) \tag{2}$$

where r is the distance from the center of the nucleus and Z is the nuclear charge. The second tem in the right side of Eq. (2) is the classical part of the potential due to the electron–electron interaction and the third tem is a local exchange potential that we will discuss later. The last term is due to the penetrating positive charges from outside of the ion-sphere, and it is absent in the IS model. The potentials V_{e} and V_{+} are classical in the sense that they satisfy Poisson's equation with the respective charge densities as the source. We assume spherical symmetry, which means that the wave functions are products of radial parts and spin-spherical harmonics. The radial parts for the nlj bound states satisfy the well known coupled Dirac equations

$$\begin{aligned} -c\hbar\frac{\mathrm{d}f}{\mathrm{d}r} - c\hbar\frac{1-\kappa}{r}f &= \left[\varepsilon - V(r) - mc^2\right]g \\ c\hbar\frac{\mathrm{d}g}{\mathrm{d}r} + c\hbar\frac{1+\kappa}{r}g &= \left[\varepsilon - V(r) + mc^2\right]f \end{aligned} \tag{3}$$

where g and f are the "large" and "small" components of the Dirac spinor and $\kappa = \pm(j+1/2)$; $l = j \pm 1/2$) with ε as the energy eigenvalue. For the bound states the normalization conditions must reflect the fact that the region of interest in the IS and IC models are different,

$$\int_0^{r_0,\infty_0} \left[g_{\mathrm{nlj}}^2(r) + f_{\mathrm{nlj}}^2(r)\right]r^2\mathrm{d}r = 1 \tag{4}$$

where the upper limits r_0 and ∞ apply to the IS or IC models, respectively, and r_0 is the ion-sphere radius. In both models the level occupancies are given by the Fermi statistics

$$p_{\mathrm{nlj}} = \frac{2j+1}{\exp\left[\left(\varepsilon_{\mathrm{nlj}} - \mu\right)\Big/kT\right] + 1} \tag{5}$$

A fundamental difference between the IS and IC models is associated with the boundary conditions imposed on the bound wave functions. In the IS model used in this paper and also in Ref. [11] the boundary conditions are given at the ion-sphere radius. The two boundary conditions are that either the wave function or the gradient must be zero. In the molecular analogy the first condition is reminiscent to an anti-bonding orbital whereas the second to a bonding orbital. In the solid state analogy the eigenvalues associated with the two boundary conditions yield a broadening of the levels into bands and sometimes two bands may overlap, a feature well known in the ground states of many metals like aluminum and cesium. The above feature is absent in the IC model, where the boundary conditions are given at infinity. The IS boundary conditions together with the band splittings were discussed in detail in Ref. [11]. It should be noted that the IS model of Ref. [5] differs from the one used here in the sense that although the charge density is normalized to the volume of the ion-sphere, but the boundary conditions for the bound states are given at infinity, thus no band structures are predicted.

From Eqs. (4) and (5) the bound electron density is

$$4\pi\rho_{\mathrm{b}}(r) = \sum_{\mathrm{nlj}} p_{\mathrm{nlj}}\Big[\tag{6}$$

The total electron density is of course the sum of the bound and free densities. We decompose the free electron density into two parts, the low to moderately high energy electrons are treated with quantum mechanics and the high energy free electrons are treated by the relativistic TFD model. This procedure is also discussed in detail in Ref. [11]; here we just give a brief survey. We have for the free electron density.

$$\rho_{\mathrm{f}}(r) = \rho_{\mathrm{f}}^{\mathrm{I}}(r) + \rho_{\mathrm{f}}^{\mathrm{II}}(r) \tag{7a}$$

$$\text{with}\quad 4\pi\rho_{\mathrm{f}}^{\mathrm{I}}(r) = \sum_{l=0}^{l_{\max}} \sum_{j=l-1/2}^{j=l+1/2} \int_0^{\varepsilon^{\mathrm{M}}} p_{\mathrm{lj}}(\varepsilon)R_{\mathrm{lj}}^2(\varepsilon, r)\mathrm{d}\varepsilon \tag{7b}$$

and $\rho_{\mathrm{f}}^{\mathrm{II}}(r)$ is given by Eq. (A16) in the Appendix. The requirement on the upper limit ε^{M} in the integral is that the partial wave with $l_{\max}$ has its classical inner turning point outside r. In this paper we give allowance for $l_{\max}$ not to be larger than 20, but pending on the density of the plasma it may be less than that. For the energy computation we need the one-particle energy density associated with the continuum states of Eq. (7b)

$$4\pi\varepsilon^{I}(r) = \sum_{l=0}^{l_{\max}} \sum_{j=l-1/2}^{j=l+1/2} \int_0^{\varepsilon^{\mathrm{m}}} p_{lj}(\varepsilon)R_{lj}^2(\varepsilon, r)\varepsilon\mathrm{d}\varepsilon \tag{7c}$$

Since Eqs. (7b) and (7c) concern low energy continuum states, for the function $R_{lj}(\varepsilon,r)$ we use a one-component relativistic