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FINAL REPORT

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EQUATION OF STATE AND CONDUCTIVITY OF HOT, DENSE MATTER

Gabor J. Kalman

Principal Investigator

Department of Physics

Boston College

Chestnut Hill, MA 02167

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I. OBJECTIVES

The purpose of the research program reported there was to develop and apply a novel method to the calculation of the Equation of State (EOS), Mean Charge State (MCS) (or degree of ionization) and conductivity of dense plasmas of moderately high Z-numbers ($Z < 30$). The method to be applied was the Thomas-Fermi model, modified and adapted to the dense plasma environment by the author and Ying [1]. The innovative elements of the approach are:

1) The plasma environment is represented by the ion-ion and ion-electron correlation functions as source densities in the TF equation.

2) The bound electron density is posited to be zero at the ion boundary: this gives a reasonably defined ion radius, separates free and bound electrons and eliminates both the unphysical extra pressure due to bound electrons (characteristic to the so-called "Confined Alom" model) and the infinite ion radius (characteristic to the TF - Debye model).

3) The MCS is determined by minimizing the free energy (F) of the combined TF-ion/plasma system, with the proper inclusion of all electron-electron, electron-ion, ion-ion correlations.

4) The method can be combined with the approach of Davis and Blaha, who solved the exact Schrodinger equation for the valence electron in the TF-potential of the core electrons.

The original program was formulated for a three-year period, and was planned to be funded on an appropriate level. In fact, after the exploratory funding of the first year, the planned second year funding was drastically reduced and third year completely eliminated. Consequently only a limited portion of the original objectives have been achieved.

II. ACCOMPLISHMENTS

1. In order to obtain a reliable description of the correlations, a hypernetted chain (HNC) integral equation has been developed for the system. The interaction potential between the ions is properly determined by the combined charge of the nucleus and the bound electrons.

but does not include the effect of the penetrating free charges. The free electron-ion interaction is represented by an effective potential which phenomenologically includes the softening quantum - effects near $\mu = 0$ and the effects of exchange with the bound electrons. [2,3] The two component HNC code has been developed and has been tested against the existing HNC computer code for pure Coulomb system, developed by the Livermore group [4].

2. The HNC and TF equations become coupled because interaction potential depends on the bound electron distribution, which, in turn, is affected by the correlations between the selected ion and its surroundings. A corresponding TF-HNC computer has been developed.

3. In order to determine the free energy of the plasma without the cumbersome and unreliable standard temperature integration, we have adopted the method of Hill [5], which requires space integrals over the pair correlation functions only.

4. We have solved the combined TF-HNC-F code for Z = 6 (Carbon), Z = 13 (Aluminum) and Z = 29 (Copper) for a wide range of temperature and density values:

T = 1, 10, 20, 50, 100, 200, 500, 1000 eV

m = 10^{19}, 10^{20}, 10^{21}, 10^{22}, 10^{23}, 10^{24}, 10^{25}, 10^{26} cm^{-3}

and determined the following quantities:

A. MCS (z):
- (i) z (T; n, Z)
- (ii) z (n; T, Z)
- (iii) equi-z contours in the (n,T) plane

B. Correlation functions g_{AB} (r):
- (i) $g_{ion\text{-}ion}$ (r)
- (ii) $g_{ion\text{-}electron}$ (r)
- (iii) $g_{electron\text{-}electron}$ (r)

C. Static structure functions S_{AB} (k)
- (i) $S_{ion\text{-}ion}$ (k)
- (ii) $S_{ion\text{-}electron}$ (k)
- (iii) $S_{electron\text{-}electron}$ (k)
- (iv) S_{charge} (k)

D. EOS: $P(n; T, Z)$ (pressure)
$E(n; T, Z)$ (energy)
$F(n; T, Z)$ (free energy)

E. Energies of the bound electrons:

$$E_{bound}(z; Z, n, T)$$

and "ionization energies"

$$I_Z(Z; n, T) = E_{bound}(z - 1; Z, n, T) - E_{bound}(z; Z, n, T)$$

Note that the ionization energies here are explicit functions of n and T.

5. We have compared our results with results available in the literature on the MCS and on the EOS: they include Davis and Blaha [6], More [7] Fen et. al. [8], the Los Alamos SESAME Code, Foster et. al. [9] Latter [10] and Soviet data provided by Professor E. Son. [11]. The results are free from the usual anomalies plaguing TF calculations, approach the Saha equation results for low densities and correctly portray pressure ionization effects at high densities.

6. In summary, we have developed a unique model, applicable over a wide range of density and temperature values for medium or high Z plasmas, which, we contend, represents the most reliable approach to hot, dense plasma MCS calculations.

7. In view of the availability of effective "ionization energies" (see above), it has become possible to abandon the average atom picture inherent in the present calculations and replace it with a Saha-like equation which can correctly describe fluctuations and integer z-numbers and describes the system in terms of integer z values only.

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III. PUBLICATIONS AND PRESENTATIONS

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