ATOMIC POTENTIALS IN VERY DENSE ALUMINUM PLASMAS

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The calculation of atomic properties is plasma is critically dependent on the form of the ion-electron interaction potential. In the case of weak collisions in a low density ionized gas, the screening of the ion under consideration by surrounding plasma is adequately described by the Debye-Hückel potential (see, e.g., Weisheit, 1983). If the plasma is very dense, the perturbation approximations leading to the Debye form break down and other techniques must be employed to incorporate additional correlative effects. The transition from classical to this strongly coupled plasma occurs when the parameter $\Gamma = (\bar{Z})^2 e^2 \beta / r_o$, where $\bar{Z}$ is the mean charge per ion, $\beta = (k_B T)^{-1}$, and r_o is the ion-sphere radius, is greater than about one.

Correlations can be introduced by a method that provides accurate particle density distribution functions in ionic systems. The hypernetted chain (HNC) approximation (see, e.g., Hansen and McDonald, 1976) to the hierarchy of equations for the distributions has been shown to closely reproduce data from computer simulations of strongly coupled plasmas (Hansen and McDonald, 1981). The method utilizes a semiclassical form for the bare two-body interaction (Deutsch, 1977) to generate charge distributions which are employed in the Poisson equation to provide the HNC effective potential (Cauble, Blaha, and Davis, 1984).

A method capable of solving for the effective potential in a quantum mechanical way is density functional theory --DFT (Gupta and Rajagopal, 1982). Since the free energy of the system is a unique functional of the charge distributions, minimization of the free energy with density profiles found from the Schrodinger equation with exchange and correlation for the free and bound electrons and a form for the ion distribution, either with (Dharma-wardana and Perrot, 1982; Perrot and Dharma-wardana, 1984) or without (Gupta, Blaha, and Davis, 1984) ion-ion correlations, leads to a unique effective ion-electron potential via a self-consistent solution of the equations.

Fig. 1 displays the ion and electron distributions around an aluminum ion located at the origin in an aluminum plasma. The plasma conditions are $n_e = 10^{25}$ cm^{-3} and T = 500 eV ($\bar{Z}$ = 10.1 and Γ = 4.75), the most extreme case considered here. The quantum mechanical DFT and the semiclassical HNC methods give very similar results except: for $\rho_i(r)$ near $r/a_o \sim 2$ and $\rho_e(r)$ near $r/a_o \sim 1$, the HNC's better treatment of ion correlations reveals the onset of spatial structure (not evident

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in the DFT) as well as plasma screening; and for $\rho_e(r)$ very close to the origin, where DFT handles the electron distribution more accurately, the curves are somewhat distinct. The Debye $\rho_i(r)$ is included for comparison; it is sigificantly in error throughout the entire range.

The remaining figures display the effective potentials for aluminum plasmas under various strongly coupled conditions. In all cases the DFT and HNC potentials are very similar, HNC ion correlations creating minor differences at large radius. The Debye potential shows excessive screening throughout. The Debye screening can be reduced by not including ions in the calculation of the Debye length, but too much of the screening effect is removed; the resulting exponential potential falls off far too slowly. The "ion-sphere" model (no ion-ion interactions at all and a uniform neutralizing electron density close to the ion being studied), thought to be valid at extremely high densities, is somewhat better than the Debye form, but is quite inaccurate even at 10^{25} cm^{-3}.

From effective potentials such as these, atomic properties of an average plasma ion can be obtained (Davis, et al, 1983). These include atomic energy levels, wavefunctions, equation of state properties (Gupta, Blaha, and Davis, 1984), photoionization cross sections (Cauble, Blaha, and Davis, 1983), and bremsstrahlung cross sections (Lamoureux, et al, 1984). These calculations show that considerable errors can be made when an inappropriately approximated potential (such as the Debye-Huckel or ion-sphere) is used. In general for atomic calculations in dense plasmas such as these considered here, the Debye-Hückel potential predicts results that have significantly greater error than those provided by the ion-sphere potential. It is quite easy, however, to use an effective interionic potential such as DFT or HNC/Poisson to account for the additional many-body effects that must be included when the plasma is close to being strongly coupled.

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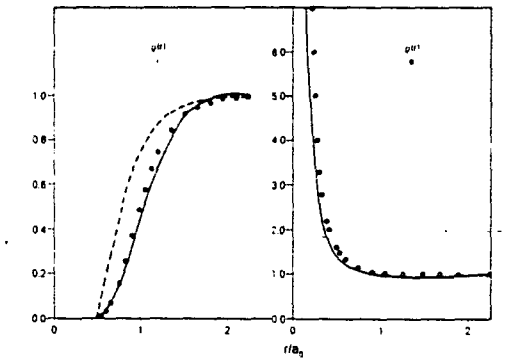

Fig. 1: Ion and electron charge distributions in Aℓ at $n_e = 10^{25}$ cm^{-3} and T = 500 eV DFT: circles; HNC: solid; and DH: dashed curve.

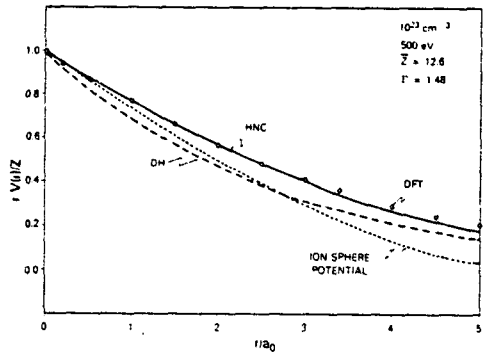

Fig. 2: Effective electron-ion potentials in Aℓ for various models. $n_e = 10^{25}$ cm^{-3}, T = 500 eV.

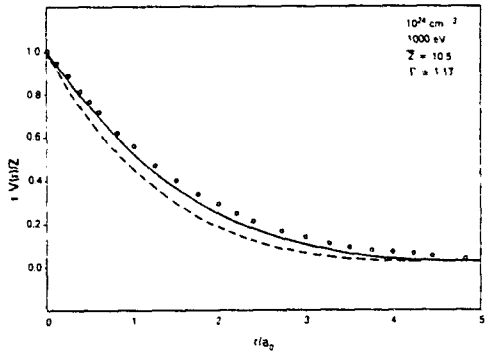

Fig. 3: Effective electron-ion potentials in Aℓ for various models. $n_e = 10^{24}$ cm^{-3} and T = 1000 eV.

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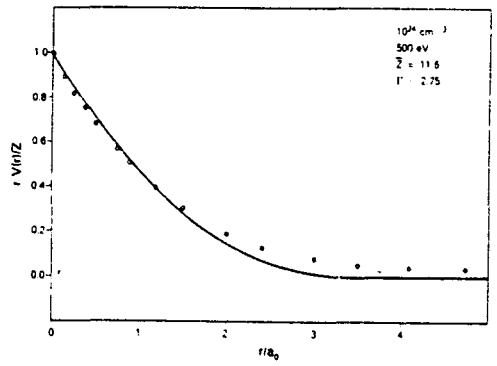

Fig. 4: Effective electron-ion potentials in Aℓ for various models. $n_e = 10^{23}$ cm^{-3} and T = 500 eV.

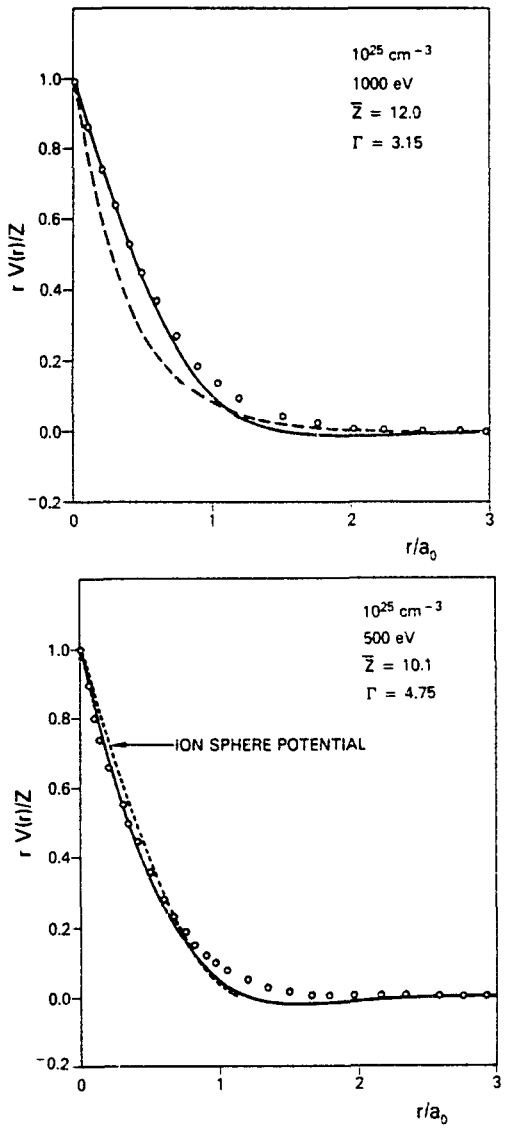

Fig. 5: Effective electron-ion potentials in Aℓ for various models. $n_e = 10^{25}$ cm^{-3}, T = 1000 eV and 500 eV.

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