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Energy level broadening effect on the equation of state of hot dense Al and Au plasma

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Abstract

In the hot dense matter regime, the isothermal equation of state (EOS) of Al and Au is calculated using an average-atom (AA) model in which the broadening of energy levels of atoms and ions are accounted for by using with a Gaussian distribution of the density of states. The distribution of bound electrons in the energy bands is determined by the continuum Fermi–Dirac distribution. With a self-consistent field average atoms scheme, it is shown that the energy-level broadening has a significant effect on the isothermal equation of state (EOS) of Al and Au in the hot dense matter regime. The jumps in the equation of state (EOS) induced by pressure ionization of the one-electron orbital with the increase in density, which often occur in the normal average-atom model and have been avoided by generally introducing the pseudo-shape resonance states, disappear naturally.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

There has been growing interest in the equation of state (EOS) of the hot dense matter regime [1], which is intermediate between the ordered solid and liquid phases and the highly disordered gas phase and is characterized by strongly coupled and partially degenerated media. This thermodynamic equilibrium regime, encountered in planetary interiors, cool dense stars, and in laboratory experiments, opens up a challenging field for both experiments and *ab initio* calculations.

Lee *et al* [2] and Bar-Shalom *et al* [3] used the modified Thomas–Fermi (TF) model, which includes shell structure by accounting for the discrete nature of the bound states and considering resonance states in the pressure ionization regions, to describe the equation of state (EOS) and the average ionization degree of the hot dense regime. This kind of shape resonance

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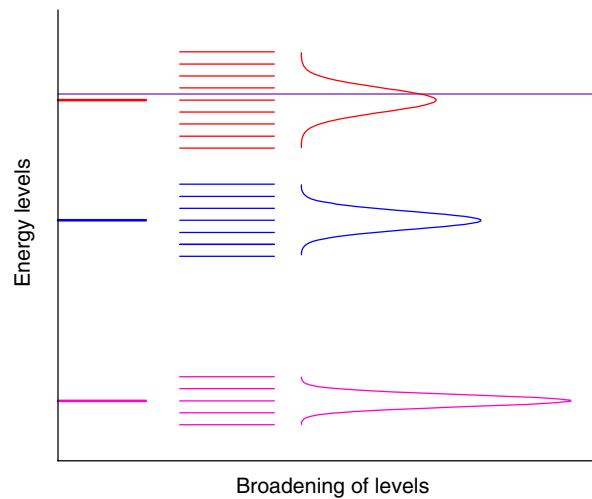


Figure 1. Splitting of bound-state energy levels into many sublevels in plasma, which are described approximately by a Gaussian distributed density of states.

state is only needed when a bound state is just emerging from the bound state to the continuum with increasing matter density. The fact is that one used an artificial localized continuum state above but very close to the ionization threshold to take into account the broadening of the bound states across the ionization threshold. However, in the special regime, the electronic energy levels of atoms and ions split many sublevels due to the strong interaction between the particles, and the space between the energy of the sublevels is very small. So the splitting of one energy level is usually described by a broad distribution of the density of states over an energy interval as shown in figure 1 [4]. The broadening is described statistically by the density of states distribution within the same number of energy intervals as that of energy levels without broadening. The electronic-energy-level broadening has been considered generally via the line shape when spectral analysis is made or radiative transfer is considered. The electronic-level broadening also has an influence on the ionization of the ions and has often been considered via the pressure-induced lowering of the ionization potentials [5–10]. For highly excited Rydberg states, one often describes the distribution of the states across the ionization threshold by approximately using a smooth function for the density of states, provided that the intervals between the Rydberg states are small enough. The broadening of the energy levels across the ionization threshold has been observed in the spectra, which is a continuum absorption band [11, 12] and no longer discrete absorption lines, and hence what can be described approximately by smooth functions of the density of states for corresponding energy bands. The broadening of the energy levels across the ionization threshold has a significant influence on the ionization of the atoms [4] and the EOS, in particular the pressure-induced ionization, which occurs at high densities of matter with large pressure-associated energy-level broadening.

The average-atom model is one of the statistical approximations applied to calculate the electronic structure of atoms and ions in hot and dense plasmas based on the statistical average over the detail of the populations and occupations of the ions and electrons [13, 14]. The average-atom model is easy to use in conjunction with a variety of treatments of electron orbitals in atoms. A widely used scheme of the average-atom calculation is to use a full self-consistent Dirac–Slater model to obtain the electron orbitals [13, 15]. With such an

appropriate treatment of the interactions between electrons and the nucleus, the average-atom model can produce reasonable results for stellar opacities and the equation of states. In the usual average-atom model, the electron orbitals of a definite pair of quantum number nl for different ionized ions of the same element and the occupation numbers of electrons on these orbitals are approximated by one pseudo-orbital with an average fractional occupation number for electrons. The energy-level shifts have been taken into account approximately by considering the environment via a static screening Coulomb potential, while the dynamical broadening caused by the interactions of free electrons and other ions is ignored. The ion splitting and the coupling splitting of the energy level have been considered approximately when one calculates the optical transitions between the pseudo-orbitals. However, the splitting of the real energy levels approximated by the pseudo-orbitals in the average-atom model are usually not considered when the average ionization degree and the EOS are calculated. The neglect of the energy-level broadening results in unreal discontinuous variations of the average ionization degree [4] and the EOS with increasing density in the dense regime. Zimmerman and More [16] developed a pressure ionization scheme, in which the bound orbital reduced with an increase in the matter density and the bound electrons merges into the continuum as a smooth function of density. In the present study, it will be shown that when the broadening of the electronic energy levels is considered implicitly by using an energy band, the irregularities in the pressure-induced electron ionization disappear naturally.

2. Method of calculation

In a full relativistic self-consistent field-based average-atom (AA) model, the influence of the environment on the atom is assumed to have spherical symmetry on average. The movement of an electron under the interactions of the nucleus and other electrons is approximated by a central field, which is determined by the standard self-consistent calculation. In the central field, the radial part of the Dirac equation has the form

$$\begin{aligned} \frac{dP_{n\kappa}(r)}{dr} + \frac{\kappa}{r}P_{n\kappa}(r) &= \frac{1}{c}[\epsilon_{n\kappa} + c^2 - V(r)]Q_{n\kappa}(r) \\ \frac{dQ_{n\kappa}(r)}{dr} - \frac{\kappa}{r}Q_{n\kappa}(r) &= -\frac{1}{c}[\epsilon_{n\kappa} - c^2 - V(r)]P_{n\kappa}(r) \end{aligned} \quad (1)$$

where $P(r)$ and $Q(r)$ are, respectively, the large and small components of the wavefunction, c is the light speed, and $V(r)$ is the self-consistent potential, which consists of three parts:

$$V_{\text{sfc}}(r) = V_s(r) + V_{\text{ex}}(r) + V_{\text{corr}}(r). \quad (2)$$

$V_s(r)$, $V_{\text{ex}}(r)$, and $V_{\text{corr}}(r)$ are, respectively, the so-called static, exchange and correlation potentials. $V_s(r)$ is calculated from the charge distributions in the atom, while $V_{\text{ex}}(r)$ and $V_{\text{corr}}(r)$ take the approximate temperature-dependent forms of Dharma-wardana and Taylor [17]. For bound states, we have the boundary conditions [13]

$$\begin{aligned} P_{n\kappa}(r) &\xrightarrow{r \rightarrow 0} ar^{l+1} \\ P_{n\kappa}(R_b) &= 0 \end{aligned} \quad (3)$$

or

$$\begin{aligned} P_{n\kappa}(r) &\xrightarrow{r \rightarrow 0} ar^{l+1} \\ \frac{d}{dr} \left[\frac{P_{n\kappa}(r)}{r} \right]_{R_b} &= 0 \end{aligned} \quad (4)$$

satisfied by the radial wavefunctions, where R_b is the radius of the atom. The difference in the two orbital energies ϵ_a and ϵ_b obtained with the boundary conditions (3) and (4) are considered

as the full width at half maximum (FWHM) of the energy band, $\Delta\epsilon = |\epsilon_a - \epsilon_b|$. The boundary conditions (3) and (4) correspond to the antibond and bond electronic states of the diatomic molecules, and ϵ_a and ϵ_b give an estimate for the variation range of one-electron energy due to interactions with the nearest-neighbor atom. For densities nearly equal to or higher than the solid density, the static interactions between the atoms dominate the whole features of the electronic states. The coupling between the electrons and the influence of the dynamical changes in the local environment produce relatively small corrections to the energies.

The electron distribution is calculated separately for the bound and free electron parts. The bound electron density is obtained according to

$$D_b(r) = \frac{1}{4\pi r^2} \sum_j \int_{\epsilon-3\Delta\epsilon}^{\epsilon+3\Delta\epsilon} b_j(\epsilon) (P_j^2(r) + Q_j^2(r)) d\epsilon \quad (5)$$

where $b_j(\epsilon)$ is density of the occupation number of the state j expressed in terms of the density of states and the Fermi–Dirac distribution

$$b_j(\epsilon) = \frac{2|\kappa_j|\rho(\epsilon)}{\exp((\epsilon_j - \mu)/T) + 1}. \quad (6)$$

The density of states $\rho(\epsilon)$ is taken to be a Gaussian function centered at the corresponding electron orbital energy of equation (3), and satisfies the requirement that

$$1 = \int_{\epsilon-3\Delta\epsilon}^{\epsilon+3\Delta\epsilon} \rho(\epsilon) d\epsilon. \quad (7)$$

Comparison between the present scheme and the full-potential linearized augmented plane wave (FLAPW) [18] formalism is made in [4]. The general shape of the density of states of the modified AA model agrees very well with the first-principles FLAPW result for Al and Au. The comparison supports the present treatment of the electronic-level broadening in the AA model.

The integration over energy in equation (5) is limited below the ionization threshold, which is chosen to be the zero point in the present calculation. As only the bound electrons are treated by equation (5), the wavefunctions are obtained with the boundary condition (3). The free electrons are considered much more simply with an assumption of the Thomas–Fermi (TF) treatment, and the local free-electron density is calculated with a Fermi–Dirac distribution of the local free electrons in the plane wave momentum k space, which can be written as

$$D_f(r) = \frac{1}{\pi^2} \int_{k_0(r)}^{\infty} \frac{k^2 dk}{e^{(\sqrt{k^2 c^2 + c^4 - c^2 - V(r) - \mu})/T} + 1} \quad (8)$$

where $k_0(r) = [2V(r)c^2 + V(r)^2]^{1/2}/c$ and μ is the so-called chemical potential. The total electron density is the sum of $D_b(r)$ and $D_f(r)$:

$$D_i(r) = D_b^i(r) + D_f^i(r). \quad (9)$$

The chemical potential μ is determined so that electrical neutrality is satisfied:

$$\sum_i n_i \int_0^{R_b^i} 4\pi r^2 D_i(r) dr = \sum_i n_i Z_i, \quad (10)$$

where n_i is the number of the i th kind of atom, and Z_i is the nuclear charge. The summation runs over all kinds of atoms. In hot and dense plasmas, the size effects on the electronic structures of atoms and ions are considerable. For pure matter, the average atomic size is taken to be

$$R_b = \left(\frac{3\Omega_0}{4\pi} \right)^{1/3}, \quad (11)$$

where Ω_0 is the average atomic volume. For mixtures, the average ionization degree and the average atomic size of each kind of element and the common chemical potential can be determined on the basis of a more general self-consistent approach, along with the atomic self-consistent potentials and the one-electron orbital energies of every kind of element, as we proposed previously [19].

3. Result and discussion

The results of the equation of state with and without broadening of the electronic states for the elements Al and Au at temperatures of 1 and 10 eV are plotted in figure 2 for comparison. The solid lines are the results calculated by the normal AA model without considering broadening of the electronic states, which have several jumps because of the pressure ionization. The jumps are caused by the same inner-shell electron ionization with increasing density. In the normal AA model, the bound states are the isolated levels; the merging of an isolated level from a bound state to an ionization state induced by the pressure would give a jump ionization of the occupied electrons on this orbital and possibly result in an unreal ionization instability. In figure 2, the result of Al at $T = 1$ eV has three jumps, caused by ionization of the inner shells of 2s, 2p and 3s, respectively. The results for Au are the same as those for Al. Because Au has more shells, it has more jumps in the results of the equation of state. In fact, for a highly dense plasma, the bound states cannot be treated as isolated energy levels and should be considered as energy bands when merging into the ionization region due to the strong interaction between particles. So, considering the splitting of the energy level as an energy band of a Gaussian distribution of the density of states, we obtained the results for the equation of state with a smooth variation in figure 2 (dot-dashed lines) with increasing density. By comparing the results between 1 and 10 eV, we found that the thermo-ionization is apparent at the low densities. Also, for Al the result at $T = 10$ eV has only two jumps, caused by ionization of the inner shells of 2s and 2p; the 3s has been ionized due to thermal ionization.

In order to exhibit the physical reason for the jumps in the EOS more explicitly, we calculate the average ionization degrees of Al and Au at $T = 1$ and 10 eV in figure 3. At $T = 1$ eV, the average charge of Al has three steps due to simultaneous ionization of the 3s, 2p and 2s, and that of Au has more steps due to simultaneous ionization of the 5d, 5p, 5s, 4f and 4d. In our considering the isolated lines of the orbital energies as energy bands of a Gaussian distribution of the density of states, the pressure-induced step-like shell ionizations in the normal average-atom model are replaced by smooth curves with much less specification of the pressure ionization of a electron shell at high density of matter. We also compare the present results with those of a super transition array (STA) calculation by including shape resonant states for the free electrons. One can find that the present treatment results in smooth curves going through the middle of the normal average-atom model and through the middle of the normal STA. However, inclusion of the shape resonant states in the STA model gives smooth curves that go like the bottom of the normal AA and normal STA zigzag curves.

4. Conclusion

The broadening of the energy levels in a hot dense plasma has been shown to have a significant influence on the equation of state by using a simple self-consistent field-based average-atom approach, in which the splitting of the one-electron orbitals caused by the interaction of the free electrons and other ions is approximated by using an energy band to replace the corresponding one-electron orbital. The unreal sharp jump increases in the EOS caused by pressure ionization

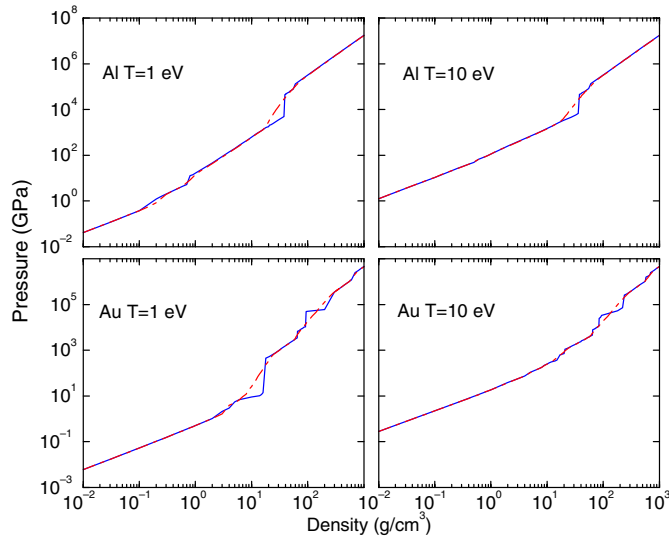


Figure 2. The equation of state for Al and Au at $T = 1$ and 10 eV: the solid line and dot-dashed line calculated by the AA model without and with the level broadening.

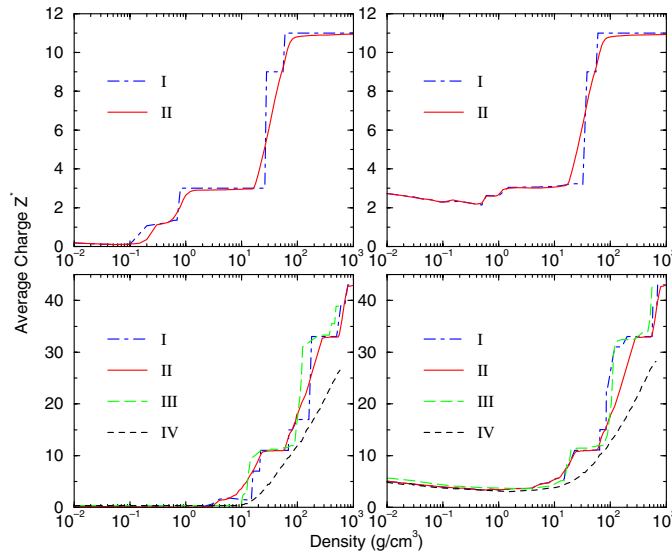


Figure 3. Density dependence of the average ionization degree of Al and Au at $T = 1$ and 10 eV. I and II label the AA results without and with the level broadening; III and IV label the STA results of [3] without and with the shape resonant orbitals.

of the electronic shells in hot dense plasmas are replaced by a smooth increase. The ionization instability related to the pressure-induced shell ionization can also be removed naturally when the level broadening is considered implicitly. The present results show that the energy-level broadening of the ions near the ionization threshold should be considered implicitly in a hot dense plasma.

Acknowledgments

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