Behavior of the coupling parameter under isochoric heating in a high-Z plasma

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Behavior of the coupling parameter under isochoric heating in a high Z plasma

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The ion-ion coupling parameter Γ is estimated for tungsten along the ρ=40 g/cm^3 isochore corresponding to twice the normal density with temperatures ranging from 10 eV to 5 keV. Using a variety approaches from a spherical Thomas-Fermi ion to a full three-dimensional orbital-free method, we show that along an isochore the effective ionic coupling parameter is almost constant over a wide range of temperatures (in our case $\Gamma \simeq 20$) due to the competition between rising temperatures and increased ionization. This Γ_plateau effect depends on the chosen density and is well delineated at normal density but almost disappears at five times the normal density. This effect could be used to obtain well defined and predictable experimental conditions.

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I. INTRODUCTION

Isochoric heating is a new technique to produce plasmas at nearly normal density. Temperatures ranging from 50 eV to 1 keV have recently been obtained by electron heating produced by picosecond laser pulses on a buried material [1, 2]. If we consider that electron and ion temperatures equilibrate on the time scale of the experiment and that the expansion of the material is negligible on the same time scale, we can deduce that the plasma is probably strongly coupled. The question is how high of a coupling parameter can be obtained by isochoric heating? For strongly coupled plasmas, we define the ion-ion coupling parameter by

$$\Gamma = \frac{Z^{*2}e^2}{4\pi\epsilon_0 a k_{\rm B} T}, \tag{1}$$

where Z^* is the ion charge state, e is the fundamental charge, $a = (3/4\pi n)^{1/3}$ is the mean ion sphere radius, n is the plasma ionic density, and T is the temperature. For a specified mass density ρ, the coupling results from the competitive effects of the ionization state $Z^*(\rho, T)$ and of the temperature. For hydrogen plasmas under inertial confinement fusion conditions, full ionization comes quickly, and for a given density any increase of the temperature translates into a decrease of the ionic coupling parameter. This is no longer true for high Z materials for which we expect a broad range of variations of the charge state in the hot dense regime. Predicting the evolution of the coupling parameter is not straightforward due to the complex relationship of ionization with density and temperature. Unfortunately, since no precise definition of the ionization state exists, we will use the usual Thomas-Fermi (TF) and Thomas-Fermi-Dirac (TFD) estimations at finite temperature. To determine the structural and transport properties, we will also use Orbital Free Molecular Dynamics simulations (OFMD), whose quality has been proven in this dense hot regime [3–9]. In this study, we focus on tungsten, which with a charge number Z=74, offers a wide range of thermodynamic states before reaching total ionization. Unless otherwise specified atomic units are used throughout, in which $\hbar = m_e = e = 1$.

II. THEORETICAL AND NUMERICAL FEATURES

In high density, hot temperature matter, ionization models based on Saha equations are no longer suitable and must be substituted with models in which density effects are included from the beginning through Pauli statistics. The Thomas-Fermi model is the basis of the description of matter in this regime. For each thermodynamic condition along the 40 g/cm^3 isochore, we have used a standard spherical code to solve the finite temperature TF or TFD equations. As usual we note that TFD estimations of Z* are 20% lower than those predicted by TF at low temperature but merge at high temperature.

We have also used OFMD to simulate a collection of 54 tungsten nuclei in a 3-dimensional box. The orbital-free method is well adapted for describing dense systems at high temperature, where methods based on orbitals such as Kohn-Sham ansatz (KS) are prohibitively expensive. Several limited studies [10–12] indicate that the transition region between KS and orbital-free calculations is sensitive to the system and conditions. However, for compressions of up to a few times normal solid density, the TFD formulations, especially with the Weiszäcker exten-

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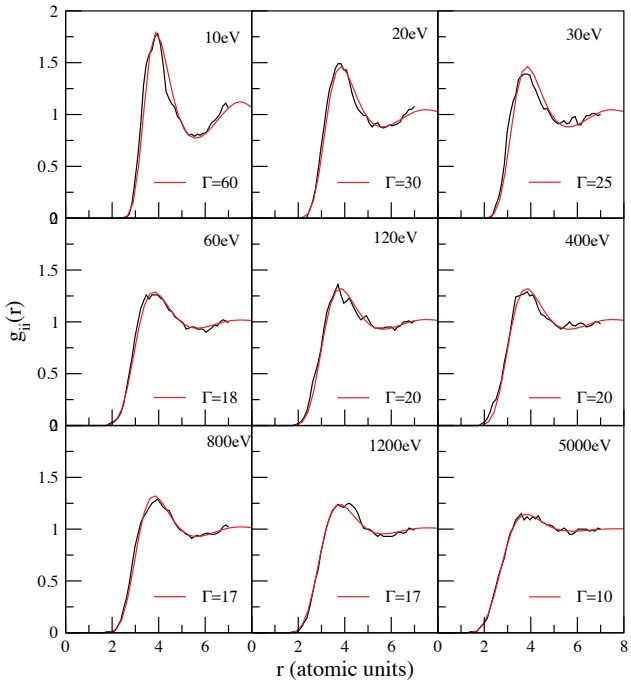

FIG. 1. (Color online) Comparison of the OFMD pair distribution function for tungsten at 40 g/cm^3 (black full line) and for 9 temperatures between 10 eV and 5000 eV with the best fitted OCP one (red-grey line).

sion (TFDW), agree within 10% or better with KS by 10 eV. As we remain generally above this transition region, we restrict this study to TF or TFD formulations.

The divergence of the electron-nucleus potential is regularized at each thermodynamical condition. The cutoff radius is chosen to be 30% of the Wigner-Seitz radius, sufficient to prevent overlap of the regularization spheres. The number of plane waves describing the local electronic density is then adjusted to converge the thermodynamic properties to within 1%. Molecular dynamics simulations are very sensitive to the value of the time-step. At each temperature the time-step must be adapted to the ionic plasma frequency[13] $\omega_p^2 = 4\pi Z^{*2} n_i^2 e^2/m_i$, where m_i and n_i are respectively the ionic mass and density. This characteristic frequency depends on the ionization Z^*. The plasma period $T_{\omega_p} = 2\pi/\omega_p$ is reported in Table I. To ensure a good energy conservation Δt has been varied from 100 a.u. at 10 eV to 10 a.u. at 5000 eV. Thermodynamical, structural, and transport properties are obtained for each simulated state. The pair distribution function (PDF) $g(r)$ gives structural information of the relative separation among the ions. We determine the self-diffusion coefficients from the standard Einstein and Green-Kubo relations for the mean-square displacement and the velocity autocorrelation function (VAF), respectively[6].

III. EFFECTIVE ONE COMPONENT PLASMA

With the one component plasma (OCP) serving as the reference model for strongly coupled plasmas [14, 15], we have performed a systematic comparison of the PDFs for each thermodynamic state. To obtain a fast evaluation of the g(r) for the OCP, we have used the fits of the static structure factor computed by Rogers et al. [16]. For each thermodynamic state, we have searched for the OCP coupling parameter Γ giving the best agreement with OFMD in terms of closest approach distance, position of the main peak and of the first minimum. This comparison between OFMD and effective OCP is shown in Fig. 1. Apart from the lowest temperatures, the g(r)'s appear the same for a large range of temperatures. A temperature of T=5000 eV must be reached to observe a significant departure from $\Gamma \simeq 20$ value. For each state, we have bracketed the g(r) to estimate the uncertainty in the coupling parameter, which can be bounded by ±2. We will call this coupling the OCP effective coupling Γ_{eff} from which we can compute an effective ionization Z_{eff}.

T	$Z_{\rm TF}$	$Z_{\rm TFD}$	Γ_{eff}	Z_{eff}	T_{ω_p}	θ	κ_{FT}
eV					a.u.		
10	8.9	7.7	60	7.1	1030	0.28	3.15
20	9.4	8.3	30	7.1	1030	0.56	2.85
30	10.3	8.8	25	8.0	922	0.78	2.65
60	12.1	10.9	18	9.6	768	1.37	2.24
120	15.4	14.9	20	14.3	515	2.11	2.02
200	20.	19.2	20	18.4	400	2.96	1.81
400	28	27.3	20	26.1	282	4.70	1.54
800	39	38.2	17	34.0	216	7.88	1.24
1200	46	45	17	41.6	177	10.3	1.12
5000	67	67	10	65.1	113	31.8	0.69
∞	74	74	0	74	-	-	-

TABLE I. Ionizations and plasma parameters for TF, TFD along the 40 g/cm^3 isochore of tungsten.

As shown in Table I, the effective ionization Z_{eff} is close to TFD, being within about 10% for temperatures above 100 eV. In addition, beyond 60 eV, the effective coupling parameter Γ_{eff} remains almost constant, which implies that behavior of the ionization just cancels the temperature effect in Eq. (1). This trend is confirmed in Fig. 2 where a slope of one-half in the effective ionization is identified at moderate temperatures on a log-log scale. This quasi-constant character of the coupling parameter is examined for a wide range of temperatures and several densities in Fig. 3; the plateau is less marked at higher density. This plateau effect is clearly related to the TFD ionization relation with temperature, but is also reminiscent of simple scaling laws at low density in the Saha regime (the well known scaling law $Z^* = 20\sqrt{T_{KeV}}$ [17] is a simplification of Saha equations [18]).

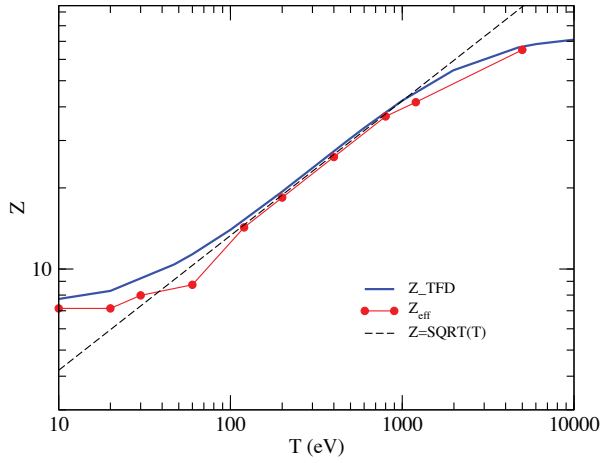

FIG. 2. (Color online) Effective ionizations for tungsten at $40\,\mathrm{g/cm^3}$.

The plasma described by OFMD is clearly strongly screened and electrons are degenerate at low temperature ($\theta = T/T_F = 0.28$ at 10 eV) but quasi-classical at high temperature ($\theta = 31$ at 5000 eV). It must be noted that the degeneracy parameter $\theta = (\mathrm{T}_{eV}/51.7)r_s^2$ depends also on the ionization through the dimensionless ratio of electronic mean radius a_e to the Bohr radius $r_s = a_e/a_B$. To quantify the screening, we use a definition of the Thomas-Fermi inverse screening length at finite temperature κ_{FT} [19] given by the fit

$$\kappa_{FT} = \sqrt{\frac{1 - 0.69\theta(1 - \exp(-2.26\theta)) + \frac{2}{3}\theta^4}{1 + \theta^5}}\kappa_0, \quad (2)$$

where κ_0 is the usual zero-temperature inverse screening length in units a^{-1}.
From the inspection of Table I, we can identify two behaviors. At low temperature the inverse screening length is high and the electronic degeneracy is high ($\theta << 1$). This suggests using an effective screened charge in a neutralizing background to make the contact with the OCP. On the contrary, at high temperature the degeneracy is low ($\theta >> 1$) as well as the inverse screening length. The electronic component is kinetic and decoupled from the ionic one, which suggests again an OCP formulation[20].

IV. COUPLING

When the ionization is converted into a coupling parameter, we can distinguish three different regimes along an isochore:

1. At low temperature, the ionization is driven by the density which gives a rather high value for the coupling parameter. This is the regime of strong coupling.

2. In the intermediate regime (between 100 eV and 1500 eV for tungsten at $40\,\mathrm{g/cm^3}$), the ionization rate exactly cancels the temperature, leading to an almost constant coupling parameter, the Γ_plateau (grey area in Fig. 3). The scaling law of the ionization with temperature ($Z \simeq T^{1/2}$) is consistent with a Thomas-Fermi description [21].

3. At high temperature for which the element is nearly fully ionized, the coupling parameter should decreases as $1/T$. This effect does not appear clearly in Fig. 3 due to the limited range in temperature (at 5000 eV, Z_{eff} is only 65 vs. 74 for full ionization).

We have found similar behavior of the coupling constant for other high Z materials, namely Pu and U (references [9] and [22]). The occurrence of the plateau is directly linked to the atomic number and density and will be the subject of a detailed subsequent paper. For light elements at normal density this plateau does not exist. Inspection of Fig. 2 suggests that the Γ_ plateau is reached for an average ionization Z_{p} in a log-log scale given by $\ln(Z_{\mathrm{p}}) = [\ln(Z) + \ln(Z_{\mathrm{min}})]/2$, where Z is the atomic number and Z_{min} the ionization at the lowest temperature (here 10 eV) given by a TFD calculation. Knowing Z_{p} we search for temperature T_{p} which gives this ionization and obtain a predicted value of the coupling parameter Γ_{p}.

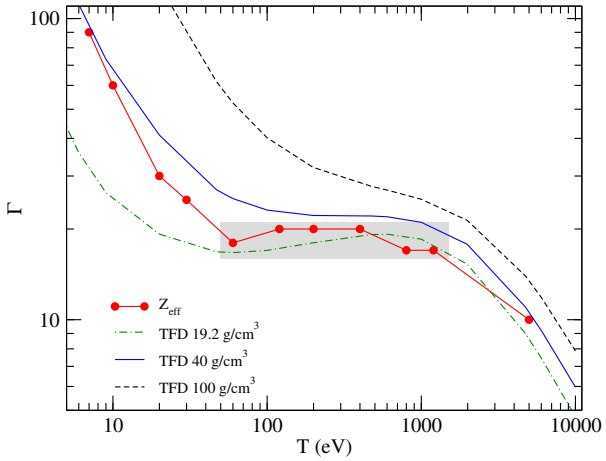

FIG. 3. (Color online) Coupling parameter for tungsten as a function of temperature for several densities. Red dots are obtained by effective matching with the OCP model for $40\,\mathrm{g/cm^3}$, and lines by a direct TFD computation. The grey area shows the quasi-constant coupling area, the Γ_plateau.

For tungsten at $40\,\mathrm{g/cm^3}$ we get $Z_{\mathrm{min}} \simeq 7$ which gives $Z_{\mathrm{p}} = 23$. This ionization is obtained for a temperature of about 300 eV leading to a plateau coupling parameter of $\Gamma_{\mathrm{p}} = 22$. One could prefer the TFDW model to get better estimations of the ionizations, particularly at low temperature, but it has been shown by Fromy et al. [23] that the improvement is very weak at the expense of much heavier calculations. At high temperature and

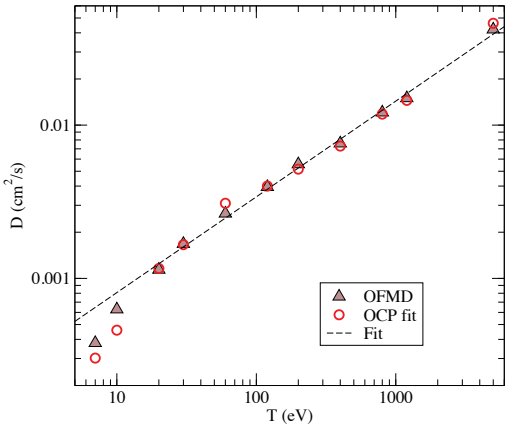

FIG. 4. (Color online) Self diffusion for tungsten at 40 g/cm^3: OFMD results compared to the effective OCP formulation.

for high Z elements ionizations predicted by TF, TFD and TFDW are almost indistinguishable (see Fig. 2 in reference [23]).

V. TRANSPORT PROPERTIES

A constant coupling means that some transport properties such as self-diffusion or viscosity are almost constant in Γ-dependent formulations when expressed in plasma units. For the self diffusion of an OCP, we can use the very simple relation established by Hansen [15] $D^* = 2.95\Gamma^{-1.34}$ and improved by Daligault [24]. In these formulations, the diffusion D^* is expressed in plasma units ($\omega_p a^2$) which again depends on the effective charge and on the ionic density. When expressed in cgs units, we see in Fig. 4 that this rough estimation is quite good compared to the OFMD results, even if the characteristic frequencies of the OCP do not match those of the screened OFMD system [4, 25]. The scaling with temperature (T^b) gives $b = 0.625$ between 100 and 1000 eV and remains consistent with the results for U (b=0.557) [22] and Pu (b=0.548) [9].

To extract further information on the characteristic frequencies of the system, we present in Fig. 5 a systematic comparison of the velocity autocorrelation functions obtained by OFMD and OCP for the effective coupling parameter. We observe that while the effective OCP may be meaningful for static structure, it fails to predict correctly the characteristic time scale at low temperature. As shown by Ohta and Hamaguchi[25], such screened systems are driven by the Einstein frequency which eventually merges with the plasma one at vanishing screening.

The use of an effective OCP plasma to represent a screened, partially-ionized plasma was first suggested by

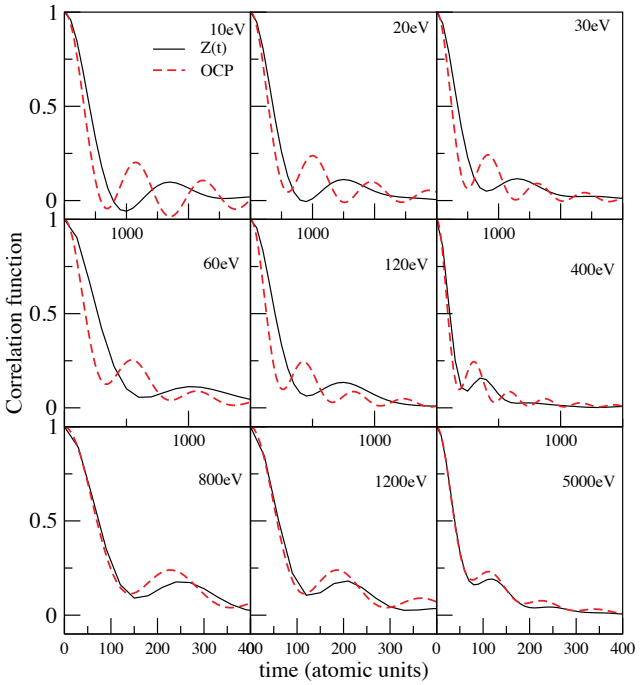

FIG. 5. (Color online) Comparison of the OFMD velocity autocorrelation function (continuous line) for 9 temperatures between 10 eV and 5000 eV with the OCP one (dashed line).

Lambert et al. [4] and developed further by Kress et al. using INFERNO average-atom code to compute the ionization [8, 22] and hence an effective OCP coupling parameter. Recently Lyon et al. [26] have suggested that the limitation of strong coupling could result from electron shielding effects. Our approach suggests that using the ionization to define an effective OCP coupling parameter Γ_{eff} gives better results than defining a screened coupling parameter.

VI. CONCLUSION

We have used orbital-free molecular dynamics simulations based on a Thomas-Fermi-like description of the electronic density to describe structural properties of tungsten along the 40 g/cm^3 isochore. In a large range of temperatures, from 60 eV to 1200 eV, the pair distribution function is essentially the same and can be successfully fitted by the one component plasma at $\Gamma = 20$ parameter. This self limitation of the ion-ion coupling, the Γ_plateau, results from a subtle compensation between the rise of the temperature (kinetic energy) and of the ionization. In particular, it appears that in the Thomas-Fermi-Dirac framework the ionization at constant density scales as the square root of the temperature in a range which depends on the compression. The value of the

plateau and its extension in temperature depends on the chosen density and disappears at high density. This effect could be used to obtain well defined and predictable experimental conditions.
The structure of a strongly screened plasma can be connected to the one of the OCP with the same pair distribution function. The effective charge is close to a TFD prediction.

VII. ACKNOWLEDGMENTS

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