Electron-ion coupling factor for temperature relaxation in dense plasmas

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We compare two formulas obtained from first principles to calculate the electron-ion coupling factor for temperature relaxation in dense plasmas. The quantum average-atom model is used to calculate this electron-ion coupling factor. It is shown that if the two formulas agree at sufficiently high temperature so that the potential energy is of limited importance, i.e., when the plasma is said to be kinetic, and are consistent with the Landau-Spitzer formula, then they strongly differ in the warm-dense-matter regime. Only one of the two is shown to be consistent with quantum molecular dynamics approach. We use this point to determine which formula is valid to describe temperature relaxation between electrons and ions in warm and hot dense plasmas.

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I. INTRODUCTION

Electrons and ions subsystems can often be found in out-of-equilibrium conditions in laboratory plasmas. This appears when matter is perturbed by intense femtosecond laser pulse, charged particles, or strong shock wave. In inertial confinement fusion, this happens also when α particles exchange their energy with the electrons and the ions of the surrounding environment at different rates due to their mass dissimilarity. This brings about a difference between electron and ion temperatures that should be treated with care to understand the ignition phenomenon of a thermonuclear plasma when the two subsystems try to reach an equilibration temperature [1]. If each species thermalizes relatively rapidly and can be considered in equilibrium at temperatures T_e and T_i, respectively, then the equilibration of the ion and electron temperatures can take time compared to their own internal equilibration time since they usually interact weakly with each other.

Since the pioneer papers of Landau [2] and Spitzer [3] on classical and weakly coupled plasmas, various attempts have been made to calculate the electron-ion coupling factor or g factor in dense plasmas. This quantity is the rate that governs the relaxation of electron and ion temperatures in plasmas while ensuring the conservation of energy between the electron and ion subsystems. Among these works, Daligault and Dimonte [4] established a practical formula to calculate the g factor including self-consistently the effects of screening and electron degeneracy and assuming a weak electron-ion interaction approximation. Recently, Daligault and Simoni [5] proposed a new formula to compute this g factor in dense plasmas that goes beyond the weak-interaction approximation. The two approaches have the property of being relatively easy to calculate with a quantum average-atom model [6–14]. Indeed, Faussurier and Blancard [15] already used an average-atom model to calculate the g factor with the expression established in Ref. [4].

In this work, we use a quantum average-atom model to calculate the g-factor formulas proposed by Daligault and Dimonte [4] and Daligault and Simoni [5]. The two expressions are compared to study the temperature relaxation between electrons and ions. If they agree with each other in kinetic plasmas and with the Laudau-Spitzer expression in these conditions, then it is shown that they deeply disagree in the warm-dense-matter regime. At electron temperature of 1 eV in solid-density plasmas, they can differ by nearly two orders of magnitude or even more. Only one of the two is consistent with quantum molecular-dynamics simulations [16], i.e., the most recent one. The paper is organized as follows. In a first, theoretical, part, we present the average-atom model used to compute the g factor in dense plasmas and the two expressions of this g factor. In a second part, we present various numerical calculations to select what is the expression of the g factor that should be used safely to study temperature relaxation between electrons and ions in warm and hot dense plasmas. The last part is the conclusion.

II. THEORY

A. The average-atom model

The nonrelativistic average-atom model in a muffin-tin approximation to describe the electronic structure in dense plasmas is well known. We assume that the electrons are in local thermodynamic equilibrium at T_e and ions at T_i. In the present approach, the electronic structure does not depend on T_i; only the equation of state depends on T_i. Using finite-temperature density-functional theory [17–19], the average-atom equations read

$$\left[-\frac{\hbar^2}{2m_e}\nabla^2 - \frac{Z^2e^2}{r} + e^2\int d\mathbf{r}'\frac{n(r')}{|\mathbf{r}-\mathbf{r}'|} + V_{xc}(r)\right]\psi_a(\mathbf{r}) = \varepsilon_a\psi_a(\mathbf{r}), \quad (1)$$

where $\hbar$ is the reduced Planck constant, e the elementary charge, m_e the electron rest mass, and Z the nuclear charge. ε_a is the one-electron energy and $a = (n, \ell)$ for bound states and $a = (\varepsilon, \ell)$ for continuum states. In this case, the one-electron

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energy is simply ε. $V_{xc}(r)$ is the finite-temperature exchange-correlation potential [20]. The wave function $\psi_a(\mathbf{r})$ is equal to

$$\psi_a(\mathbf{r}) = \frac{1}{r} P_a(r) Y_{\ell_a}^{m_a}(\theta,\phi)\chi_{\sigma_a}, \tag{2}$$

where $Y_\ell^m(\theta,\phi)$ is a spherical harmonic and χ_σ is a two-component electron spinor. The bound and free radial wave functions are normalized such that

$$\int_0^{+\infty} dr P_{n\ell}(r) P_{n'\ell}(r) = \delta_{nn'} \tag{3}$$

and

$$\int_0^{+\infty} dr P_{\varepsilon\ell}(r) P_{\varepsilon'\ell}(r) = \delta(\varepsilon-\varepsilon'). \tag{4}$$

The total electron density of the average-atom $n(r) = n_b(r) + n_f(r)$, where

$$4\pi r^2 n_b(r) = \sum_{n\ell} \frac{2(2\ell+1)}{1+e^{(\varepsilon_{n\ell}-\mu)/k_BT_e}} P_{n\ell}(r)^2 \tag{5}$$

and

$$4\pi r^2 n_f(r) = \sum_{\ell} \int_0^{+\infty} d\varepsilon \frac{2(2\ell+1)}{1+e^{(\varepsilon-\mu)/k_BT_e}} P_{\varepsilon\ell}(r)^2, \tag{6}$$

where k_B is the Boltzmann constant. The chemical potential μ is such that

$$\int_0^{R_{\rm WS}} 4\pi r^2 [n_b(r) + n_f(r)] dr = Z, \tag{7}$$

where $R_{\rm WS}$ is the Wigner-Seitz radius with $4\pi R_{\rm WS}^3 N_i/3 = 1$, where N_i is the ion density. For $r > R_{\rm WS}$, $V_{ei}(r) = 0$, where

$$V_{ei}(r) = -\frac{Z^2e^2}{r} + e^2 \int d\mathbf{r}' \frac{n(r')}{|\mathbf{r}-\mathbf{r}'|} + V_{xc}(r). \tag{8}$$

The Kohn-Sham potential $V_{ei}(r)$ is short range. These equations are solved self-consistently using the RADIAL package [21]. Particular attention should be paid to the calculation of phase shifts for the continuum wave functions, especially at high temperature. Another point to consider is that these self-consistent equations may not converge due to sharp resonances in the continuum or oscillations of a subshell that can be bound or free. The maximum orbital quantum number is set to 15. We do not describe the density of states between -0.0001 Ry and 0.0001 Ry.

B. The *g* factor

Let us introduce the basic equations to describe the electron-ion temperature relaxations in dense plasmas [15]. Ions are classical particles, whereas electrons are treated as an ideal Fermi gas that can be degenerate or not. By definition,

$$\frac{d}{dt} U_i(T_i) = -g(T_i - T_e) \tag{9}$$

and

$$\frac{d}{dt} U_e(T_e) = -g(T_e - T_i), \tag{10}$$

where $U_i(T_i) = \frac{3}{2} N_i k_B T_i$. This system of equations ensures the conservation of the energy density $U = U_i + U_e$. The relaxation rate g or g factor is usually expressed in $\mathrm{W/m^3K}$. In the present work, it depends only on T_e like U_e. U_i depends only on T_i. Daligault and Dimonte [4] proposed to calculate the g factor as follows:

$$g = -\frac{N_i k_B}{2\pi^2 m_i} \int_0^{+\infty} dk k^4 |\hat{V}_{ei}(k)|^2 \frac{\partial Im\chi_e^0(k,\omega)}{\partial\omega}\bigg|_{\omega=0}, \tag{11}$$

where m_i is the atomic mass of the element. In this expression, $\hat{V}_{ei}(k)$ is the Fourier transform of the electron-ion interaction-potential $V_{ei}(r)$ and $\chi_e^0(k,\omega)$ is the dynamic density response function of the electron gas. $\chi_e^0(k,\omega)$ is related to the dynamic dielectric function in the random-phase approximation [4,15]. To obtain this expression, we have neglected electron-ion correlations and assumed a weak interaction between electrons and ions. Another expression for the g factor that goes beyond this approximation has been proposed by Daligault and Simoni [5]. The g factor now reads

$$g = \frac{\hbar^3 N_i}{\pi^2 m_e m_i T_e} \int_0^{+\infty} dk k^5 f(\varepsilon_k)[1-f(\varepsilon_k)]\sigma_{\rm tr}(k), \tag{12}$$

where $\varepsilon_k = \hbar^2k^2/2m_e$ and $f(\varepsilon)=1/(e^{\varepsilon/k_BT_e-\eta}+1)$, $\eta=\mu/k_BT_e$ is the reduced chemical potential, and $\sigma_{\rm tr}(k)$ is the transport cross section for the binary collisions which reads

$$\sigma_{\rm tr}(k) = \frac{4\pi}{k^2} \sum_\ell (\ell+1) \sin^2[\delta_\ell(k) - \delta_{\ell+1}(k)], \tag{13}$$

where $\delta_\ell(k)$ is the phase shift of the ℓth partial wave at wave number k for the electron-ion potential $V_{ei}(r)$. As stated in Ref. [5], formula (12) is applicable to any temperature T_e. In particular at $T_e = 0$, we have [22]

$$g = \frac{\hbar k_B N_i k_F^4}{\pi^2 m_i} \sigma_{\rm tr}(k_F), \tag{14}$$

where k_F is the Fermi wave number. We can clearly see why Eqs. (11) and (12) are well suited for the average-atom model. For clarity, the acronym JD09 is associated with Eq. (11) and JD19 with Eq. (12). Note that the ionic internal energy could depend on T_e if, for instance, we introduce the ion-ion interaction energy using an OCP approach [23]. The dependence with respect to T_e is then due to the average ionization that allows to define a plasma coupling parameter. The calculation of the internal ion-ion energy can be complicated, especially at low temperature in the warm-dense-matter regime. Since our aim is to see what happens on the temperature relaxation using either the JD09 or the JD19 approaches, we prefer not to add another ingredient. In Ref. [23], it has been seen that the internal ion-ion energy has a noticeable but small impact on the temperature relaxation process. It mainly modifies the equilibration temperature.

III. NUMERICAL APPLICATIONS

We plot in Figs. 1 and 2 the g factor as a function of T_e in solid-density aluminum and gold plasmas, respectively. Note that the JD09 and JD19 formulas to calculate the g factor in the average-atom model do not depend on T_i. This temperature is thus irrelevant and is not specified. This explains why we only consider T_e in Figs. 1 and 2. Formulas (11) and (12) are compared to the Landau-Spitzer (LS) formula [24,25]. We can

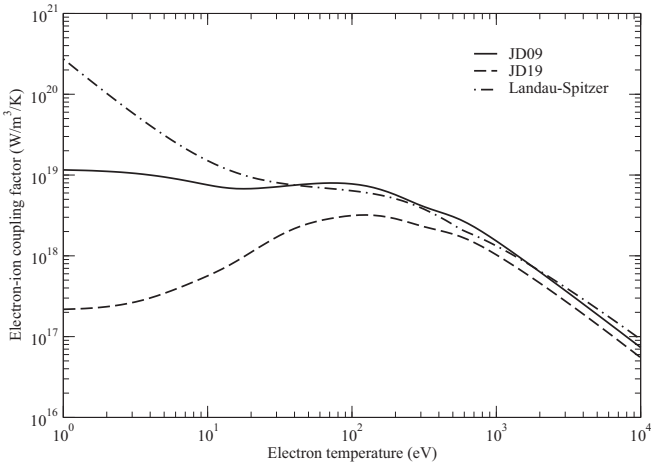

FIG. 1. Electron-ion coupling factor as a function of electron temperature in a solid-density aluminum plasma (see text).

see that the various formulas agree with each other at high temperature in kinetic plasmas. In this regime, the potential energy is of limited importance [26]. The Landau-Spitzer is not valid at low temperature. As for JD09 and JD19, we can see that they disagree at low temperature by nearly two orders of magnitude. In Fig. 2, we can see that JD19 agrees with quantum molecular dynamics (QMD) approach [16] even if the curvatures are not the same between QMD and JD19. The fact that Eq. (12) leads to better results compared to QMD may by due to the scattering phase shifts that are very sensitive to the electronic structure compared to Eq. (11) in which appears the Fourier transform of the electron-ion potential times the dynamic density response function. The key point could be the assumption that the interaction between electrons and ions is weak to established Eq. (11), whereas no such assumption is made to obtain Eq. (12). So, from a theoretical point of view, we may expect that Eq. (12) leads to results that are in better agreement with QMD at low temperature in the warm-dense-matter regime where electron-ion interaction is strong and the electronic structure difficult to calculate, especially for an element like gold. At high temperature, we may expect that both approaches lead to similar results since in this case the electron-ion potential is weak compared to the kinetic energy. This situation can be viewed as a reminiscence of the calculation of the electrical resistivity in dense plasma using the Ziman approach in the weak and strong isolated scatterers [27]. In the weak isolated scatterer, the Born approximation may be used to get the differential scattering cross section. The electron-ion interaction potential is weak and can be treated as a pseudopotential. In the formula for the differential scattering cross-section appears the Fourier transform of this weak electron-ion interaction potential. On the contrary, for strong isolated scatterers, the Born approximation should be abandoned and one should use the phase shifts of the electron-ion potential to obtain the differential scattering cross section. We can conclude that JD19 is sound at low temperature, whereas JD09 should not be used in this warm-dense-matter regime. Note that the JD19 g factor is an increasing function of T_e at low temperature and then reaches a maximum before decreasing with T_e at high temperature. For solid-density aluminum, the maximum temperature is equal to 123.1 eV and for solid-density gold, we find 984.4 eV. Since this result appears to be new and only relies on a few cases, more calculations should be performed to confirm this observation. Another point to be mentioned concerns the Landau-Spitzer approach in which the average ionization $\bar{Z}$ is calculated using the Thomas-Fermi model [25]. In the present regime, the LS g factor is proportional to $\bar{Z}^3/T_e^{3/2}$, i.e., to $\Gamma^{3/2}$, where Γ is the ion-ion coupling factor. We have the ratio of two quantities that increase with T_e. There is thus a competition between the way $\bar{Z}$ increases as a function of T_e compared to the way $T_e^{3/2}$ is rising. We have a phenomenon similar to the Γ plateau [28] for the LS g factor. We call this fact the g-plateau phenomenon. At some densities, the LS g factor can be almost constant over a wide range of electron temperatures. In Fig. 1 we are above the density at which this phenomenon takes place and in Fig. 2, we are below. There is a density at which we have something similar to a critical point in log-log graph. For aluminum, this happens near

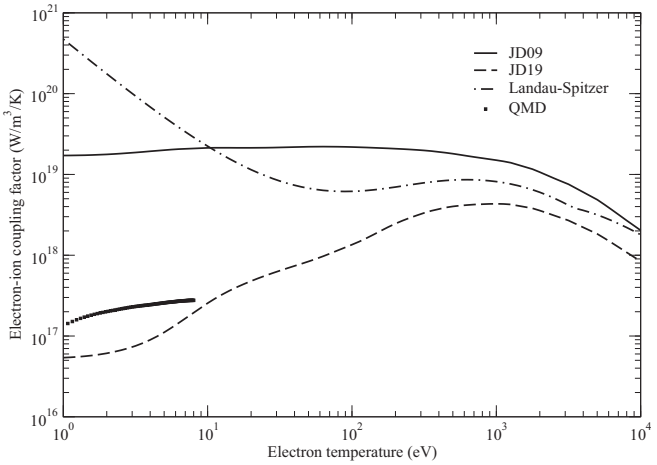

FIG. 2. Electron-ion coupling factor as a function of electron temperature in a solid-density gold plasma (see text).

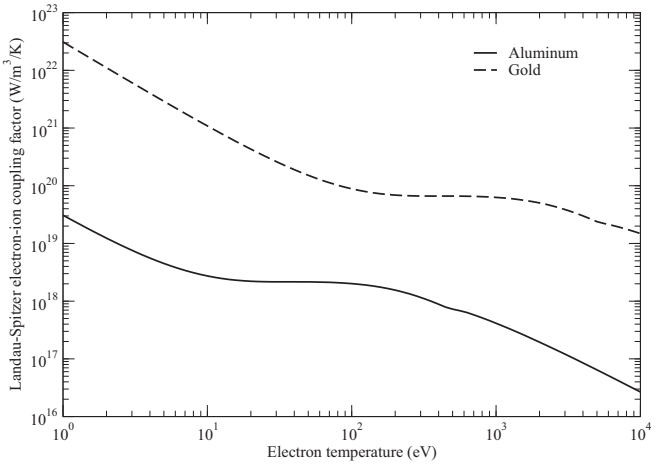

FIG. 3. Landau-Spitzer electron-ion coupling factor as a function of electron temperature in aluminum plasma at 1.4 g/cm^3 and gold plasma at 62 g/cm^3.

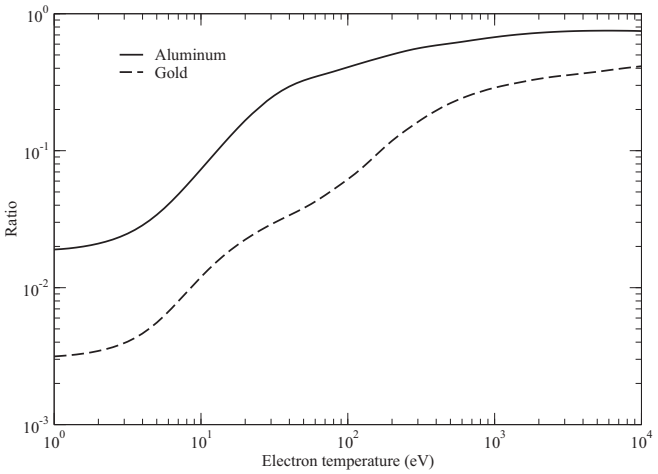

FIG. 4. Ratio of the JD19 g factor with respect to the JD09 g factor as a function of electron temperature in solid density aluminum and gold plasmas (see text).

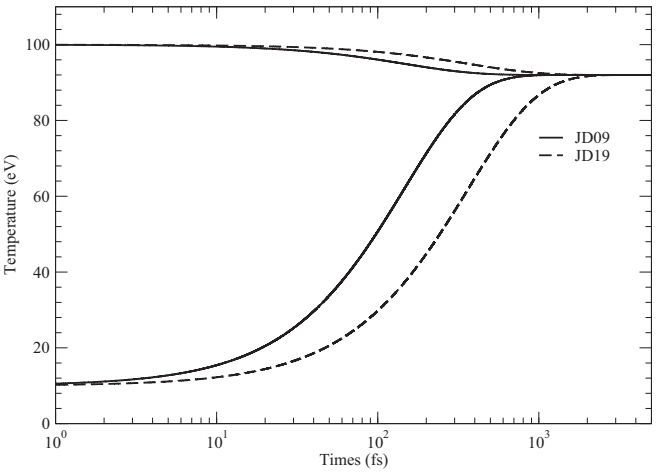

FIG. 5. Temperature relaxation in solid-density aluminum plasma starting with initial temperatures $T_e^0 = 100$ eV and $T_i^0 = 10$ eV.

1.4 g/cm^3 and for gold near 62 g/cm^3. We plot in Fig. 3 the LS g factor in aluminum and gold plasmas at these densities to appreciate the g-plateau phenomenon. In Fig. 4, we plot the ratio of the JD19 g factor with respect to the JD09 g factor as a function of electron temperature in aluminum and gold solid-density plasmas. We can appreciate the way they differ at low temperature and how they match at high temperature. In this regime, the convergence of the ratio with respect to one is rather slow. To keep on studying the difference between JD09 and JD19, we plot in Fig. 5 the temperature relaxation in an aluminum plasma at solid density starting with initial temperatures $T_e^0 = 100$ eV and $T_i^0 = 10$ eV. The difference between JD09 and JD19 is noticeable. For JD09, the relaxation temperature is reached around 0.8 ps, whereas for JD19, it is between 2 and 3 ps. The equilibration temperature is equal to 92 eV.

IV. CONCLUSION

We have used a nonrelativistic average-atom model to compare two ways to calculate the electron-ion coupling factor for temperature relaxation in dense plasmas. If they agree at high temperature, then they greatly disagree at low temperature where only the more recent expression is consistent with quantum molecular dynamics approach. At high temperature, both approaches are consistent with the Landau-Spitzer formula. The numerical examples shown in this work indicate that the more recent formula for the g factor should be preferred in practical applications.

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