Electrical resistivity calculations in dense plasmas

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We present calculations of electrical resistivity in dense plasmas using the average-atom model. The Born approximation is proposed to improve the computations especially in the hot domain of the density and temperature plane. Both the nonrelativistic and relativistic regimes are considered. Numerical examples are given.

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I. INTRODUCTION

The calculation of electrical resistivity in dense plasmas by coupling the density-functional theory and the Ziman approach has a long history [1–10]. Using the quantum average-atom model [7,8,11–17] and the Ziman-Evans formula [18], we can compute the electrical resistivity of dense plasmas in local thermodynamic equilibrium (LTE) in a large part of the density and temperature plane and for a great variety of elements. Comparisons with the scarce experimental data have shown that this general approach makes sense [19–21].

However, it appears that this method should be improved in hot dense plasmas. Indeed, calculations have shown that the electrical resistivity usually decreases when the temperature increases in the plasma phase at constant density. Then sometimes, the electrical resistivity still decreases with temperature but with a change of slope at some threshold temperature in a log-log graph. The reason is to be found in the limited number of partial waves that are taken into account to calculate the differential elastic-scattering cross section [22–24]. In practice, we limit the maximum orbital quantum number ($\ell_>$). If this is acceptable in the warm dense matter, then it is questionable in the hot dense regime. One way to correct this deficiency could be to increase $\ell_>$. Yet this can be problematic to calculate the continuum wave functions for large ℓ. We rather propose to use the Born approximation to calculate the phase shifts [25,26]. This method is inspired from the technique used to calculate the continuum density using an identity concerning the spherical Bessel functions [14]. Our approach works in the nonrelativistic and relativistic regimes. It is much simpler than using an effective Yukawa potential [3,9]. It is also more efficient since we use the same short-range Kohn-Sham potential that appears in the average-atom model and which is employed to calculate the phase shifts. In clear, we use the fact that the exact phase shifts are nearly equal to the Born phase shifts for sufficiently large ℓ [25,26]. This is the case in dense plasmas.

This paper is organized as follows. In Sec. II, we present the method to improve the calculation of the differential elastic cross section that is used to calculate the resistivity from the Ziman-Evans formula. Both the nonrelativistic and relativistic conditions are considered. In Sec. III, we apply our formalism to calculate the electrical resistivity in hot dense matter. Section IV is the conclusion. Particular developments are presented in the Appendix.

II. THEORY

We consider LTE dense plasmas at temperature T and density ρ of single element. The Wigner-Seitz radius $R_{\rm WS}$ is related to the ion density N_i through the equation $4\pi R_{\rm WS}^3 N_i/3 = 1$. The average ionization $\bar{Z}$ is calculated [27] by the formula $\bar{Z} = n(R_{\rm WS})/N_i$, where $n(r)$ is the radial electron density. The electrical resistivity ϱ is calculated as follows [3,9,18]:

$$\varrho = -\frac{\hbar}{3\pi e^2 \bar{Z}^2 N_i} \int_0^\infty dk \frac{df_0}{dk} \int_0^{2k} q^3 \sigma(q) S(q) dq, \quad (1)$$

where $\hbar$ is the reduced Planck constant, e the elementary charge, $\bar{Z}$ the average ionization, N_i the ion density, $S(q)$ the structure factor, and $\sigma(q)$ is the differential elastic-scattering cross section [3,9]. The quantity f_0 is the Fermi-Dirac factor,

$$f_0 = \frac{1}{1 + e^{\beta\left(\frac{\hbar^2 k^2}{2m_e} - \mu\right)}}. \quad (2)$$

$\beta = 1/k_B T$, where k_B is the Boltzmann constant and m_e is the electron rest mass. The scattering cross section $\sigma(q)$ is calculated quantum mechanically [3,9] using the phase shifts found in the electronic potential $V(r)$ of the quantum average-atom model. The chemical potential μ is calculated such that

$$\int_0^{R_{\rm WS}} 4\pi r^2 n(r) dr = Z, \quad (3)$$

where Z is the nuclear charge of the element. q is the wave number transferred from the incident electron with wave number k. We have $q^2 = 2k^2(1 - \cos\theta)$, where θ is scattering angle between the incident wave vector $\mathbf{k}$ and the scattered wave vector $\mathbf{k}'$. We recall that the wave number k is equal to the wave number k' in the elastic-scattering process. To calculate $S(q)$, we use the approach proposed by Bretonnet and Derouiche [28]. These authors have determined a simple analytic formula to calculate the structure factor of the OCP system.

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A. Nonrelativistic regime

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

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

and

$$4\pi r^2 n_f(r) = \int_0^{+\infty} d\varepsilon \sum_{\ell} \frac{2(2\ell+1)}{1+e^{\beta(\varepsilon-\mu)}} P_{\varepsilon\ell}(r)^2. \tag{5}$$

$P_{n\ell}(r)$ and $P_{\varepsilon\ell}(r)$ satisfy the self-consistent Schrödinger equation

$$-\frac{\hbar^2}{2m_e}\Delta\psi_s + V(r)\psi_s = \varepsilon_s\psi_s, \tag{6}$$

where

$$\psi_s = (1/r)P_{n\ell}(r)Y_\ell^m(\theta,\phi)\chi_\sigma \tag{7}$$

is the bound wave function and

$$\psi_s = (1/r)P_{\varepsilon\ell}(r)Y_\ell^m(\theta,\phi)\chi_\sigma \tag{8}$$

is the free wave function. $Y_\ell^m(\theta,\phi)$ is a spherical harmonics and χ_σ a spinor. Moreover, n is the principal quantum number, m is the magnetic quantum number [29], and s is a generic quantum number. The continuum eigenfunctions are normalized such that

$$\int_0^{+\infty} dr P_{\varepsilon\ell}(r)P_{\varepsilon'\ell}(r) = \delta(\varepsilon-\varepsilon'), \tag{9}$$

whereas for the bound eigenfunctions, we have

$$\int_0^{+\infty} dr P_{n\ell}(r)P_{n'\ell}(r) = \delta_{nn'}. \tag{10}$$

The self-consistent field potential

$$V(r) = -\frac{Ze^2}{r} + e^2\int d\mathbf{r}'\frac{n(r')}{\mid \mathbf{r}-\mathbf{r}'\mid} + V_{xc}(r) \tag{11}$$

is such that $V(r) = 0$ when $r \geqslant R_{\mathrm{WS}}$. This electronic potential $V(r)$ contains the electrostatic interaction between the nucleus and the electrons, the electrostatic interaction between the electrons, and the finite-temperature exchange and correlation potential $V_{xc}(r)$ using an unpublished work by Perrot based on Ref. [30]. $V_{xc}(r)$ is deduced from the exchange and correlation energy of an electron gas at finite temperature evaluated in the static local-field approximation using the Singwi-Tosi-Land-Sjölander scheme and parametrized in analytic formulas.

The elastic-scattering cross section $\sigma(q)$ is calculated quantum mechanically [3,9,23] using the phase shifts found in this electronic potential $V(r)$. It reads

$$\sigma(q) = \mid f_k(\theta) \mid^2, \tag{12}$$

where

$$f_k(\theta) = \frac{1}{k}\sum_{\ell}(2\ell+1)e^{i\delta_\ell(k)}\sin\delta_\ell(k)P_\ell(\cos\theta) \tag{13}$$

is the scattering amplitude [23]. $\delta_\ell(k)$ is the phase shift and P_ℓ the Legendre polynomial of order ℓ [31]. Introducing

$$W(k) = \int_0^{2k} q^3\sigma(q)S(q)dq, \tag{14}$$

we find the compact formula

$$\begin{aligned} W(k) \simeq 2k^2 &\sum_{\ell=0}^{\ell_>}\sum_{\ell'=0}^{\ell_>}(2\ell+1)(2\ell'+1)\sin\delta_\ell(k) \\ &\times \sin\delta_{\ell'}(k)\cos[\delta_\ell(k)-\delta_{\ell'}(k)] \\ &\times \int_{-1}^{1} dx(1-x)S[k\sqrt{2(1-x)}]P_\ell(x)P_{\ell'}(x). \end{aligned} \tag{15}$$

The expression (15) can be calculated numerically but suffers from the fact that the summation on the orbital quantum numbers are restricted by $\ell_>$. This is fine for the warm dense matter regime but questionable in hot dense matter. The border between the warm dense matter and hot dense matter regimes is around 100 eV. We propose to use the Born approximation as follows. In this approximation, the phase shifts are small and given by the expression [24]

$$\delta_\ell^B(k) = -k\frac{2m_e}{\hbar^2}\int_0^{+\infty} drr^2V(r)j_\ell^2(kr), \tag{16}$$

where j_ℓ is the spherical Bessel function of order ℓ [31]. The Born expression of the scattering amplitude (13) is given by

$$f_k^B(\theta) = \frac{1}{k}\sum_{\ell}(2\ell+1)\delta_\ell^B(k)P_\ell(\cos\theta). \tag{17}$$

What is interesting is that for the Born approximation $f_k^B(\theta)$, we can sum this series. Injecting in this expression the expression (16) of the Born phase shifts $\delta_\ell^B(k)$ and using the identity [31]

$$\frac{\sin(qr)}{qr} = \sum_{\ell}(2\ell+1)j_\ell^2(kr)P_\ell(\cos\theta), \tag{18}$$

where $q = 2k\sin(\frac{\theta}{2})$ is the transferred wave number, we find that

$$f_k^B(\theta) = -\frac{2m_e}{\hbar^2}\int_0^{+\infty} drr^2V(r)\frac{\sin(qr)}{qr}. \tag{19}$$

This expression is the scattering amplitude obtained in the Born approximation [23]. We now use this formula as follows. Instead of calculating $\sigma(q)$ using Eq. (12), we consider the expression [26]

$$\sigma(q) = \left|f_k^B(\theta) + f_k(\theta) - f_k^B(\theta)\right|^2. \tag{20}$$

The first term in this formula is calculated using Eq. (19), whereas for the last term we use Eqs. (16) and (17). The middle term is calculated using Eq. (13). At this stage, this expression is equivalent to Eq. (12) since we just add and subtract the same quantity calculated differently. However, $\delta_\ell(k) \to \delta_\ell^B(k)$ when ℓ is large in a short-range potential as it is the case here. This means that when $\ell > \ell_>$, $\delta_\ell(k) \approx \delta_\ell^B(k)$ with $\mid \delta_\ell^B(k) \mid \ll 1$. Thus, the contribution due to $\ell > \ell_>$ in Eqs. (13) and (17) are seen to cancel if we use this approximation. The physical meaning of Eq. (20) is now clear. Each sum in Eq. (20) is limited from $\ell = 0$ to $\ell = \ell_>$ using

the smooth transition between the phase shift $\delta_\ell(k)$ and its Born equivalent $\delta_\ell^B(k)$ for large ℓ. So doing, we correct the fact that in the sum in Eq. (15) we have neglected the contribution of $\ell > \ell_>$ that is taken into consideration using Eq. (19) in Eq. (20). Note also that contrary to Eq. (15), we obtain an expression for $W(k)$ in which the integral and the sum on the orbital quantum number are interchanged. Moreover, we have no more a double sum on ℓ and ℓ' but only one sum on ℓ using the real and imaginary parts of the expression that appears in Eq. (20). Here the Born approximation only correct the real part of the scattering amplitude since $f_k^B(\theta)$ given either by Eq. (17) or Eq. (19) is real. In practice, we integrate only between 0 and $R_{\rm WS}$ in Eq. (19) since $V(r) = 0$ when $r \geqslant R_{\rm WS}$.

B. Relativistic regime

In the relativistic regime [32], the total electron density of the average-atom $n(r) = n_b(r) + n_f(r)$, where

$$4\pi r^2 n_b(r) = \sum_a \frac{2 \mid \kappa_a \mid}{1 + e^{\beta(\varepsilon_a - \mu)}} [P_a(r)^2 + Q_a(r)^2] \tag{21}$$

and

$$4\pi r^2 n_f(r) = \int_0^{+\infty} d\varepsilon \sum_\kappa \frac{2 \mid \kappa \mid}{1 + e^{\beta(\varepsilon - \mu)}} [P_{\varepsilon,\kappa}(r)^2 + Q_{\varepsilon,\kappa}(r)^2]. \tag{22}$$

$P_a(r)$, $Q_a(r)$, $P_{\varepsilon,\kappa}(r)$, and $Q_{\varepsilon,\kappa}(r)$ satisfy the Dirac equation for the spherically symmetric potential $V(r)$,

$$\begin{cases} [V(r) + m_e c^2] P_a(r) + \hbar c \left[\frac{dQ_a(r)}{dr} - \frac{\kappa_a}{r} Q_a(r) \right] = E_a P_a(r) \\ -\hbar c \left[\frac{dP_a(r)}{dr} + \frac{\kappa_a}{r} P_a(r) \right] + [V(r) - m_e c^2] Q_a(r) = E_a Q_a(r) \end{cases}, \tag{23}$$

where c is the speed of light, $a = (n, \kappa)$ for bound states, and $a = (\varepsilon, \kappa)$ for continuum states. In this case, the one-electron energy is simply E. In both cases, κ_a means κ of index a. Note that the eigenvalue E_a contains the rest-mass energy. For bound states $E_a = \varepsilon_a + m_e c^2$ and for free states $E = \varepsilon + m_e c^2$. We have $\kappa = -1 - \ell$ for $j = \ell + 1/2$ and $\kappa = \ell$ for $j = \ell - 1/2$. This can be summarized as $\kappa = \mp(j + 1/2)$ for $j = \ell \pm 1/2$. As for the bound large (P) and small (Q) components, we have the orthogonality relations [33]

$$\int_0^{+\infty} dr [P_{n,\kappa}(r) P_{n',\kappa}(r) + Q_{n,\kappa}(r) Q_{n',\kappa}(r)] = \delta_{nn'}, \tag{24}$$

where $\delta_{nn'}$ is the Kronecker symbol. Concerning the free large (P) and small (Q) components, we have

$$\int_0^{+\infty} dr [P_{\varepsilon,\kappa}(r) P_{\varepsilon',\kappa}(r) + Q_{\varepsilon,\kappa}(r) Q_{\varepsilon',\kappa}(r)] = \delta(\varepsilon - \varepsilon'). \tag{25}$$

The relativistic generalization of Eqs. (12) and (13) reads [5,8]

$$\sigma(q) = \mid f_k(\theta) \mid^2 + \mid g_k(\theta) \mid^2, \tag{26}$$

where

$$f_k(\theta) = \frac{1}{k} \sum_\kappa \mid \kappa \mid e^{i\delta_\kappa(k)} \sin \delta_\kappa(k) P_\ell(\cos\theta) \tag{27}$$

and

$$g_k(\theta) = \frac{1}{k} \sum_\kappa \frac{\mid \kappa \mid}{i\kappa} e^{i\delta_\kappa(k)} \sin \delta_\kappa(k) P_\ell^1(\cos\theta). \tag{28}$$

P_ℓ^1 is the associated Legendre function [24,29,34]. Using ℓ instead of κ, we find the equivalent expressions [22,24,35]

$$f_k(\theta) = \frac{1}{2ik} \sum_{\ell=0}^{+\infty} \{(\ell+1)[e^{2i\delta_{-\ell-1}(k)} - 1] + \ell[e^{2i\delta_\ell(k)} - 1]\} P_\ell(\cos\theta) \tag{29}$$

and

$$g_k(\theta) = \frac{1}{2k} \sum_{\ell=1}^{+\infty} [e^{2i\delta_{-\ell-1}(k)} - e^{2i\delta_\ell(k)}] P_\ell^1(\cos\theta) \tag{30}$$

since $P_0^1(\cos\theta) = 0$; $f_k(\theta)$ and $g_k(\theta)$ are the direct and spin-flip scattering amplitudes [22]. As in the nonrelativistic regime, we are limited by $\ell_>$. We can do the same thing by using the Born approximation. As shown in Appendix, the Born approximation of the phase shift reads

$$\delta_\kappa^B(k) = -\frac{k}{\hbar^2 c^2} \int_0^{+\infty} dr r^2 V(r) [(E + m_e c^2) j_\ell^2(kr) + (E - m_e c^2) j_{\ell'}^2(kr)], \tag{31}$$

where $\ell = \ell(\kappa)$ and $\ell' = \ell(-\kappa)$. This is the relativistic generalization of the nonrelativistic expression (16) which is recovered when $E \simeq m_e c^2$. In the Born approximation, we have

$$f_k^B(\theta) = \frac{1}{k} \sum_\kappa \mid \kappa \mid \delta_\kappa^B(k) P_\ell(\cos\theta) \tag{32}$$

and

$$g_k^B(\theta) = \frac{1}{k} \sum_\kappa \frac{\mid \kappa \mid}{i\kappa} \delta_\kappa^B(k) P_\ell^1(\cos\theta). \tag{33}$$

Using Eqs. (18) and (31), and the fact that

$$\sum_\kappa \mid \kappa \mid j_\ell^2(kr) P_\ell(\cos\theta) = \frac{\sin(qr)}{qr} \tag{34}$$

and [36]

$$\sum_\kappa \mid \kappa \mid j_{\ell'}^2(kr) P_\ell(\cos\theta) = \cos\theta \frac{\sin(qr)}{qr}, \tag{35}$$

we find that

$$f_k^B(\theta) = -\frac{E\left(2 - \frac{q^2}{2k^2}\right) + m_e c^2 \frac{q^2}{2k^2}}{\hbar^2 c^2} \int_0^{+\infty} dr r^2 V(r) \frac{\sin(qr)}{qr}. \tag{36}$$

Concerning the spin-flip Born scattering amplitude, we have

$$g_k^B(\theta) = -\frac{(E - mc^2)}{i\hbar^2 c^2} \frac{q}{k} \sqrt{1 - \frac{q^2}{4k^2}} \int_0^{+\infty} dr r^2 V(r) \frac{\sin(qr)}{qr}. \tag{37}$$

To prove this identity, we have used the formula

$$P_{\ell+1}^1(\cos\theta) - P_{\ell-1}^1(\cos\theta) = (2\ell+1)\sqrt{1 - \cos^2\theta} P_\ell(\cos\theta) \tag{38}$$

for $\ell > 0$ with [22,24,29,34]

$$P_1^1(\cos\theta) = \sqrt{1-\cos^2\theta} \tag{39}$$

and Eq. (18). One should be careful because there is a phase factor $(-1)^m$ in the definition of the associated Legendre function $P_\ell^m(x)$ in Refs. [31,38,39] that is not present in Refs. [22,24,29,34], for instance. In the nonrelativistic regime, $E \simeq m_e c^2$ and we recover Eq. (19) from Eq. (36). Moreover, $g_k^B(\theta)$ cancels. In the Born approximation, one can see that the direct scattering amplitude is real, whereas the spin-flip scattering amplitude is purely imaginary. We can use the Born approximation in the relativistic regime as follows. We write instead of Eq. (26)

$$\sigma(q) = \left|f_k^B(\theta) + f_k(\theta) - f_k^B(\theta)\right|^2 + \left|g_k^B(\theta) + g_k(\theta) - g_k^B(\theta)\right|^2. \tag{40}$$

For the first terms in $f_k^B(\theta)$ and $g_k^B(\theta)$, we use Eqs. (36) and (37). For $f_k(\theta)$ and $g_k(\theta)$, we use the series expansions (27) and (28), whereas for the last terms $f_k^B(\theta)$ and $g_k^B(\theta)$, we use the series expansions given in Eqs. (32) and (33) based on Eq. (31). In each case, we consider only $\ell \leqslant \ell_>$. As in the nonrelativistic regime, we integrate only between 0 and $R_{\rm WS}$ in Eqs. (31), (36), and (37). Note that in practice, the relativistic calculation of the electrical resistivity is usually close to the nonrelativistic one. What is important is that the calculation of the electrical resistivity is now consistent with the equation of state model in the nonrelativistic and relativistic regimes.

III. APPLICATIONS

As an illustration, we consider Li at solid density between 100 eV and 10 keV in temperature with or without the Born correction. At these conditions, calculations are done in the nonrelativistic regime. We plot in Fig. 1 the electrical conductivity of solid density Li plasma as a function of temperature calculated using the average atom model without the Born correction (Wo Born) and with the Born correction (Wi Born). We compare these calculations with the Kramers-Kubo-Greenwood (KKG) [40,41] and the Spitzer models. The Spitzer formula used in this work is extracted from the Lee and More formula [42]. Both KKG and Spitzer are semiclassical approaches. KKG is based on the calculation of the electrical conductivity using the Kubo-Greenwood approach developed by Johnson *et al.* [15] in the framework of the average-atom model. The free-free component is calculated using the Kramers approach [36], hence the acronym KKG. The Spitzer formula we use is taken from Ref. [42] in which is proposed a conductivity model for dense plasmas. The average ionization is calculated from the Thomas-Fermi approach [27]. We are interested by the high-temperature limit when electrons are nondegenerate, hence our use of the Spitzer formula taken from this reference. We can see that the calculations made without or with the Born correction agree below 100 eV. Beyond this temperature, we can see that the Born correction becomes important with increasing temperature. Indeed, we are in rather close agreement with KKG and Spitzer at high temperature using the Born correction. There is clearly lacking partial waves if we do not use the Born correction. Above 100 eV, KKG and the calculations done using the Born approximation reach an asymptotic regime. The Born correction behaves as $T^{1.31}$ and KKG as $T^{1.48}$, so close to a $T^{3/2}$ behavior. The Spitzer curve shows a behavior $T^{3/2}/\ln(T)$ due to the Coulomb logarithm [42]. Similar results are found for Be, B, and C solid density plasmas between 1 eV and 10 000 eV. Calculations have been done with $\ell_> = 10$. On Fig. 2 we plot the same things for an aluminium plasma at solid density. One can see that Wi Born calculations are in rather good agreement at high temperature with KKG and Spitzer compared to Wo Born. Calculations have been done with $\ell_> = 15$. Note that below 100 eV there is a conductivity minimum or a resistivity saturation [10] for quantum-mechanical calculations without or with the Born

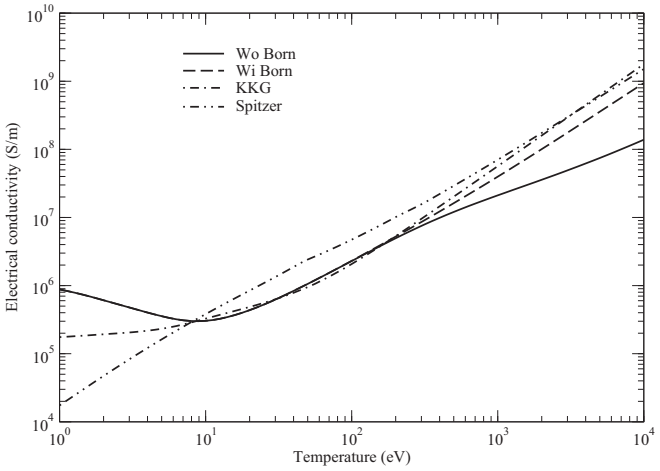

FIG. 1. Electrical conductivity of solid density lithium plasma as a function of temperature calculated using the quantum average-atom model without the Born correction (Wo Born) and with the Born correction (Wi Born). We compare these calculations with the Kramers-Kubo-Greenwood (KKG) and the Spitzer approximations.

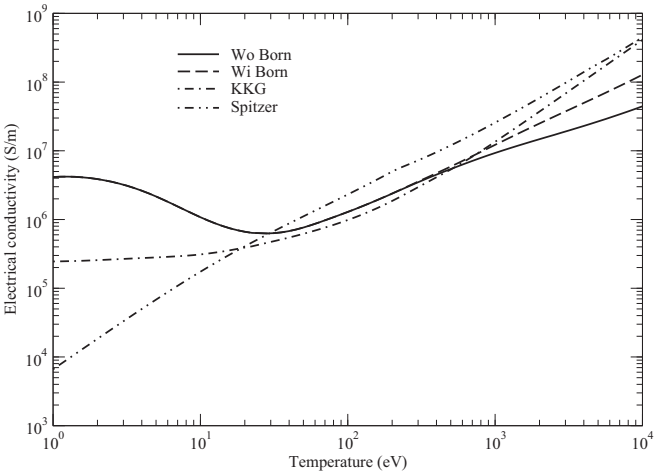

FIG. 2. Electrical conductivity of solid density aluminum plasma as a function of temperature calculated using the quantum average-atom model without the Born correction (Wo Born) and with the Born correction (Wi Born). We compare these calculations with the Kramers-Kubo-Greenwood (KKG) and the Spitzer approximations.

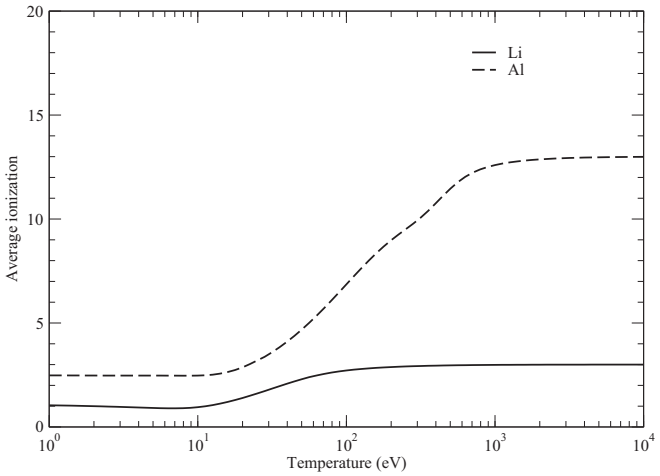

FIG. 3. Average ionization of solid-density Li and Al plasmas as a function of temperature using the quantum average-atom model.

correction. KKG is a semiclassical expression valid in hot dense plasmas but not in the warm dense matter in the range 1–10 eV. It is not surprising that the Ziman-Evans formula and KKG differ in this regime. KKG does not predict any resistivity saturation, as far as we know. The agreement at high temperature indicates that our approach using the Born approximation is sound. For information, we plot in Fig. 3 the average ionization $\bar{Z}$ of solid-density Li and Al plasmas as a function of temperature obtained using the nonrelativistic quantum average-atom model. We can see the ionization of the two materials between 1 eV and 10 keV. The curves are smooth, thanks to the way $\bar{Z}$ is calculated. At 10 keV, Li and Al are fully ionized. Between 1 keV and 10 keV, the plasmas are kinetics in which regime KKG and Spitzer are sound and can be compared to.

As for relativistic effects, they are small in the thermodynamic regime encountered in this study. Taking into account relativistic effects in the calculation of the electrical resistivity is recommended if the equation of state model is also relativistic. This is important for the internal consistency of the approach. Note that we use the same Ziman-Evans formula (1) for both nonrelativistic and relativistic regimes. This formula has been obtained using a nonrelativistic method. To be really consistent, we should also use the relativistic equivalent of Eq. (1). To our knowledge, this relativistic formula has not been derived from first principles as was done for the nonrelativistic formula [18]. This means that our relativistic treatment is partial since we should use the relativistic extension of the nonrelativistic Ziman-Evans formula (1).

IV. CONCLUSION

We have proposed a method to calculate the electrical resistivity in hot dense matter. We use the Born approximation to take into account the phase shifts that are neglected by calculating directly the electrical resistivity using the Ziman-Evans formula. Doing this, we use the fact that the exact phase shifts are nearly equal to the Born phase shifts for large angular quantum number ℓ. This avoids adding large angular quantum numbers in the Ziman-Evans formula for which the continuum wave functions are difficult to calculate. We have presented the nonrelativistic and relativistic cases. The calculation of the electrical resistivity is now consistent with the equation of state model in both cases. By consistent, we mean that we can calculate an electrical resistivity using the Born approximation nonrelativistically or relativistically if the quantum average-atom model, i.e., the equation of state model, is nonrelativistic or relativistic, respectively. Using the Born approximation to calculate the elastic-scattering cross section without using summation over large angular quantum numbers is important at high temperature. Relativistic effects are small in the thermodynamic regime considered in this work.

APPENDIX: RELATIVISTIC BORN APPROXIMATION FOR PHASE SHIFTS

In this Appendix, we present the relativistic generalization of the nonrelativistic Born expression for the phase shifts. The derivation is similar to the nonrelativistic case. Let us start with the average-atom Dirac equations (23). We have

$$\begin{cases} [V(r)+m_ec^2]P_{\varepsilon,\kappa}(r)+\hbar c\left[\frac{dQ_{\varepsilon,\kappa}(r)}{dr}-\frac{\kappa}{r}Q_{\varepsilon,\kappa}(r)\right]=EP_{\varepsilon,\kappa}(r) \\ -\hbar c\left[\frac{dP_{\varepsilon,\kappa}(r)}{dr}+\frac{\kappa}{r}P_{\varepsilon,\kappa}(r)\right]+[V(r)-m_ec^2]Q_{\varepsilon,\kappa}(r)=EQ_{\varepsilon,\kappa}(r) \end{cases}, \tag{A1}$$

where $\varepsilon = E - m_ec^2$ in a potential $V(r)$. In a potential $\bar{V}(r)$, we have at the same energy

$$\begin{cases} [\bar{V}(r)+m_ec^2]\bar{P}_{\varepsilon,\kappa}(r)+\hbar c\left[\frac{d\bar{Q}_{\varepsilon,\kappa}(r)}{dr}-\frac{\kappa}{r}\bar{Q}_{\varepsilon,\kappa}(r)\right]=E\bar{P}_{\varepsilon,\kappa}(r) \\ -\hbar c\left[\frac{d\bar{P}_{\varepsilon,\kappa}(r)}{dr}+\frac{\kappa}{r}\bar{P}_{\varepsilon,\kappa}(r)\right]+[\bar{V}(r)-m_ec^2]\bar{Q}_{\varepsilon,\kappa}(r)=E\bar{Q}_{\varepsilon,\kappa}(r) \end{cases}. \tag{A2}$$

Let us multiply the first equation of Eq. (A1) by $\bar{P}_{\varepsilon,\kappa}(r)$ and the first equation of Eq. (A2) by $P_{\varepsilon,\kappa}(r)$. In the same spirit, we multiply the second equation of Eq. (A1) by $\bar{Q}_{\varepsilon,\kappa}(r)$ and the second equation of Eq. (A2) by $Q_{\varepsilon,\kappa}(r)$. We find that

$$\begin{cases} [V(r)+m_ec^2]\bar{P}_{\varepsilon,\kappa}(r)P_{\varepsilon,\kappa}(r)+\hbar c\bar{P}_{\varepsilon,\kappa}(r)\left[\frac{dQ_{\varepsilon,\kappa}(r)}{dr}-\frac{\kappa}{r}Q_{\varepsilon,\kappa}(r)\right]=E\bar{P}_{\varepsilon,\kappa}(r)P_{\varepsilon,\kappa}(r) \\ -\hbar c\bar{Q}_{\varepsilon,\kappa}(r)\left[\frac{dP_{\varepsilon,\kappa}(r)}{dr}+\frac{\kappa}{r}P_{\varepsilon,\kappa}(r)\right]+[V(r)-m_ec^2]\bar{Q}_{\varepsilon,\kappa}(r)Q_{\varepsilon,\kappa}(r)=E\bar{Q}_{\varepsilon,\kappa}(r)Q_{\varepsilon,\kappa}(r) \end{cases} \tag{A3}$$

and

$$\begin{cases} [\bar{V}(r)+m_ec^2]P_{\varepsilon,\kappa}(r)\bar{P}_{\varepsilon,\kappa}(r)+\hbar cP_{\varepsilon,\kappa}(r)\left[\frac{d\bar{Q}_{\varepsilon,\kappa}(r)}{dr}-\frac{\kappa}{r}\bar{Q}_{\varepsilon,\kappa}(r)\right]=EP_{\varepsilon,\kappa}(r)\bar{P}_{\varepsilon,\kappa}(r) \\ -\hbar cQ_{\varepsilon,\kappa}(r)\left[\frac{d\bar{P}_{\varepsilon,\kappa}(r)}{dr}+\frac{\kappa}{r}\bar{P}_{\varepsilon,\kappa}(r)\right]+[\bar{V}(r)-m_ec^2]Q_{\varepsilon,\kappa}(r)\bar{Q}_{\varepsilon,\kappa}(r)=EQ_{\varepsilon,\kappa}(r)\bar{Q}_{\varepsilon,\kappa}(r) \end{cases}. \tag{A4}$$

We now subtract the first equation of Eq. (A3) by the first equation of Eq. (A4) and the second equation of Eq. (A3) by the second equation of Eq. (A4). We find that

$$[V(r)-\bar{V}(r)]P_{\varepsilon,\kappa}(r)\bar{P}_{\varepsilon,\kappa}(r)+\hbar c\left[\bar{P}_{\varepsilon,\kappa}(r)\frac{dQ_{\varepsilon,\kappa}(r)}{dr}-\frac{\kappa}{r}\bar{P}_{\varepsilon,\kappa}(r)Q_{\varepsilon,\kappa}(r)-P_{\varepsilon,\kappa}(r)\frac{d\bar{Q}_{\varepsilon,\kappa}(r)}{dr}+\frac{\kappa}{r}P_{\varepsilon,\kappa}(r)\bar{Q}_{\varepsilon,\kappa}(r)\right]=0 \tag{A5}$$

and

$$-\hbar c\left[\bar{Q}_{\varepsilon,\kappa}(r)\frac{dP_{\varepsilon,\kappa}(r)}{dr}+\frac{\kappa}{r}\bar{Q}_{\varepsilon,\kappa}(r)P_{\varepsilon,\kappa}(r)-Q_{\varepsilon,\kappa}(r)\frac{d\bar{P}_{\varepsilon,\kappa}(r)}{dr}-\frac{\kappa}{r}Q_{\varepsilon,\kappa}(r)\bar{P}_{\varepsilon,\kappa}(r)\right]+[V(r)-\bar{V}(r)]Q_{\varepsilon,\kappa}(r)\bar{Q}_{\varepsilon,\kappa}(r)=0. \tag{A6}$$

We now add these two equations. The terms in κ/r disappear. We are left with

$$\begin{aligned}[V(r)-\bar{V}(r)][P_{\varepsilon,\kappa}(r)\bar{P}_{\varepsilon,\kappa}(r)+Q_{\varepsilon,\kappa}(r)\bar{Q}_{\varepsilon,\kappa}(r)]+\hbar c[\bar{P}_{\varepsilon,\kappa}(r)\frac{dQ_{\varepsilon,\kappa}(r)}{dr} \\ -P_{\varepsilon,\kappa}(r)\frac{d\bar{Q}_{\varepsilon,\kappa}(r)}{dr}-\bar{Q}_{\varepsilon,\kappa}(r)\frac{dP_{\varepsilon,\kappa}(r)}{dr}+Q_{\varepsilon,\kappa}(r)\frac{d\bar{P}_{\varepsilon,\kappa}(r)}{dr}]=0\end{aligned} \tag{A7}$$

or

$$\bar{P}_{\varepsilon,\kappa}(r)\frac{dQ_{\varepsilon,\kappa}(r)}{dr}-P_{\varepsilon,\kappa}(r)\frac{d\bar{Q}_{\varepsilon,\kappa}(r)}{dr}-\bar{Q}_{\varepsilon,\kappa}(r)\frac{dP_{\varepsilon,\kappa}(r)}{dr}+Q_{\varepsilon,\kappa}(r)\frac{d\bar{P}_{\varepsilon,\kappa}(r)}{dr}=\frac{d}{dr}[\bar{P}_{\varepsilon,\kappa}(r)Q_{\varepsilon,\kappa}(r)-P_{\varepsilon,\kappa}(r)\bar{Q}_{\varepsilon,\kappa}(r)]. \tag{A8}$$

Consequently,

$$[\bar{P}_{\varepsilon,\kappa}(r)Q_{\varepsilon,\kappa}(r)-P_{\varepsilon,\kappa}(r)\bar{Q}_{\varepsilon,\kappa}(r)]_0^R=-\frac{1}{\hbar c}\int_0^R dr[V(r)-\bar{V}(r)][P_{\varepsilon,\kappa}(r)\bar{P}_{\varepsilon,\kappa}(r)+Q_{\varepsilon,\kappa}(r)\bar{Q}_{\varepsilon,\kappa}(r)]. \tag{A9}$$

As usual, there is no contribution from the origin in the left-hand side of this equation. Assuming that R is large, we can use the asymptotic expressions of the different functions. Moreover, we choose $\bar{V}(r)=0$. Since [32,37]

$$P_{\varepsilon,\kappa}(r)=f(k)v_{\varepsilon,\kappa}(r) \tag{A10}$$

and

$$Q_{\varepsilon,\kappa}(r)=g(k)w_{\varepsilon,\kappa}(r), \tag{A11}$$

where

$$v_{\varepsilon,\kappa}(r)\underset{r\to+\infty}{\sim}\sin\left[kr-\frac{\ell\pi}{2}+\delta_\kappa(k)\right] \tag{A12}$$

and

$$w_{\varepsilon,\kappa}(r)\underset{r\to+\infty}{\sim}-\cos\left[kr-\frac{\ell\pi}{2}+\delta_\kappa(k)\right] \tag{A13}$$

when $r\to+\infty$. $\delta_\kappa(k)$ is the phase shift,

$$f(k)=\sqrt{\frac{E+m_ec^2}{\hbar^2\pi c^2k}} \tag{A14}$$

and

$$g(k)=\sqrt{\frac{E-m_ec^2}{\hbar^2\pi c^2k}}. \tag{A15}$$

$f(k)$ and $g(k)$ are smooth functions of k. Let us note that

$$f(k)g(k)=\frac{1}{\hbar\pi c}. \tag{A16}$$

So at R we have

$$P_{\varepsilon,\kappa}(r)\sim f(k)\sin\left[kR-\frac{\ell\pi}{2}+\delta_\kappa(k)\right] \tag{A17}$$

and

$$Q_{\varepsilon,\kappa}(r)\sim -g(k)\cos\left[kR-\frac{\ell\pi}{2}+\delta_\kappa(k)\right]. \tag{A18}$$

For the free wave functions, we have

$$\bar{P}_{\varepsilon,\kappa}(r)=f(k)krj_\ell(kr) \tag{A19}$$

and

$$\bar{Q}_{\varepsilon,\kappa}(r)=-sgn(\kappa)g(k)krj_{\ell'}(kr), \tag{A20}$$

where $\ell=\ell(\kappa)$ and $\ell'=\ell(-\kappa)$. $sgn(\kappa)$ is the sign of κ. Asymptotically, we have

$$\bar{P}_{\varepsilon,\kappa}(r)\underset{r\to+\infty}{\sim}f(k)\sin\left(kr-\frac{\ell\pi}{2}\right) \tag{A21}$$

and

$$\bar{Q}_{\varepsilon,\kappa}(r)\underset{r\to+\infty}{\sim}-g(k)\cos\left(kr-\frac{\ell\pi}{2}\right). \tag{A22}$$

Consequently, Eq. (A9) becomes

$$\begin{aligned}f(k)g(k)\sin[\delta_\kappa(k)]\sim-\frac{1}{\hbar c}\int_0^{+\infty}drV(r)[P_{\varepsilon,\kappa}(r)\bar{P}_{\varepsilon,\kappa}(r) \\ +Q_{\varepsilon,\kappa}(r)\bar{Q}_{\varepsilon,\kappa}(r)],\end{aligned} \tag{A23}$$

where we have taken $R \to +\infty$. We know assume that $\delta_\kappa(k)$ is small for large angular momentum number. We call this the Born approximation. We can replace $P_{\varepsilon,\kappa}(r)$ by $\bar{P}_{\varepsilon,\kappa}(r)$ and $Q_{\varepsilon,\kappa}(r)$ by $\bar{Q}_{\varepsilon,\kappa}(r)$. We find that

$$f(k)g(k)\delta_\kappa^B(k) = -\frac{k^2}{\hbar c}\int_0^{+\infty} drr^2V(r)\left[\frac{E+m_ec^2}{\hbar^2\pi c^2k}j_\ell^2(kr) + \frac{E-m_ec^2}{\hbar^2\pi c^2k}j_{\ell'}^2(kr)\right], \tag{A24}$$

where we have used Eqs. (A14) and (A15). So, using Eq. (A16), we find that

$$\delta_\kappa^B(k) = -\frac{k}{\hbar^2c^2}\int_0^{+\infty} drr^2V(r)\big[(E+m_ec^2)j_\ell^2(kr) + (E-m_ec^2)j_{\ell'}^2(kr)\big]. \tag{A25}$$

This is Eq. (31). We have obtained the relativistic generalization of the nonrelativistic expression (16).

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