Electrical resistivity of hot dense plasmas

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We present calculations of the dc electrical resistivity of a variety of plasmas using rigorous generalizations of the Ziman formula which extend from the usual weak-isolated-scatterer limit to the hitherto inaccessible regime of strong multiple scatterers. All the ingredients necessary for the calculation are computed from first principles in a self-consistent manner, using a density-functional description of the electrons and ions in the plasma. As is usual in density-functional calculations, electron exchange correlation is handled in the local-density approximation. The method uses an average-ion distribution of the plasma environment, together with the assumption of spherical symmetry. The numerical procedures for the regime of strong multiple scatterers turn out to be no more difficult than for the weak-isolated-scatterer limit.

I. INTRODUCTION

The objective of this paper is to demonstrate how results from density-functional-theory (DFT) calculations could be used to calculate linear transport properties of strongly coupled plasmas of arbitrary degeneracy and density without making many of the restrictive assumptions found in existing calculations. We shall use the calculation of the electrical resistivity to illustrate the implementation of the method, merely noting that other related transport coefficients (e.g., thermal conductivity, thermal power, diffusion coefficients) can be handled by similar methods.

The linear transport coefficients, e.g., the electrical conductivity σ, can be expressed in terms of Kubo-type formulas[1,2] which, although formally elegant, lead to poor results unless extreme care is taken in handling the integral equations for the vertex functions which are submerged in the correlation functions.[3] On the other hand, methods based on the Boltzmann equation easily lead to good results and proceed via the *inverse* transport coefficients, e.g., the resistivity $R=1/\sigma$. The Boltzmann equation naturally embodies a number of conservation principles[4] which may not be present in some other approximate kinetic equations or approximations based on Kubo-type theories. A very successful variational solution to the Boltzmann equation is the Ziman formula[5] for the electrical conductivity. The Ziman formula and its generalizations which go beyond the simple Boltzmann equation can be derived using Green's-function methods. Such generalized Ziman formulas for the inverse transport coefficients have been derived by several authors[6–9] using the formalism of multiple-scattering theory. We shall use such generalizations of the Ziman formula and depend upon density-functional theory[10–13] to calculate the various quantities (e.g., structure factors, scattering cross sections) needed to evaluate them for various plasmas situations.

The main contribution to R is R_{ei}, i.e., the resistivity due to the scattering of electrons by the ions (usually having some bound electrons) which have an effective charge $\bar{Z}$. On this basis a plasma may be classified into three regimes: (i) weak-*isolated*-scatterer limit (WIS), i.e., the "single-site" model where the ions are well separated and the electron-ion interaction V_{ei} is weak, or formally weak in that a pseudopotential is available; (ii) strong but *isolated* scatterers (SIS), i.e., V_{ei} is strong so that linear response methods, Born approximation, etc., are inapplicable but scattering from several ionic centers is unimportant; and (iii) strong multiple scattering (SMS) occurs, i.e., V_{ie} is strong and the scattering centers are too close together to use the *isolated*-scatterer model. These three regimes, WIS, SIS, and SMS, present increasingly difficult theoretical problems. Nevertheless, it will be shown that DFT can be used in all three regimes with no significant increase in computational tractability. In this paper we shall only treat R_{ei}.

A density-functional calculation for a plasma requires the plasma temperature T, the material density $\bar{\rho}$, and the bare nuclear charge Z as inputs. The DFT calculation solves two coupled equations self-consistently. One of these is the Kohn-Sham (KS) equation which is an effective one-particle Schrödinger equation for the electron density distribution $n(r)$ in the external potential of the scattering center and the associated ion distribution. The other self-consistent equation has the form of a screened hypernetted-chain (HNC) equation and yields the ion distribution $\rho(r)$ in the field of the central ion and the associated electron distribution $n(r)$ obtained from the KS equation. The latter also provides the atomic structure of the "average atom" in the plasma, i.e., the bound states, scattering phase shifts $\delta_l(\varepsilon)$, and the effective ionic charge $\bar{Z}$. The phase shifts can be used to construct the T matrix. The screened HNC equation provides the ion-density profile $\rho(r)=\bar{\rho}g(r)$ where $g(r)$ is the ion-ion radial distribution function. Hence the ion-ion structure factor

for the plasma is also known. Thus all the ingredients necessary for the evaluation of Ziman-type formulas are available with no essential approximations except for the use of (i) local-density approximation (LDA) for the exchange and correlation potential[13] V_{xc} in the KS equation, (ii) the HNC approximation for the treatment of ion-ion correlations, and (iii) average-atom description of the scattering centers in the plasma. This last feature neglects the effects of electron- and ion-configuration fluctuations; for instance, the mean ionic charge $\bar{Z}$ may be an average over many values of the effective charge Z_c of a given short-lived configuration c. Fluctuation effects are particularly important in dilute plasmas in the WIS and SIS regimes. Most of the existing calculations treat these two regimes and do not consider fluctuation effects. There is some reason to believe that fluctuation effects cancel out (to lowest order), and we will examine this subsequently.

The available experimental data for the resistivity are of modest accuracy in the plasma phase but are more accurate for solid-state materials. Practical plasma codes require values of transport coefficients of modest accuracy but over a wide region of the phase diagram of a material. For instance, Lee and More[14] present a model for the efficient calculation of all the transport coefficients (including those in a magnetic field) for a wide range of physical situations. Rinker[15] has presented a single-site calculation which is quite close to ours in approach but he uses many simplifications to achieve a relatively rapid computational procedure. The objective of the present calculations is to treat a few cases carefully and consistently. The results are useful as bench marks for the present method, and in the construction of more approximate models, or in incorporating DFT models where the more traditional methods fail. In Sec. II we discuss the Ziman formula and its generalizations, and touch upon some existing calculations of the resistivity. In Sec. III we present the results obtained from the present calculations where density-functional theory is used to model the plasma. The discussion and conclusions are relegated to Sec. IV. Some calculational details are given in the Appendix.

II. THE ZIMAN FORMULA

In this section we shall review the Ziman formula and discuss how it has been used in existing calculations before we proceed to consider the DFT model.

A. Regime of isolated scatterers

The most familiar form of the Ziman formula applies to plasmas and liquid metals in the WIS and SIS regimes—i.e., weak and strong but *isolated* scatterers. The resistivity R is given by

$$R=\frac{\hbar}{3\pi\bar{Z}^{2}e^{2}\bar{\rho}}\int_{0}^{\infty}d\varepsilon f'(\varepsilon)\int_{0}^{2k}dq\, q^{3}S(q)\sigma(q)\ , \tag{2.1}$$

where $q^{2}=2k^{2}(1-\cos\theta)$. Here $\mathbf{q}$ is the momentum transferred from the incident electron with energy $\varepsilon=k^{2}$. The derivative of the Fermi distribution for the electrons at a mean density $\bar{n}=\bar{Z}\bar{\rho}$ is denoted by $f'(\varepsilon)$. The mean ion density is $\bar{\rho}$. The ion distribution is specified by the structure factor $S(q)$. The differential scattering cross section $\sigma(q)$ depends on the incident-electron momentum $\mathbf{k}$ and the transferred momentum $\mathbf{q}$. For strong scatterers $\sigma(q)$ has to be obtained from the phase shifts of V_{ei}. In the weak-isolated-scatterer limit the Born approximation may be used to obtain $\sigma(q)$. Then

$$\sigma(q)=|V_{ei}(q)/4\pi\epsilon(q)|^{2}\ , \tag{2.2}$$

where $V_{ei}(q)$ is the weak electron-ion interaction or a pseudopotential[16] which is *weak by construction*. $\epsilon(q)$ is the exact interacting uniform electron-gas dielectric function at a density $\bar{n}$ and temperature T. Generally speaking, both $V_{ei}(q)$ and $\epsilon(q)$ are not readily available except in certain limiting cases.

The ion-ion structure factor $S(q)$ is determined by the ion density $\bar{\rho}$, temperature T, and the ion-ion pair interaction $V_{ii}(q)$. Once $V_{ei}(q)$ and $\epsilon(q)$ are chosen for a fluid in the WIS regime, then to second order in perturbation theory we have ($e=\hbar=1$)

$$V_{ii}(q)=\bar{Z}^{2}V_{q}+|V_{ie}(q)|^{2}X(q)\ , \tag{2.3}$$

where

$$X(q)=\frac{1}{V_{q}}\left[\frac{1}{\epsilon(q)}-1\right]\ , \tag{2.4}$$

$$V_{q}=4\pi/q^{2}\ . \tag{2.5}$$

Hence $S(q)$ should be determined using the ion-ion pair potential of Eq. (2.3) for a consistent application of the Ziman formula.

In practical applications of the Ziman formula, various approximations have been made. The early form of the Ziman equation contained the form (2.2) for $\sigma(q)$ and the applications were to simple liquid metals[17] using a variety of pseudopotentials and dielectric functions. However, $S(q)$ was not obtained from the assumed $V_{ei}(q)$ and $\epsilon(q)$. Ashcroft and Leckner[17] used a hard-sphere model for liquid metals near the melting point. In plasma applications Minoo, Deutsch, and Hensen,[18] and other authors used the $S(q)$ from machine simulation results for the one component plasma (OCP). In the calculations for plasmas the electron-ion interaction V_{ei} was taken to be the *bare* Coulomb potential (rather than a pseudopotential) and linear screening using the Thomas-Fermi form was used for $\epsilon(q)$. Such assumptions restrict the validity of the theory to weakly charged ions in a dense electron gas. In the more recent work of Ichimaru and collaborators,[19,20] the Born approximation is still used with a linearly screened *bare* Coulomb potential. But the $S(q)$ used is consistent with the V_{ei} since it is calculated from the corresponding V_{ii} and the HNC equation.

The scattering cross section for an *isolated* nucleus of charge Z immersed in an electron gas can be calculated using a suitable Schrödinger code which builds up the internal structure of the ion and gives it an effective charge $\bar{Z}$. Such a calculation would in fact be a density-functional calculation for an ion in jellium of the appropriate electron density and temperature. This DFT calculation can be approximated by various models of increasing simplicity (e.g., Thomas-Fermi models). This

leads to various average-atom models giving the electron potential around the scatterer. Rozsnyai[21] and Rogers[22] construct analytic forms of $V_{ei}(r)$ from the potentials obtained from their quantum calculations. Rogers *et al.*[23] computed quantum mechanical phase shifts $\delta_l(\varepsilon)$ from the analytic potentials and used them in the Williams-DeWitt kinetic equations. In the work of Rinker[15] model potentials for V_{ie} are constructed by interpolating between low-density self-consistent atomic calculations and Thomas-Fermi-type calculations more suitable for high temperatures and high densities. (The LDA is implicit in the atomic models of all these calculations.) These model potentials are then used to calculate phase shifts by solving the Schrödinger equation. The structure factor $S(q)$ is *not* obtained from the electron-ion interactions as in Eq. (2.3) but form an heuristic model. Rinker's calculations are motivated by the need to calculate the resistivity with moderate accuracy for a wide regime of plasma conditions.

In the DFT calculations presented here the isolated (i.e., single-site) scatterer is represented by an ion immersed in jellium of infinite extent. (Note that this is slightly different to Liberman's[24] model which uses a jellium background containing a cavity.) The total plasma is made up of the individual ions and their *overlapping* charge clouds, as in standard pseudopotential theories[25] of simple metals. The DFT calculation[11] using the Kohn-Sham equation solves for continuum electron states $\phi_{kl}(r)$ having the asymptotic behavior

$$\phi_{kl}(r)\rightarrow\sin[kr-l\pi/2+\delta_l(k)]/kr \quad \text{as } r\rightarrow\infty \ . \tag{2.6}$$

Hence the phase shifts $\delta_l(k)$ are a necessary result of the calculation. Further, at self-consistency *the phase shifts satisfy the finite-temperature version of the Friedel sum rule,* thus guaranteeing the correct construction of the continuum electron density of states as modified by the scattering potential. Note that any model which treats the continuum by a Thomas-Fermi approximation will (a) not give the correct continuum density of states, and (b) not correctly incorporate the effects of electron-electron interactions in the electron-ion phase shifts. Thus such a model will not be reliable for the evaluation of the scattering cross section.

The scattering cross section is given in terms of the phase shifts by[26]

$$\sigma(q,\theta)=t_{kk'}(\varepsilon)=\left|\frac{1}{2ik}\sum_l(2l+1)(e^{2i\delta_l(k)}-1)\times P_l(\cos\theta_{kk'})\right|^2 , \tag{2.7}$$

where, for elastic scattering $k^2=(k')^2=\varepsilon$. The corresponding δ functions in the t matrix have been left out for brevity. The scattering angle is θ and the momentum transferred, $\mathbf{q}=\mathbf{k}'-\mathbf{k}$, is given by

$$q^2=2k^2(1-\cos\theta) \ . \tag{2.8}$$

Hence the density-functional calculation avoids the need to construct an explicit pseudopotential $V_{ei}(q)$ and does not require an explicit form for the dielectric function $\epsilon(q)$. Instead $\sigma(q)$ is directly obtained from the density-functional ion-in-jellium calculation. To obtain $S(q)$ we now solve not just the Kohn-Sham equation but also the screened HNC equation for the ions to determine the ion profile $\rho(r)=\bar{\rho}g(r)$. Hence $g(r)$ and $S(k)$ are also known, leading to a self-contained and consistent determination of the quantities needed to evaluate the t-matrix version of the Ziman formula, viz., Eq. (2.1).

The form (2.1) of the Ziman equation containing $\sigma(q)$ instead of (2.2) follows from the work of Edwards.[6] It was introduced by Evens *et al.*[7] as a method of calculating the electrical conductivity of liquid transition metals. Its actual practical applicability to liquid transition metals is still controversial[27] since the scatterers in, say, liquid Fe may not be well treated by a model of independent scattering centers due to the nature of d-electron interactions. This leads us to the question of multiple-scattering effects.

B. The regime of strong multiple scatterers

In this regime the ion-ion interactions are such that the system cannot be treated as a sum of independent scattering centers, be they weak scatterers or strong scatterers. Thus the electron is scattered from a given quasistatic ion distribution consisting of many centers. Following the work of Edwards,[6] and also Rousseau *et al.*,[8] the resistivity corresponding to a definite configuration c of ions can be written as

$$R_c=\frac{\hbar}{3\pi e^2\bar{n}^2}\int_0^\infty d\varepsilon\tilde{f}'(\varepsilon)\int_0^{2k}dq\,q^3T^c_{\mathbf{kk}'}(\varepsilon) \ , \tag{2.9}$$

where, as before, we have left out the δ functions for brevity, it being understood that $k^2=(k')^2=\varepsilon$ and $q^2=2k^2(1-\cos\theta_{\mathbf{kk}'})$.

The actual measured resistivity is obtained by averaging over all ion configuration to give $\langle R_c\rangle$ and this involves the configuration-averaged total T matrix $T_{k,k'}(\varepsilon)$, viz.,

$$T_{k,k'}(\varepsilon)=\langle T^c_{\mathbf{k},\mathbf{k}'}\rangle \ . \tag{2.10}$$

In the DFT calculation $\langle T^c_{\mathbf{k},\mathbf{k}'}\rangle$ is approximated by $\bar{T}_{k,k'}$,

$$\langle T^c_{\mathbf{k},\mathbf{k}'}(\varepsilon)\rangle\rightarrow\bar{T}_{k,k'}(\varepsilon) \ , \tag{2.11}$$

where $\bar{T}_{k,k'}(\varepsilon)$ is calculated from the *average-ion distribution* $\rho(r)$. Thus the configuration-averaged T is replaced by the T for an average configuration derived essentially from a pair fluid description of the plasma. At present (2.11) is one of the few approximations that is computationally practicable. The total T matrix of the average distribution, viz., $\bar{T}_{k,k'}(\varepsilon)$, is obtained from the phase shifts $\Delta_l(k)$ of the Kohn-Sham equation solved in the external field of the scattering ion *and* its associated distribution $\rho(r)$ [recall that in the isolated scatterer case we use the jellium model where $\rho(r)=\bar{\rho}$]. The formula (2.9) does *not* contain an ion-ion structure factor and the *evaluation of (2.9) is actually simpler* than evaluating the usual Ziman formula. The structure factor can be made explicit in the isolated-scatterer limit when

$$T_{\mathbf{k},\mathbf{k}'}(\varepsilon)\rightarrow\bar{\rho}S(|\mathbf{k}-\mathbf{k}'|)t(|\mathbf{k}-\mathbf{k}'|) \ . \tag{2.12}$$

Here $t(|\mathbf{k}-\mathbf{k}'|)$ is the single-center scattering matrix of Eq. (2.7). Thus, in the isolated-scatterer limit we expect that the T matrix of the DFT calculation using the ion profile $\rho(r)$ will be simply related to the t matrix of the jellium calculation via Eq. (2.12). In the multiple-scattering regime the individual scatterers interact with each other and the electronic structure, i.e., the bound electron structure, $\bar{Z}$, etc.—obtained from the DFT calculation with the ion profile could be *different* from that obtained for the ion immersed in jellium of the same mean electron density and temperature.

Equation (2.9) contains a modified distribution function $\tilde{f}(\varepsilon)$. In the individual-scatterer limit this was just the Fermi function. In the multiple-scattering case the mean free path l_e of the electrons may become comparable to the characteristic correlation lengths of the ion configurations which scatter the electron. In our model this would correspond to the "correlation distance" d_c within which the ion distribution $\rho(r)$ tends to the mean density $\bar{\rho}$. Since $g(r)$ decays slowly for strongly coupled plasmas, l_e may become comparable to d_c. Then $\tilde{f}(\varepsilon)$ must be calculated from the one-electron Green function via

$$\tilde{f}(\varepsilon)=-\frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{\mathrm{Im}G(\omega)}{1+e^{\beta\omega}}d\omega\ , \tag{2.13}$$

with

$$G(\omega)\simeq\frac{1}{\omega-\varepsilon-\Sigma_k^+(\omega)}\ ,$$

where $\Sigma_k^+(\omega)$ is the self-energy of the electron arising from the ion-electron scattering process which also produces the resistivity. Hence $\Sigma_k^+(\omega)$ can be obtained from the T matrix which is already known from the phase shifts. Thus we have, from the Dyson equation,

$$G=G^0+G^0\Sigma^+(\omega)G$$

$$=G^0+G^0T^+(\omega)G^0\ ,$$

with

$$G^0=(\omega-\varepsilon+i0^+)^{-1}\ .$$

Hence we approximate $\Sigma_k^+(\omega)$ by

$$\Sigma_k^+(\omega)=\int\frac{d\mathbf{k}'}{(2\pi)^3}T_{\mathbf{k},\mathbf{k}'}(\omega)\delta(\omega-\varepsilon)\ . \tag{2.14}$$

This procedure leads to a consistent inclusion of mean-free-path effects in the resistivity calculations in the multiple-scattering regime where $\mathbf{k}$ is not a good quantum number over the distance d_c defining the ion correlations in the fluid.[28]

The inclusion of self-energy corrections also raises the question as to whether the following many-body corrections are important.

(i) The electron mass renormalization, viz.,

$$m/m_k^*=Z_k\left[1+\frac{m}{\hbar k}\frac{\partial\,\mathrm{Re}\Sigma_k^+(\omega)}{\partial k}\right]\ ,$$

where Z_k is the quasiparticle renormalization factor;

(ii) renormalization of the T matrices to the form $Z_kT_{k,k'}(\varepsilon)Z_{k'}$; and

(iii) the inclusion of the true $\mathbf{k},\varepsilon$ dispersion form given by the solution of $\omega-\varepsilon-\Sigma_k(\omega)=0$.

These questions have been discussed carefully by Itoh and Watabe[29] in the context of the electrical resistivity of liquid metals. Since $T_{k,k'}(\varepsilon)$ is available from the DFT calculation, it is indeed quite practicable to obtain $\Sigma_k^+(\omega)$ and hence Z_k, m_k^*, and also the dispersion $\varepsilon(k)$ for a realistic plasma. In fact such a dispersion was studied by us in Ref. 12. In the present calculation we have neglected all these many-body effects and the mean-free-path effect arising from $\mathrm{Im}\Sigma_k(\omega)$. The relative importance of these effects in plasmas and liquid metals will be treated in detail in a future paper.

C. Fluctuation effects

The discussion of Sec. II B touched upon the question of taking the configuration average over the matrix $T_{k,k'}^c(\varepsilon)$ for a given ionic configuration c, having a definite electronic configuration. We noted that in the dilute plasma limit (isolated scatterers) we can ignore the effects of the ionic distribution and assume that the individual ion $t_{k,k'}(\varepsilon)$ could be used, together with the structure factor $S(k,k')$, as in the standard Ziman formula. However, fluctuation effects are even more important in the dilute plasma limit as a statistical consequence of the small number density of electrons and ions in such plasmas. The isolated-ion t matrix needed in the Ziman formula is

$$t_{\mathbf{k},\mathbf{k}'}(\varepsilon)=\langle t_{k,k'}^c(\varepsilon)\rangle\ , \tag{2.15}$$

where the average is over the many possible electronic configurations of a single ion (i.e., an isolated ion in jellium). The average over t^c is replaced in our calculations by a t matrix for the average configuration given by the DFT calculation for the isolated ion in jellium. Thus

$$t_{\mathbf{k},\mathbf{k}'}(\varepsilon)\rightarrow\bar{t}_{\mathbf{k},\mathbf{k}'}(\varepsilon)\ . \tag{2.16}$$

It is this approximate $\bar{t}$ that is used in calculating the resistivity. The DFT atom (or any average-atom model) contains mean electronic occupation numbers given by the Fermi factor $f(\varepsilon_{nlm})$ at the energy of the bound state ε_{nlm}. The true, fluctuating configurations have occupation numbers 0 or 1 with statistical weights such that the average reduces to $f(\varepsilon_{nlm})$. Associated with each electronic configuration there is also an effective ionic charge Z_c such that

$$\bar{Z}=\langle Z_c\rangle\ . \tag{2.17}$$

Perrot[30] has recently given a configurational analysis of probable atomic configurations in a plasma using DFT concepts. He discusses the spectrum of Z_c and evaluates the statistical weights of each configuration. His method can be extended to the calculation of $t_{k,k'}^c(\varepsilon)$ and the evaluation of $t_{k,k'}(\varepsilon)$, of Eq. (2.15), thus avoiding the approximation of (2.16). However, a simpler method of approximately correcting for configuration fluctuation effects is to

note that the most important correction probably occurs in the use of $\bar{Z}$ rather than Z_c since this occurs as Z_c^2 in the scattering cross section. That is, we need to use $\langle Z_c^2 \rangle$ rather than $\langle Z_c \rangle^2$. This can be estimated via the compressibility of the plasma as follows.

The fluctuations in Z_c are intimately related to the fluctuations in the electron- and ion-particle densities in the plasma. We assume that ion fluctuation effects are too slow to follow the electron-density fluctuations which determine the electronic configurations and electron-scattering processes. Hence we consider only the fluctuations in the electron subsystem. We have

$$\bar{n} k_B T \kappa_e = \langle n \rangle^{-1} (\langle n^2 \rangle - \langle n \rangle^2) , \tag{2.18}$$

where n is an operator for the number of electrons and κ_e is the *electron-gas* compressibility at a density $\bar{n}$ and temperature T. We write

$$n = Z_c \bar{\rho} ,$$

where $\bar{\rho}$ is used instead of the operator ρ since ion-density fluctuations are considered negligible during the time scales relevant to electron scattering. Then, from (2.18), assuming that the electron correlation volume is essentially equal to an atomic volume, we get

$$\langle Z_c^2 \rangle = \langle Z_c \rangle^2 (1 + \bar{\rho} k_B T \kappa_e) . \tag{2.19}$$

Taking $\langle Z_c \rangle = \bar{Z}$ we see that fluctuation effects can be approximately incorporated into the Ziman formula if $\langle Z^2 \rangle$ is calculated using (2.19) instead of it being approximated by $\bar{Z}^2$. The finite-temperature interacting electron as compressibility κ_e can be obtained from the electron-gas response function via the static structure factor since

$$\bar{Z} \bar{\rho} k_B T \kappa_e = S_{ee}(0) . \tag{2.20}$$

The $q \to 0$ limit of the local field to be used in evaluating $S_{ee}(0)$ would be $\partial V_{xc}(n,T)/\partial n$ where V_{xc} is the exchange-correlation potential[13] used in the density-functional calculation.

The above analysis suggests that $t_{k,k'}(\varepsilon)$ evaluated from an average atom should be corrected by the factor $[1 + S_{ee}(0)/\bar{Z}]$. However, the constant in front of the integral in the Ziman formula also contains a $1/\bar{n}^2$ factor, or equivalently, $1/\bar{Z}^2$ factor. It is not immediately clear that this $1/\bar{Z}^2$ should be treated in the same way as $1/\langle n^2 \rangle$ and included in the averaging. If this is so, the total effect of electron-density fluctuations would cancel out, to this order of analysis. Hence we provisionally conclude that the use of an average-atom model may be quite reasonable in the context of the Ziman formula for the *static* resistivity.

Another aspect of the evaluation of the electrical resistivity is related to the question of evaluating the mean free path $\langle l \rangle$ or $1/\langle l^{-1} \rangle$. Even if configuration fluctuation effects are negligible in the sense that the electronic configuration and $\bar{Z}$ are fixed, the difference in the two estimates of the mean free path arises from the width of the free-electron Fermi distribution and appears as corrections to the lowest-order variational solutions to the Boltzmann equation. In the classical limit, this amounts to the use of a convergent expansion in Sonine polynomials and the effect of higher-order terms have been sometimes approximated by including a factor of the form $8 + 13\sqrt{2}\bar{Z})/(8 + 4\sqrt{2}\bar{Z})$ in the conductivity. At intermediate degeneracies the effect of this contribution is expected to decrease and give a factor of unity at full degeneracy if the fluctuations in $\bar{Z}$ are neglected. However, a more detailed analysis is needed at intermediate degeneracies since the ratio of the first-order and second-order polynomial approximations is not expected to depend simply on $\bar{Z}$ alone. hence, in presenting the results of our calculations, the Sonine polynomial corrections will not be included.

In the SIS and SMS models used in this paper we have assumed an averaged spherical ion distribution. Fluctuations of the ion distribution will also clearly affect the electrical conductivity. One way to include their effects would be to make use of static ion microfields. Thus we take the SIS model and calculate the scattering with a given ion microfield E imposed on the scatterer. The re-

TABLE I. Resistivities of H plasmas calculated in the strong-isolated-scatterer (SIS) model and the strong-multiple-scatterer (SMS) models. The last seven rows correspond to the H plasmas previously studied by DFT in Ref. 12. The coupling parameter Γ is given for reference only and is not used in calculations. $\Gamma = \bar{Z}^2/(r_I k_B T)$ where r_I was taken to be r_s in all cases. The comparisons are free of the Sonine polynomial corrections.

					$\times 10^{-5}$ Ω cm			Other
r_s	T/T_F	$T \times 10^{-6}$ K	Γ	$\bar{Z}_{SIS}$	R_{SIS}	R_{SMS}	$\bar{Z}_{SMS}$	calculations
0.333	0.191	1.00	0.95	1.0	0.109	0.091	1.0	0.099[a]
0.500	0.430	1.00	0.63	1.0	0.315	0.293	1.0	0.282[a]
0.750	0.967	1.00	0.42	1.0	0.809	0.733	1.0	0.683[a]
1.00	0.271	0.158	2.00	1.0	2.034	2.332	1.0	1.56[a]
1.00	0.108	0.063	5.00	1.0	1.822	2.170	1.0	N.A.[b]
1.00	0.054	0.032	10.0	1.0	1.619	1.967	1.0	N.A.[b]
2.00	4.00	0.581	0.213	0.88	4.261	4.570	0.89	(2.67[a])
2.00	2.00	0.291	0.314	0.74	8.578	9.029	0.78	N.A.
2.00	1.00	0.145	0.563	0.65	13.25	15.32	0.79	N.A.
3.00	4.00	0.258	0.267	0.80	13.07	13.84	0.82	N.A.

[a]Ichimaru and Tanaka (Ref. 20).
[b]Not available.

TABLE II. Details of the H atomic structure for the partially ionized hydrogen plasmas treated in Table II. (See Ref. 12.) The value of $\bar{Z}$ given is consistent with the SMS model. r_s is the electron-sphere radius, Eq. (3.3). Thus $r_s=3$ corresponds to $\bar{n}=5.96\times10^{22}$ electrons/cm^3 and $T/T_F=4$ corresponds to 66.8 eV.

r_s	T/T_F	k_BT (a.u.)	ε_{1s} (a.u.)	$2f_{1s}$	$\bar{Z}$
2	4	3.68	−0.121	0.188	0.89
2	2	1.84	−0.057	0.237	0.78
2	1	0.92	−0.012	1.00	0.79
3	4	2.45	−0.183	0.217	0.82

sulting cross section is now used to calculate the resistivity for each microfield and the actual resistivity can be obtained by averaging over the ion-microfield probability function $P(E)$. In the present study we have not evaluated these effects.

III. RESULTS

In this section we present the results obtained from numerical calculations based on the preceding theory. Two types of calculations are presented.

(i) Strong-isolated- (i.e., independent) scatterer (SIS) model,

$$R=\frac{\hbar}{3\pi^2\bar{Z}^2e^2\bar{\rho}}\int_0^\infty d\varepsilon f'(\varepsilon)\int_0^{2k}dq\,q^3S(q)\bar{t}(q)\ . \tag{3.1}$$

(ii) Strong-multiple-scatter (SMS) model,

$$R=\frac{\hbar}{3\pi^2\bar{n}^2e^2}\int_0^\infty d\varepsilon f'(\varepsilon)\int_0^{2k}dq\,q^3\bar{T}(q)\ . \tag{3.2}$$

In (3.1) $\bar{t}(q)$ is the isolated average-atom scattering cross section [see Eqs. (2.7), (2.15), and (2.16)] calculated with a single ion immersed in a uniform electron gas of density $\bar{n}$ and temperature T and a compensating uniform positive background. In Eq. (3.2) $\bar{T}(q)$ is calculated with the scattering center immersed in an electron gas of mean density $\bar{n}$ and an ion distribution $\rho(r)$ which tends to $\bar{\rho}$ for large r. In (3.2) no electron self-energy corrections (e.g., $m\to m^*$, $Z_k\neq1$, corrections to $f(\varepsilon)$ due to lifetime effects, etc., discussed in the Sec. II) were included in the numerical work. Fully and partially ionized plasmas at several densities and temperatures, as well as an iron plasma and a xenon plasma, have been studied. The examples chosen overlap some existing calculations but also treat regimes for which no other calculations are available.

Hydrogen plasma. In Table I we present results for ten different hydrogen plasmas of varying degeneracy, density, and coupling strength. Four of the plasmas carry shallow 1s bound states and hence have $\bar{Z}<1$. The plasma can be characterized by the electron-sphere radius r_s ($e=\hbar=m_e=1$),

$$r_s^3=3/(4\pi\bar{n})\ , \tag{3.3}$$

and the coupling parameter

$$\Gamma=\bar{Z}/(r_Ik_BT)\ ,$$

where r_I is the ion-sphere radius. Since Γ is used merely to give a measure of the coupling strength of the plasma, and not for use in calculation, r_I is replaced by r_s for these H plasmas. We also define

$$\tilde{T}=T/T_F,\quad T_F=E_F/k_B\ , \tag{3.4}$$

where E_F is the Fermi energy, given in hartree atomic units by $1.8416r_s^{-2}$. The electrons are fully degenerate when $\tilde{T}\to0$ and essentially classical for $\tilde{T}>5$. The three plasmas with $r_s<1$ given in Table I correspond to cases studied by Minoo, Deutsch, and Hansen assuming full electron degeneracy and Thomas-Fermi screening. Ichimaru and Tanaka[20] have used a more appropriate dielectric function inclusive of degeneracy effects and given a parametrization of the Coulomb logarithm. We have used the latter to obtain the results attributed to Ref. 20 in Table I. The remaining plasmas were studied by us in Refs. 11 and 12 using DFT but the resistivities of these

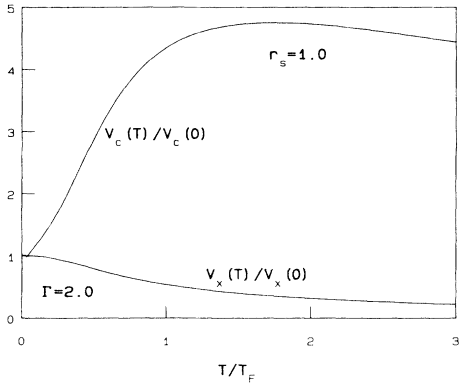

FIG. 1. The exchange potential $V_X(T)$ and the correlation potential $V_C(T)$ as a function of T for electrons at a density where $r_s=1$. $V_x(0)$ and $V_c(0)$ are the zero temperature values and T_F is the Fermi temperature. The arrow marked $\Gamma=2.0$ is at $T/T_F=0.271$ and corresponds to the conditions of the MD simulation of Ref. 31.

TABLE III. Resistivities of two plasmas where the ions have significant internal structure (see Table IV).

	SIS		SMS		Other	
T	$\bar{Z}$	R (Ω cm)	$\bar{Z}$	R (Ω cm)	$\bar{Z}$	R
Xe 2.12 eV	0.70	0.315×10^{-2}	0.75	not calculated	1.0[a]	0.271×10^{-2}
Fe 5 keV	22.87	0.956×10^{-6}	24.85	1.441×10^{-6}	22.99[b]	0.827×10^{-6}

[a]Ichimaru and Tanaka, Ref. 20; their Sonine polynomial factor 1.97 has been removed.
[b]Rinker, Ref. 15.

plasmas were not calculated at that stage. The case $r_s=1$, $\Gamma=2$ has been studied[31] using molecular-dynamics (MD) simulation and also with classical integral equation methods. Four of the plasmas given in Table I carry significant but shallow bound states, as reflected in the value of $\bar{Z}$. These weak bound states have extensions which overlap the nearest-neighbor ions and hence the isolated-scatterer model is not appropriate. The atomic structures of the *average atoms* in these plasmas are given in Table II. Although the energy levels are very shallow, ε_{1s}/k_BT being 1% to 7%, their effect on $\bar{Z}$, etc., is not negligible and is discussed in detail in Ref. 12. The question at issue is: Do we ignore these shallow levels and treat these plasmas as fully ionized ($\bar{Z}=1$) as far as the conductivity is concerned? No clear-cut answer can be given at this stage since, as already noted, the resistivity is determined by an average over the scattering from many atomic configurations, but the approximation (2.16) uses the scattering from an average configuration. In the calculations reported in Table I, the value of $\bar{Z}$ consistent with the model has been included.

The values obtained in the SIS and SMS models for a hydrogen plasma at $r_s=1$, $\Gamma=2$ turn out to be significantly larger than the MD (Ref. 31) result: 1.11×10^{-5} Ω cm. This case corresponds to a temperature $T/T_F=0.271$ and hence the electrons are probably poorly approximated by the classical model implicit in the MD calculation. As shown in Fig. 1, the exchange potential V_x as well as the correlation potential V_c for the electrons clearly indicate that at $T/T_F=0.271$ electron screening would be closer to that of a degenerate system than to a classical system. the Ichimaru-Tanaka (IT) (Ref. 20) calculation is more appropriate to the plasma conditions. However, IT uses linear response theory and this is probably one of the main reasons for the difference between our results and theirs. Even though they suggest that their parametrization is appropriate for $r\leq2$, $T/T_F>0.1$, their approach is not *a priori* applicable to systems with bound states. Thus the case $r_s=2$, $T/T_F=4$, and $\Gamma=0.213$ gives $R=2.67\times10^{-5}$ Ω cm with $\bar{Z}=0.88$. This low estimate is due to the linear response approximation and the lack of inclusion of bound-state effects.

In Table III we give the results for two plasmas having relatively large bound electronic structures. The presence of the inner shells makes the electron-ion interaction relatively weak and hence methods valid in the WIS or SIS regime should be adequate provided the electronic structure of the ion does not change when going from a jellium model (SIS) to a full plasma model (SMS). This is essentially the case for the Xe plasma which is a relatively dilute system at $T=2.12$ eV and with a Wigner-Seitz radius $R_{WS}\simeq7$ a.u. In the case of the Fe plasma, $R_{WS}\simeq0.45$ a.u., $T=5$ keV, and the isolated-scatterer model is not valid. The notoriously difficult d-electron problem of low-temperature plasmas (viz., liquid metals[27]) surfaces here to some extent and further pushes the problem to the SMS regime. The structure factors for the Fe and Xe plasmas calculated from the DFT equations are given in Fig. 2. The change in the electronic structure when going from a SIS model to a SMS model for Fe is seen from Table IV. This is consequently reflected in the different values of $\bar{Z}$ obtained from the two models.

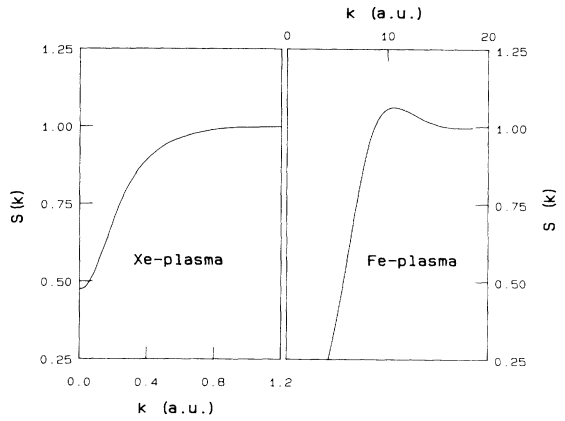

FIG. 2. Structure factors of the Xe plasma ($T=2.12$ eV, $R_{WS}=7$ a.u.) and Fe plasma ($T=5$ keV, $R_{WS}=0.45$ a.u.) calculated using DFT and used in evaluating the electrical resistivity.

IV. CONCLUSION

We have presented calculations of the dc electrical resistivity of a variety of plasmas using generalizations of the Ziman formula to cover situations which extend from

TABLE IV. Energy level structure of an Fe ion in an iron plasma at a temperature of 5 keV and electron density of 60.9 electrons per atomic unit of volume. The plasma is modeled by (a) jellium, i.e., SIS model with $\bar{Z}=22.87$; (b) using the most probable ion distribution of Fig. 4, i.e., SMS model with $\bar{Z}=24.85$. Here the Wigner-Seitz radius is 0.424 a.u.

	Energy (Ry)		Occupation		⟨Radius⟩ (a.u.)	
Level	(a)	(b)	(a)	(b)	(a)	(b)
1s	556.998	478.33	0.484	0.430	0.0583	0.0583
2s	77.301	7.940	0.203	0.174	0.2495	0.3139
2p	72.656	0.428	0.200×3	0.171×3	0.2188	0.3388
3s	9.214		0.174		0.6955	
3p	7.070		0.174×3		0.6801	
3d	2.911		0.172×5		0.6358	

the weak-isolated-scatterer limit to the strong-multiple-scatterer limit. The calculations do not use any model potentials, model dielectric functions, or structure data, but proceed via first-principles calculations based on density-functional theory in the local-density approximation. The electronic structure of an average scatterer is constructed using the Schrödinger equation. Unlike in most of the other available methods for resistivity, our calculations generate phase shifts which satisfy the finite-temperature Friedel sum rule. The calculated phase shifts and ion-ion structure factors are the essential ingredients of the resistivity calculation. We also discuss the approximations in the method arising from the use of an average atom in an average plasma model having spherical symmetry. Numerical results are given for ten different hydrogen plasmas, a Xe plasma, and an iron plasma to illustrate the method. The methods presented in this study provide a self-contained and self-consistent approach to the calculation of the electrical conductivity of plasmas of arbitrary degeneracy, structure, and density, where all the necessary ingredients are calculated in the LDA with the nuclear charge, mean matter density, and temperature as the input data.

APPENDIX: NUMERICAL METHODS

The evaluation of the resistivity requires the calculation of integrals of the form:

$$W(k)=\frac{1}{8k^4}\int_0^{2k} dq\, q^3 S(q)\,|\,\phi(q,k)\,|^2 \tag{A1}$$

with

$$\phi(q,k)=\sum_l (2l+1)(e^{2i\delta_l}-1)P_l(\cos\theta) \tag{A2}$$

depending on k and the momentum transfer

$$q=k\sqrt{2(1-\cos\theta)}\ . \tag{A3}$$

Taking $x=\cos\theta$ as a new integration variable, we get

$$W(k)=\sum_{l,l'=0}^{\infty}(2l+1)(2l'+1)\sin\delta_l\sin\delta_{l'}\cos(\delta_l-\delta_{l'})I_{ll'}\ , \tag{A4}$$

$$I_{ll'}(k)=\int_{-1}^{1} dx\,(1-x)S[k\sqrt{2(1-x)}]P_l(x)P_{l'}(x)\ . \tag{A5}$$

The functions $I_{ll'}(k)$ have been computed using a step $\Delta x=0.01$ and interpolating the structure factor $S(q)$ of the DFT program by means of the four-point Lagrange formula. This "exact" calculation of the $I_{ll'}$'s has been performed for angular momenta $l,l'\leq 9$. However, larger values of l must be included in (A4) for high energies, i.e., large values of k. In order to save computing time, we introduced a correction for large momenta in the following way.

At high electron energies, it is appropriate to use the classical scattering cross section for a screened potential:

$$\sigma_{cl}(q)=\left[\frac{A}{q^2+\lambda^2}\right]^2 \tag{A6}$$

with $A=2m\bar{Z}e^2/\hbar^2$ and λ a screening constant to be determined. In analogy with (A1), we can define a function $\tilde{\phi}(k,q)$ such that

$$\sigma_{cl}(q)=\frac{1}{4k^2}\,|\,\tilde{\phi}(k,q)\,|^2\ . \tag{A7}$$

One finds easily that

$$\tilde{\phi}(k,q)=\frac{A}{k}\frac{1}{z-\cos\theta} \tag{A8}$$

with

$$z=1+\frac{\lambda^2}{2k^2}\ .$$

Now, $\tilde{\phi}(k,q)$ may be expanded in Legendre polynomials:

$$\tilde{\phi}(k,q)=\frac{A}{k}\sum_l (2l+1)iQ_l(z)P_l(\cos\theta)\ , \tag{A9}$$

where Q_l is an associated Legendre function.[32] Now, for the large angular momenta where this approximation is relevant, the phase shift $\delta_l(k)$ is small and, consequently,

$$e^{2i\delta_l}-1\sim 2i\delta_l=i\frac{A}{k}Q_l(z)\ . \tag{A10}$$

Since $\delta_l(k)$ is known (from the DFT results) for $l=0,\ldots,9$, one fits the ratio $\delta_9(k)/\delta_8(k)$ to $Q_9(z)/Q_8(z)$ in order to determine z and then $\lambda^2=2k^2(z-1)$. Thus, *the "best" λ is obtained as a function of k.* The practical formula to be used instead of (A4) is

$$W(k)=\sum_{l,l'=0}^{9}(2l+1)(2l'+1)\left[\sin\delta_l\sin\delta_{l'}\cos(\delta_l-\delta_{l'})-\frac{A^2}{4k^2}Q_l(z)Q_{l'}(z)\right]I_{ll'}(k)+\frac{A^2}{2k^2}\int_0^{2k} dq\frac{q^3S(q)}{(q^2+\lambda^2)^2}\ . \tag{A11}$$

It has been checked that the fitted $\lambda(k)$ goes to the normal screening constant (linearized Thomas-Fermi screening constant, reducing to the Debye constant when degeneracy effects are negligible) at very high energies.

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