Transport properties of strongly coupled plasmas

I. M. Tkachenko* and P. Fernández de Córdoba
Department of Applied Mathematics, Polytechnic University of Valencia, Valencia E-46022, Spain
(Received 12 May 1997; revised manuscript received 16 October 1997)

A self-consistent field theory is proposed of transport properties of strongly coupled, fully ionized, multicomponent plasmas. The results are compared with those of simulation and experimental studies [for molecular-dynamics one-component plasmas see J. P. Hansen *et al.*, Phys. Rev. A **23**, 2041 (1981); for capillary discharges see J. F. Benage, Jr. *et al.*, Phys. Rev. E **49**, 4391 (1994); for vaporization of copper wires in water see A. W. DeSilva (private communication)]. Like in previously considered cases [V. M. Adamyan *et al.*, J. Phys. D **27**, 927 (1994), and references therein], the agreement is good or reasonable; the approach possesses no adjustable parameters. [S1063-651X(98)06302-8]

PACS number(s): 52.25.Fi

I. INTRODUCTION

Recently, there has been an increasing amount of work both theoretical and experimental, on electrical conductivity of strongly coupled Coulomb systems. The experimental studies have been carried out by measuring the resistivity of a plasma channel produced by strong electrical (capillary) discharges in dense materials such as polyurethane [1] and copper [2,3].

Recent experimental data, especially those of DeSilva and Kunze and DeSilva, have invited a number of researchers to compare their theoretical predictions with these data; see [4,5] and also [6].

These theoretical approaches either are based, like [7], on generalizations of the Ziman formula for resistivity of metals (see also [8]) or, as in [9], construct appropriate interpolation formulas between the Ziman and Spitzer theories [8]. One should also take into consideration the semiempirical results of [10].

More references can be found in the review article by Iakubov [11], where it was also pointed out that there was no theoretical approach capable of describing all experimental data, despite its ambiguity. In an early work [12] a correlation-function expression for the collision frequency was found and shown to reduce to the Ziman and Lenard-Balescu results in the appropriate limits. The realm of validity of this expression is limited by the possibility of applying and solving the hypernetted-chain equations.

In this paper we want to show that the theory of transport coefficients of dense cold plasmas based on the concept of self-consistent field and the generalized random-phase approximation (RPA) also possesses correct low- and high-density limiting properties and is in reasonable, taking into account a low level of precision of resistivity measurements, agreement with all available experimental data. This theory considers only fully ionized plasmas and has not yet been extended to the description of data corresponding to alleged Mott phase transition conditions.

*Electronic address: imtk@iqn.upv.es

II. MODEL

We consider dense relatively cold plasmas with temperature T of about $T \geqslant 10^4$ K and electronic number density $n_e \geqslant 10^{21}$ cm^{-3} [13]. Under such conditions all characteristic lengths such as the Wigner-Seitz radius $d=(3/4\pi n_e)^{1/3}$, the electronic Debye radius $\lambda_{De}=(4\pi n_e e^2\beta)^{1/2}$ ($\beta^{-1}=k_BT$, k_B is the Boltzmann constant), and the de Broglie wavelength $\lambda=\pi\hbar(2\beta/m)^{1/2}$ ($\hbar$ is the Planck constant) are of the same order of a few atomic units and the Debye correction to the ionization energy becomes comparable to the (hydrogen) ionization energy itself. Thus, at least the valent atomic electrons become collectivized and one cannot distinguish between charged and neutral components of the plasma.

The basic idea considered in the present approach is that of self-consistent field: Each electron (carrier) moves in a self-consistent field generated by all other free charges in the system. The finite values of the transport coefficients result from the electron's scattering on the self-consistent field fluctuations.

This approach was outlined and applied in [13]. This work was based on the paper [14] by Edwards, which related the Lorentz-model expression for the fully ionized plasma electrical conductivity to the strict quantum-statistical calculation involving the Green's-function formalism with the self-consistent field potential.

III. THEORY

The starting point for the conductivity calculation is the quantum-mechanical expression

$$\sigma=\mathrm{Re}\frac{\partial}{\partial F}j_x(\vec{r},t)|_{F=0}, \tag{1}$$

where $\vec{j}(\vec{r},t)$ is the averaged current density generated in the system by an external electric field $\vec{F}(F,0,0)$. We presume that

$$F(\vec{r},t)=F\exp(\delta t), \tag{2}$$

with $\delta>0, \delta\to 0^+$. This specific time dependence of the field is introduced to avoid coherent currents inducted at the switch-on moment $t=-\infty$. Thus

$$j_x(\vec{r},t)=\mathrm{Tr}\hat{\rho}(t)\left\{-\frac{i\hbar e}{2m}\left[\Psi^\dagger(\vec{r},-\infty)\frac{\partial}{\partial x}\Psi(\vec{r},-\infty)-\frac{\partial}{\partial x}\Psi^\dagger(\vec{r},-\infty)\Psi(\vec{r},-\infty)\right]\right\}, \tag{3}$$

where only the density matrix operator $\hat{\rho}(t)$ depends on the external field (2), so that

$$\left[\frac{\partial\hat{\rho}(t)}{\partial F}\right]_{F=0}=\frac{ie}{\hbar}\int_0^\infty e^{-\delta s}ds\times\int_\Omega x[\Psi^\dagger(\vec{r},s)\Psi(\vec{r},s),\hat{\rho}(-\infty)]d\vec{r}. \tag{4}$$

[$(-e)$ and m are the electronic charge and mass.] Here

$$-eFe^{-\delta t}\int_\Omega x\Psi^\dagger(\vec{r},s)\Psi(\vec{r},s)d\vec{r}$$

is the interaction contribution to the system Hamiltonian $H(t)$ and

$$\hat{\rho}(-\infty)=\exp\{-\beta[H(-\infty)-\phi]\},$$
$$\exp(-\beta\phi)=\mathrm{Tr}\exp[-\beta H(-\infty)], \tag{5}$$

ϕ being the system free energy of Helmholtz and Ω the system volume. Thus,

$$\sigma=\frac{e^2}{2m}\mathrm{Re}\int_0^\infty e^{-\delta s}ds\int_\Omega d\vec{r}'x'\,\mathrm{Tr}\hat{\rho}(-\infty)\times\left[\Psi^\dagger(\vec{r},-\infty)\frac{\partial}{\partial x}\Psi(\vec{r},-\infty)-\frac{\partial}{\partial x}\Psi^\dagger(\vec{r},-\infty)\times\Psi(\vec{r},-\infty),\Psi^\dagger(\vec{r}',s)\Psi(\vec{r}',s)\right]. \tag{6}$$

The second-quantized wave function $\Psi(\vec{r},t)$ is expressible in terms of the one-electron wave function $\psi_\nu(\vec{r})$ of the one-electron free Hamiltonian H_0,

$$H_0\psi_\nu(\vec{r})=\varepsilon_\nu\psi_\nu(\vec{r}), \tag{7}$$

$$\Psi(\vec{r},s)=\sum_\nu a_\nu\exp\left(-\frac{i}{\hbar}\varepsilon_\nu s\right)\psi_\nu(\vec{r}), \tag{8}$$

a_ν being the corresponding annihilation operator, for which we have the averaged commutator

$$\mathrm{Tr}\hat{\rho}(-\infty)[a_{\mu'}^\dagger a_\mu,a_{\nu'}^\dagger a_\nu]=\delta_{\mu\nu'}\delta_{\mu'\nu}[w_\nu-w_\mu], \tag{9}$$

where

$$w_\nu=w(\varepsilon_\nu)=\{\exp[\beta(\varepsilon_\nu-\mu)]+1\}^{-1}$$

is the Fermi-Dirac distribution, μ being the electronic subsystem chemical potential.

The trace in Eq. (6) can thus be simplified to get

$$\sigma=\frac{e^2}{2m}\mathrm{Re}\int_0^\infty\int_0^\infty d\varepsilon_1 d\varepsilon_2\int_\Omega d\vec{r}'x'\times\left\langle G(\vec{r},\vec{r}';\varepsilon_1)\frac{\partial}{\partial x}G(\vec{r},\vec{r}';\varepsilon_2)-G(\vec{r},\vec{r}';\varepsilon_2)\frac{\partial}{\partial x}G(\vec{r},\vec{r}';\varepsilon_1)\right\rangle\frac{\hbar[w(\varepsilon_1)-w(\varepsilon_2)]}{i(\varepsilon_1-\varepsilon_2-i\hbar\delta)}. \tag{10}$$

Here

$$G(\vec{r},\vec{r}';\varepsilon)=\sum_\nu\psi_\nu^\dagger(\vec{r})\psi_\nu(\vec{r}')\delta(\varepsilon_\nu-\varepsilon)$$

is the electronic Green's function of the Schrödinger equation involving the self-consistent field $V(\vec{r})$:

$$-\frac{\hbar^2}{2m}\Delta G+eV(\vec{r})G=\varepsilon G+\delta(\vec{r}-\vec{r}),$$
$$G(\vec{r},\vec{r}';\varepsilon)=G(\vec{r}',\vec{r};\varepsilon). \tag{11}$$

Averaging in Eq. (10) is to be carried out over the self-consistent field fluctuations. The symmetry properties of the Green's function lead to

$$\sigma=\frac{\pi e^2\hbar^3}{m^2}\mathrm{Re}\int_0^\infty d\varepsilon\frac{d\omega(\varepsilon)}{d\varepsilon}\int_\Omega d\vec{r}'\times\left\langle\frac{\partial G(\vec{r}',\vec{r};\varepsilon)}{\partial x'}\frac{\partial G(\vec{r},\vec{r}';\varepsilon)}{\partial x}\right\rangle. \tag{12}$$

An important advantage of formula (12) for σ is that it is analogous to the expression that describes the interaction of electrons with quantized electromagnetic field and there already exists the diagrammatic perturbation theory technique of calculation of the right-hand side of Eq. (12). In addition, the present problem lacks the divergence difficulties characteristic of quantum electrodynamics and various approximate methods of the quantum field theory can be applied to evaluate Eq. (12) without complications.

There is an important difference between Eqs. (1) and (3), on the one hand, and Eq. (12), on the other. The latter permits one to carry out the self-consistent field averaging procedure before the coordinate integration.

Edwards [14], who previously obtained Eq. (12), developed and applied to it a diagrammatic technique analogous to that of the quantum field theory. He showed that if the interaction operator $\hat{I}$ could be introduced by the equation

$$\langle GG\rangle=\langle G\rangle\langle G\rangle+\langle G\rangle\langle G\rangle\hat{I}\langle GG\rangle \tag{13}$$

and estimated within a perturbation theory, the *free* Green's function

$$G_0(\vec{r},\vec{r}';\varepsilon)=\frac{m}{2\pi^2\hbar^2}\frac{\sin(k|\vec{r}-\vec{r}'|)}{|\vec{r}-\vec{r}'|} \tag{14}$$

[here $k=(2m\varepsilon/\hbar^2)^{1/2}$] in the presence of the self-consistent field $V(\vec{r})$ fluctuations should be substituted by

$$\langle G(\vec{r},\vec{r}';\varepsilon)\rangle=\frac{m}{2\pi^2\hbar^2}\frac{\sin(k|\vec{r}-\vec{r}'|)}{|\vec{r}-\vec{r}'|}\exp\left(-\frac{|\vec{r}'-\vec{r}|}{\gamma(\varepsilon)}\right), \tag{15}$$

where $\gamma(\varepsilon)$ is the electronic mean free path. Then integration in Eq. (12) yields

$$\sigma=-\frac{2me^2}{3\pi^2\hbar^3}\int_0^\infty E\frac{dw(E)}{dE}\gamma(E)dE. \tag{16}$$

Since, as in the kinetic theory,

$$\gamma(E)=(2E/m)^{1/2}\tau(E), \tag{17}$$

$\tau(E)$ being the mean relaxation time, Eq. (16) coincides with the Lorentz formula

$$\sigma=-\frac{4e^2}{3m}\int_0^\infty E\,dE\frac{dw(E)}{dE}\rho(E)\tau(E), \tag{18}$$

where $\rho(E)=(2m^3E)^{1/2}/2\pi^2\hbar^3$ is the density of one-electron states in the energy space. Generally speaking, the mean free path $\gamma(E)$ or the mean relaxation time $\tau(E)$ of Eq. (18) is determined by the exact pairwise scattering cross section. Notice also that the averaging over the self-consistent field thermal fluctuations includes *configurations* for which the conductivity is infinite. We attribute to such contributions of $V(\vec{r})$ a negligible statistical weight.

IV. CALCULATION OF CONDUCTIVITY

It was shown in [14] that Eq. (15) for the averaged one-electron Green's function $\langle G\rangle$ is a result of summation of infinite series in powers of the pairwise-interaction transport cross section. That is why, though we substitute the latter by its first Born approximation and thus neglect a good deal of diagrammatic contributions to $\langle G\rangle$ [13], we can consider Coulomb systems with relatively strong interactions. Thus we express the inverse mean relaxation time in terms of the self-consistent field correlation function

$$\tau^{-1}(E)=\frac{me^2}{4\pi(2mE)^{3/2}}\int_0^Q q^3dq\int_{-\infty}^{\infty}\langle|\hat{V}(\vec{q},\omega)|^2\rangle d\omega. \tag{19}$$

Here $Q=(8mE/\hbar^2)^{1/2}$, the momentum $\hbar Q$ being the maximum possible variation of the electronic momentum as a result of the scattering process, and

$$\hat{V}(\vec{q},\omega)=\frac{4\pi e}{q^2\varepsilon(q,\omega)}\sum_a\kappa_a(q)\hat{\rho}_a(\vec{q},\omega) \tag{20}$$

is the field potential operator complete Fourier transform, $\hat{\rho}_a(\vec{q},\omega)$ being the a-species density operator in $(\vec{q},\omega)$ space and $\varepsilon^{-1}(q,\omega)$ the plasma dynamic screening function. The system is presumed to contain electrons (e) and p ionic species $(i_1,i_2,\ldots,i_p)$ characterized by their respective form factors $\kappa_a(q)$, $a=e,i_1,i_2,\ldots,i_p$, which describe the internal charge distribution of the species a, $\kappa_e=-1$, and $\kappa_i(0)=Z_i$, the charge number of ions i. The field potential correlation function thus equals

$$\langle|\hat{V}(\vec{q},\omega)|^2\rangle=\left(\frac{4\pi e}{q^2\varepsilon(q,\omega)}\right)^2\sum_{a,b}\kappa_a(q)\kappa_b(q)S_{ab}(\vec{q},\omega). \tag{21}$$

The dynamic structure factor of the species a and b,

$$S_{ab}(\vec{q},\omega)=\langle\hat{\rho}_a^*(\vec{q},\omega)\hat{\rho}_b(\vec{q},\omega)\rangle, \tag{22}$$

is related, by the fluctuation dissipation theorem [15]

$$S_{ab}(\vec{q},\omega)=\frac{\hbar}{2\pi}\coth(\beta\hbar\omega/2)\mathrm{Im}X_{ab}(\vec{q},\omega), \tag{23}$$

to the partial density-response (Green's) function

$$X_{ab}(\vec{q},\omega)=\Pi_a(q,\omega)\delta_{ab}-\Pi_a(q,\omega)\Pi_b(q,\omega)J^{ab}(\vec{q},\omega), \tag{24}$$

$$J^{ab}(\vec{q},\omega)=\frac{4\pi e^2}{q^2}\frac{\kappa_a(q)\kappa_b(q)}{\varepsilon(q,\omega)} \tag{25}$$

being the full vertex part and $\Pi_a(q,\omega)$ the a-species polarization operators, which also determine the dielectric function in Eq. (20) and

$$\varepsilon(q,\omega)=1+\frac{4\pi e^2}{q^2}\sum_a\kappa_a^2(q)\Pi_a(q,\omega). \tag{26}$$

Substitution of Eqs. (21)–(25) into Eq. (19) and integration [15] yields

$$\tau^{-1}(E)=\frac{4\pi me^4}{\beta(2mE)^{3/2}}\int_0^Q\frac{dq}{q}\sum_{a,l}\frac{\kappa_a^2(q)\Pi_a(q,l)}{\varepsilon^3(q,l)}. \tag{27}$$

(A corresponding expression from [16] is valid for hydrogen plasmas only.) Here the l summation is spread over the poles

$$\Omega_l=2\pi l/\beta\hbar\quad(l=0,\pm1,\pm2,\ldots) \tag{28}$$

of $\coth(\beta\hbar z/2)$ on the imaginary z-axis, i.e., over the Matsubara frequencies [17], and $\Pi_a(q,l)$ are the real parts of the $\Pi_a(q,\omega)$ operators at $\omega=i\Omega_l$. Equation (27) together with Eq. (18), forms a general algorithm of conductivity calculation, as soon as specific approximate expressions are used for the density-response functions and the polarization operators.

In our computations we evaluated the real part $\Pi_a(q,l)$ of the a-species polarization operator beyond the standard RPA, using the temperature-dependent static local-field correction $G_e(q)$ [18,16,19] parametrized to satisfy both the compressibility sum rule [with the electronic subsystem compressibility determined from the one-component plasma excess interaction energy determined by the Monte Carlo (MC) simulation [20]] and the long-wavelength limiting condition of Kimball [21]

$$G_e(q)=G_e(z)=[b+a/(2z)^2]^{-1}. \tag{29}$$

Here $b=[1-g_e(0)]^{-1}$ and a was estimated as in [19]:

$$a=-(12\pi^2)^{-1/3}\left(\frac{A}{9}+\frac{B}{12}\Gamma^{-1}+\frac{2C}{27}\Gamma^{-4/3}+\frac{5D}{54}\Gamma^{-2/3}\right)^{-1}. \tag{30}$$

Here $\Gamma=\beta e^2(4\pi n_e/3)^{1/3}$ measures the rate of Coulomb coupling in the system, $z=q/k_F$, $k_F=(3\pi^2 n_e)^{1/3}$ is the Fermi wave vector, and $A=-0.899\,374\,9$, $B=-0.224\,469\,9$, $C=-0.017\,874\,7$, $D=-0.517\,575\,3$, [20].

The model parameter $g_e(0)$, which is the zero-separation value of the electronic radial distribution function was determined by a self-consistent procedure: It was computed via a simultaneous solution of two integral equations

$$S_e(z)=\sum_{l=-l_1}^{l_1}\frac{P_e(z,l)}{\varepsilon_e(z,l)}, \tag{31}$$

$$g_e(0)=1+12\int_0^\infty (S_e(z)-1)z^2dz. \tag{32}$$

In Eq. (31) the summation is spread over the Matsubara dimensionless frequencies

$$v_l=\pi l/2Dz; \tag{33}$$

$$\varepsilon_e(z,l)=1+\frac{\Gamma}{(12\pi^2)^{1/3}}\frac{P_e(z,l)}{z^2} \tag{34}$$

is the electronic dielectric function; the value of l_1 in Eq. (31) was determined by the numerical precision.

Here $D=\theta^{-1}=\beta\hbar^2k_f^2/2m$ is another dimensionless parameter measuring the plasma degeneracy rate; notice that the Brueckner parameter

$$r_s=\Gamma\theta/0.543. \tag{35}$$

$P_e(z,l)$ in Eq. (31) is the dimensionless polarization operator $\Pi_e(q,l)=\Pi_e(q,i\Omega_l)$ with the local-field correction included:

$$P_e(z,l)=P_e^0(z,l)\left(1-\frac{\Gamma}{(12\pi^2)^{1/3}}\frac{G_e(z)P_e^0(z,l)}{z^2}\right)^{-1}. \tag{36}$$

The RPA dimensionless polarization operator $P_e^0(z,l)$ can be calculated (for each value of density and temperature, z and l) by simple integration [22],

$$P_e^0(z,l)=\frac{3\theta}{4z}\int_0^\infty\frac{y\,dy}{e^{y^2/\theta-\eta}+1}\ln\left|\frac{z+y+iv_l}{z-y+iv_l}\right|, \tag{37}$$

while the dimensionless chemical potential $\eta=\beta\mu$ is determined by the normalization condition

$$\int_0^\infty\frac{t^{1/2}}{e^{(t-\eta)}+1}=\frac{2}{3}\theta^{-3/2}. \tag{38}$$

Thus we used in Eq. (27)

$$\Pi_e(q,l)=n_e\beta P_e^0(z,l) \tag{39}$$

for the electronic polarization operator and [8]

$$\Pi_i(z,l)=\beta n\,\delta_{l,0}\left(1-\frac{\Gamma}{(12\pi^2)^{1/3}}\frac{G_i(z)}{z^2}\right)^{-1} \tag{40}$$

with

$$G_i(z)=\{b[\varepsilon_e(z,l)]+a/(2z)^2\}^{-1}, \tag{41}$$

for the ionic one ($\delta_{l,m}$ is the Kronecker delta symbol) and thus obtained a closed expression for the conductivity coefficient. Notice that the influence of the value of $g_e(0)$ proved to be quite small; see, nevertheless, Sec. VII A.

V. LIMITING CASES

Despite the approximations made to obtain our expression for the plasma conductivity, it possesses correct limiting forms corresponding to the cases of dilute gas plasma and metal-density Coulomb systems. In particular, if we omit the electronic contribution in Eq. (27) and neglect the screening effects (i.e., set $\varepsilon(q,l)=1$) and the momentum dependence of the ionic form factors, the sum on the right-hand side of Eq. (27) becomes a constant

$$\beta\sum_i Z_i^2 n_i.$$

If further we presume E to be equal to the mean kinetic energy of an electron, we retrieve from Eq. (27) the Coulomb logarithm, and Eq. (18) with $w(E)$ substituted by the Boltzmann distribution takes the form of the Spitzer formula without corrections due to electron-electron interactions [23]. We have estimated the relative weight of this last correction. In particular, in the dilute plasma regime, we calculated the conductivity contribution due to scattering on ions only. Hydrogenlike plasmas were considered in these computations with $n_e=Zn_i$ and the screening function was substituted by its long-range static limiting form

$$\varepsilon(q,\omega)\to(1+q^2/k_s^2)^{-1}$$

with the screening length k_s^{-1} chosen to be either the electronic Debye radius $k_1^{-1}=(4\pi n_e e^2\beta)^{-1/2}$ or the complete Debye radius $k_2^{-1}=[4\pi(1+Z)n_e e^2\beta]^{-1/2}$. Thus we employed instead of the relaxation time of Eq. (27) the limiting expression

$$\tau_s^{-1}(E)=\frac{4\pi mZ^2e^4n_i}{(2mE)^{3/2}}\int_0^Q\frac{q^5dq}{(q^2+k_s^2)^3}. \tag{42}$$

These estimates are provided in Table I, labeled σ_1 and σ_2, along with the results of our complete calculations, labeled σ and obtained as explained in Sec. VII C. It is seen that the electron-electron interactions are responsible for up to 45% of the resistivity value.

On the other hand, if we consider the low-temperature limiting case ($\beta^{-1}\to0$), the Fermi-Dirac distribution derivative in Eq. (18) turns into $-\delta(E-E_F)$ with $E_F=\hbar^2k_F^2/2m$ and Q becomes equal to $2k_F$, so that we immediately regain the Ziman specific resistance formula [24].

Notice that no special effort was done *ab initio* to guarantee the correct limiting behavior of our model. Neverthe-

TABLE I. Relative contributions to the plasma conductivity σ of Table III, σ_s ($s=1,2$), are calculated according to Eq. (18) but with $\tau_s(E)$ from Eq. (40) with $k_1=\sqrt{4\pi n_e e^2\beta}$ and $k_2=\sqrt{4\pi(1+Z)n_e e^2\beta}$, respectively. T, n_e are the temperature and electronic number density in copper and Ze is the effective ion charge.

T (kK)	$n_e\times10^{-21}$ (cm^{-3})	Z	$\sigma\times10^{-4}$ (S/m)	$\sigma_1\times10^{-4}$ (S/m)	$\sigma_2\times10^{-4}$ (S/m)
20	3.18	1.3	2.12	3.13	4.07
20	7.69	1.2	2.94	4.55	6.34
30	4.07	1.6	3.03	4.02	5.21
30	6.03	1.6	3.42	4.47	5.97
40	4.33	2.0	3.66	4.37	5.72

less, further studies of the limiting behavior of our model and a comparison with other general expressions for the collision frequency (e.g., [12]) or for the conductivity itself (see [25]) are to be carried out.

In general, the difference between our expression and that of Ziman (widely used lately to calculate conductivity [4–6]) is that we include the energy-dependent relaxation time [Eq. (27)] and the Ziman formula takes it at $E=E_F$. In addition, we have the electron-electron interaction included explicitly via the structure factor $S_{ee}(q,\omega)$.

The $\sigma(T)$ dependence at constant density (see [16]) is characterized by a minimum corresponding to a transition from the low-temperature regime with decreasing (with growing T) conductivity characteristic for metals and liquid metals (Ziman regime) to that of increasing conductivity at higher temperatures, characteristic for dilute plasmas (Spitzer regime). Thermodynamic conditions were specified in [16] corresponding to the domain of values of the electronic concentration and the plasma temperature (in hydrogen plasmas) where our expression asymptotically approaches the Spitzer regime with $\sigma_{Sp}(T)\propto T^{3/2}$.

Finally, relative contributions due to various factors in Eq. (27) were also estimated. We found that at least for $T=20$ kK and $n_e\geqslant10^{21}$ cm^{-3} (conditions considered earlier in [13]), the value of conductivity calculated with the sum in Eq. (27) substituted by

$$[\Pi_e(q,0)+Z^2\Pi_i(q,0)]/\varepsilon(q,0)$$

(as in [13]) was about 50% higher than the complete calculation results given in Tables I and III.

VI. OTHER TRANSPORT COEFFICIENTS

If the initial state of plasma is not far from that of thermodynamic equilibrium, the generalized transport equations for the mean current density $\vec{J}$ and for the thermal flux $\vec{Q}$ can be written as [26]

$$\vec{J}=e^2K_0\vec{F}+T^{-1}eK_1(-\vec{\nabla}T), \tag{43}$$

$$\vec{Q}=eK_1\vec{F}+T^{-1}K_2(-\vec{\nabla}T). \tag{44}$$

T is the plasma temperature and no magnetic effects are taken into account. The transport coefficients K_i ($i=0,1,2$) in Eqs. (43) and (44) satisfy the Onsager relations [26] and within the same approximation instead of Eq. (18) we have

$$K_i=-\frac{4}{3m}\int_0^\infty E\rho(E)\tau(E)\frac{dw(E)}{dE}(E-\mu)^i dE, \tag{45}$$

where μ is the electronic subsystem chemical potential and $\tau(E)$ is the same relaxation time defined by Eq. (27). The transport coefficient K_0 determines the static conductivity

$$\sigma=e^2K_0, \tag{46}$$

while the static thermal conductivity

$$\kappa=\frac{1}{T}(K_2-K_1^2/K_0) \tag{47}$$

and the thermal electromotive potential

$$\alpha=K_1(eTK_0)^{-1}. \tag{48}$$

In the case of complete degeneracy of the electronic subsystem the conductivities κ and σ are related by the Wiedemann-Franz law

$$\frac{\kappa}{\sigma}=\frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2T. \tag{49}$$

If the degeneracy is incomplete, like in our case, there appear temperature-dependent corrections to Eq. (49). Nevertheless, we will see that these corrections under the conditions we consider are quite small.

VII. RESULTS AND CONCLUSIONS

Extensive studies of electrical and thermal conductivities in a wide range of variation of temperature and electronic density in hydrogenlike plasmas (with $n_e=Zn_i$) were carried out in [16,27,28]. Here we report our results on the conductivities obtained for the conditions corresponding to (i) model Coulomb plasmas [29], (ii) capillary discharges in polyurethane [1], and (iii) copper plasmas obtained by vaporizing copper wire in a water bath [3].

A. Microscopic simulation of hydrogen plasma

Fully ionized strongly coupled hydrogen plasmas were simulated using the method of molecular dynamics (MD) in well-known studies by Hansen and McDonald [29]. Quantum effects were taken into account in these simulations through the use of effective pair potentials; at short distances these differed significantly from the bare Coulomb potential. Reasonable agreement with the conductivity results of [29]

TABLE II. σ_L^* are the results of the extrapolation procedure according to Eq. (50) and σ_D^* were calculated in terms of the diffusion coefficients as explained in Sec. VII A. σ_{Cp}^* are the results of the present work computed using the Coulomb potential and σ_{pp}^* represent our results calculated with the model pseudopotential suggested in [31] and employed in [29]; σ_{BRD}^* stands for the results of [12].

$n_e\times10^{-24}$ (cm^{-3})	$T\times10^{-5}$ (K)	Γ	r_s	σ_L^*	σ_D^*	σ_{Cp}^*	σ_{pp}^*	σ_{BRD}^*
1.611	1.579	2.0	1.00	1.1	0.60	0.59	1.20	3.72
1.610	6.315	0.5	1.00	2.15	0.86	1.00	1.40	2.13
25.170	15.79	0.5	0.40	3.6	1.47	1.80	2.70	4.13

was obtained in [12] (see Table II, where the results are presented for the dimensionless conductivity $\sigma^*=\sigma/\omega_{pe}$ ($\omega_{pe}=(4\pi n_e e^2/m)^{1/2}$ being the electronic plasma frequency). The *dynamical* results of [29] were successfully considered in [30].

The static conductivity of model plasmas was obtained in [29] on the basis of the Nernst-Einstein law in terms of electronic and ionic diffusion coefficients directly estimated by MD simulations:

$$\sigma_D=\beta n_e e^2(D_i+D_e). \tag{50}$$

In addition, σ was determined, at least for $\Gamma=2$ and $r_s=1$, through the electric current autocorrelation function in the relaxation time approximation [29].

Notice that the simulation data for $\Gamma=2$ and $r_s=1$ were obtained in [29] by MD calculations; in this case the value σ_D^* was calculated as

$$\sigma_D^*=\frac{3\Gamma}{4\pi}\left\langle\frac{m}{M}\right\rangle D_i^*+D_e^*, \tag{51}$$

D_e^* and D_i^* being the dimensionless diffusion coefficients determined in [29]. Other results were found in [29] by extrapolation. In these cases D_i^* was set equal to zero (not determined in [29]); M is the proton mass.

The value of σ_L^* was obtained in [29] by a limiting procedure over the dynamic conductivity $\sigma(k,\omega)$,

$$\sigma_L=\lim_{\omega\to0}\lim_{k\to0}\mathrm{Re}\sigma(k,\omega), \tag{52}$$

and thus related via the fluctuation-dissipation theorem to the dynamic *charge-charge* structure factor. The limiting value of Eq. (50) could be found in [29] only by extrapolation of long-wavelength MD data (see Table IV of [29]). The point with $\Gamma=2.0$ was the only point really simulated in [29]. The other two points were obtained in this work using an extrapolation procedure; its precision is unknown to us. We would rather not consider $\sigma_L^*=\sigma_L/\omega_{pe}$ (characterized in [29] as the *true* value) to be much more reliable than σ_D^*.

We computed the conductivity of strongly coupled hydrogen plasma for all three cases considered in [29] and using the static local field correction of Eq. (29). The calculations were carried out for both the Coulomb interaction and the model pseudopotential suggested by Deutsch and co-workers in [31] and employed in [29]. In the case of Coulomb interactions the relaxation time was calculated according to Eq. (27) with $\kappa_a^2(q)=1, a=e,i$; see the σ_{Cp}^* data in Table II.

The model pseudopotential of [31,29] is determined by the interacting particles charge numbers and their reduced masses. The species form factors cannot be introduced, so that Eq. (21) should be modified:

$$\langle|\hat{V}(\vec{q},\omega)|^2\rangle=\left(\frac{4\pi e}{q^2\varepsilon(q,\omega)}\right)^2\sum_{a,b}Y_{ab}(q)S_{ab}(\vec{q},\omega), \tag{53}$$

where

$$Y_{ab}(q)=Y_{ba}(q)=Z_aZ_b[1+(q\lambda_{ab})^2]^{-1}, \tag{54}$$

$$\varepsilon(q,\omega)=1+\frac{4\pi e^2}{q^2}\sum_a Y_{aa}^2(q)\Pi_a(q,\omega), \tag{55}$$

and

$$\lambda_{ab}=\left[\frac{\hbar\beta}{2\pi}(m_a^{-1}+m_b^{-1})\right]^{1/2}, \tag{56}$$

m_a and Z_a being the a species mass and charge number. In hydrogen plasmas $m_e=m$ and $m_i=M$, while $Z_e=-1$ and $Z_i=1$.

The pseudoparticles screened interaction energy is equal to $4\pi e^2Y_{ab}/q^2\varepsilon(q,\omega)$ and the relaxation time expression of Eq. (27) becomes more complicated:

$$\tau_{pp}^{-1}(E)=\frac{4\pi me^4}{\beta(2mE)^{3/2}}\int_0^Q\frac{dq}{q}\sum_l[Y_{ee}^2\Pi_e+Y_{ii}^2\Pi_i+2(Y_{ee}Y_{ii}-Y_{ei}^2)\Pi_e\Pi_i]/\varepsilon^3(q,l). \tag{57}$$

The results of our computations with all these changes included, labeled σ_{pp}^*, are also provided in Table II. We cannot overestimate the fact that σ_{pp}^* virtually coincides with the *true* conductivity value σ_L^* at $\Gamma=2.0$. More simulation results on both transport and dynamic plasma properties are needed to decide whether, and to what extent, the behavior of the classical pseudoparticles with the pseudopotential of [31,29] imitates that of the true quantum system. We conclude that overall satisfactory agreement with available plasma-simulation data is achieved.

B. Capillary discharge in polyurethane

Dense strongly coupled plasmas were created in a well-diagnosed uniform discharge in polyurethane with density 1.265×10^{-2} g/cm^3 and temperatures in the 25–30 eV range

TABLE III. σ are the results of the present work, the experimental values σ^{expt} are by DeSilva [3], T and ρ are the temperature and mass density of copper, Ze is the effective ion charge, and f is the dimensionless Wiedemann-Franz ratio (59).

T (kK)	ρ (g/cm^3)	Z	Γ	θ	$\sigma^{expt}\times10^{-4}$ (S/m)	$\sigma\times10^{-4}$ (S/m)	f
20	0.7930	1.5	2.97	1.020	5.1	10.50	0.99
10	2.4550	2.3	10.12	0.167	32.1	21.00	0.99
14	1.2036	1.7	5.15	0.460	9.5	11.95	0.98
20	0.1557	1.2	1.62	3.240	2.2	4.12	1.11
26	0.0580	1.4	0.94	7.340	3.9	3.44	1.11
30	0.0400	1.6	0.75	9.930	4.8	3.42	1.11
40	0.0230	2.0	0.51	16.50	5.8	3.66	1.10
10	1.3546	1.7	7.51	0.304	8.3	11.27	0.99
14	0.3500	1.1	2.95	1.401	1.3	4.90	1.05
20	0.0260	1.3	0.92	10.13	2.0	2.12	1.11
10	2.2616	2.2	9.70	0.182	27.1	19.10	0.99
14	0.9704	1.5	4.60	0.577	6.4	9.86	0.99
16	0.1323	1.1	1.87	3.060	1.2	3.27	1.11
20	0.0680	1.2	1.62	5.630	2.2	2.94	1.11
30	0.0270	1.6	0.66	12.61	4.4	3.03	1.11

[1]. These results were compared in [1] with several dense plasma theories [32,33,12,34] and showed to be in a significant disagreement.

Preliminary experiments of this type were reported in [35–37]. Reasonable agreement with these data was obtained in [16], especially at $T=17$–18 eV [37], but within the hydrogen model.

An effective average ionic charge number $Z=2.3$ was obtained in [1] presuming Saha equilibrium. This permitted us to carry out the calculation of the electrical conductivity of a multiply ionized two-component plasma in the range $n_e=(4.8-5.2)\times10^{21}$ cm^{-3} and $T=(2.5-4.0)\times10^5$ K. The same local field correction as in Sec. VII A was employed with $g_e(0)=0$ (see [19] and above).

The experimental data of [1] (provided graphically for the resistivity) range between 2.0×10^5 and 3.3×10^5 $(\Omega\,\mathrm{m})^{-1}$. Our results varied between 3.3×10^5 $(\Omega\,\mathrm{m})^{-1}$ (for $n_e=5.2\times10^{21}$ cm^{-3} and $T=2.5\times10^5$ K) and about 10^6 $(\Omega\,\mathrm{m})^{-1}$ (for $n_e=4.8\times10^{21}$ cm^{-3} and $T=4.0\times10^5$ K), taking the value of $\sigma=5.0\times10^5$ $(\Omega\,\mathrm{m})^{-1}$ at about 3×10^5 K and $n_e=5\times10^{21}$ cm^{-3}. This last value is characteristic for the results of *dense plasma theories* [32,33,12,34] referred to in [1]. Notice that the lowest conductivity value reached by these theories is about 4.2×10^5 $(\Omega\,\mathrm{m})^{-1}$ [1] and also that under these specific conditions, i.e., at $\Gamma=0.18$–0.12, the dimensionless (normalized to the plasma frequency) computed plasma conductivity can be fitted to a simple potential function of the coupling parameter Γ only:

$$\sigma^*(\Gamma)=u/\Gamma^v \tag{58}$$

with $u=1.70\times10^{-2}$ and $v=2.27$.

C. Discharges in water

We have also carried out a broad comparison with the conductivity data measured by vaporizing copper wires in a water bath [3]. Plasma densities observed ranged from about 2.5 g/cm^3 down to 0.025 g/cm^3 and temperatures varied between 10 and 30 kK. The ionization state used by DeSilva and in our computations was taken from the Fermi-Thomas model by More [38]. The plasma coupling and degeneracy parameters ranged from $\Gamma=0.66$ to $\Gamma=10.12$ and $\theta=0.167$ to $\theta=16.5$, respectively; see Table III.

We considered three shots of data of [3] and calculated both electrical and thermal conductivities. The results are provided in Table III, where f is the dimensionless Wiedemann-Franz ratio

$$f=\frac{3}{\pi^2}(\kappa e^2/\sigma k_B^2 T). \tag{59}$$

First of all, we observe a good level of verification of the Wiedemann-Franz law: We neglected the ionic transport. A reasonable 30% agreement is observed in the majority of points, especially at higher densities. A factor of 2–3 disagreement detected at 14–16 kK and low densities is attributable to the possible onset at the conductor-dielectric phase transition: The copper plasma begins to undergo a transformation from the fully ionized state corresponding to our model into the partially ionized state where charge-atom interactions are to be taken into account. The SESAME code ''is increasingly inaccurate with the onset of strong Coulomb interaction'' [39] and cannot include the possible Mott-type phase transition. The precision level of this code is not known. In addition, the experimental measurements are quite difficult [2,3] and we believe that an overall precision of the experimental data of [3] is of the order of 30–100 %.

Notice once more that no adjustable parameters were used in our computations. The only input data were the plasma temperature (T) and density (ρ) (provided by the SESAME code; see [3]) and the precalculated charge number Z (see above).

Calculations were carried out for different values of the local-field correction static parameter $g_e(0)$, ranging according to its definition between zero and unity. No appreciable dependence on the value of $g_e(0)$ was detected; further cal-

culations were carried out with $g_e(0)$ set to be zero. Thus the only *experimental* data our results are based on is the computer fit to the one-component plasma interaction energy obtained by MC simulations [20].

In conclusion, a theory of transport coefficients of fully ionized strongly coupled plasmas, based on the self-consistent field concept and having no adjustable parameters, is presented. The self-consistent field theory suggested in [13], outlined in detail, modified, and applied here to various model and real plasmas, is not based on the solution of kinetic equations. In particular, we do not have to introduce into our expression the order of 2 correction [40] (see also [12,7,8]) that takes into account higher-order Sonine polynomials contributions to the solution of the kinetic equation. The theory is applicable to multiple-component (non-hydrogen-like) plasmas with variable ionization states, and is shown to possess correct low-density (Spitzer) and metal-density (Ziman) limiting forms.

ACKNOWLEDGMENTS

The authors are grateful to A. W. DeSilva for providing his numerical data on conductivity and ionization state and also to V. M. Adamyan, W. Ebeling, J. Ortner, and A. A. Mihajlov for valuable discussions.

[1] J. F. Benage,Jr. *et al.*, Phys. Rev. E **49**, 4391 (1994).
[2] A. W. DeSilva and H. J. Kunze, Phys. Rev. E **49**, 4448 (1994).
[3] A. W. DeSilva, in *Physics of Strongly Coupled Plasmas*, edited by W. D. Kraeft and M. Schlanges (World Scientific, Singapore, 1995), p. 216 and private communication.
[4] J. K. Yuan, Y. S. Sun, and S. T. Zhang, Phys. Rev. E **53**, 1059 (1996).
[5] E. Nardi, Phys. Rev. E **54**, 1899 (1996).
[6] H. Reinholz, R. Redmer, and S. Nagel, Phys. Rev. E **52**, 5368 (1995).
[7] S. Ichimaru and S. Tanaka, Phys. Rev. A **32**, 1790 (1985).
[8] S. Ichimaru, *Statistical Plasma Physics* (Addison-Wesley, Reading, MA, 1991), Vol. II.
[9] G. Röpke and R. Redmer, Phys. Rev. A **39**, 907 (1989).
[10] W. Ebeling *et al.*, *Thermophysical Properties of Hot Dense Plasmas* (Teubner Verlagsgeselschaft, Stuttgart, 1991), pp. 210–212.
[11] I. T. Iakubov, Usp. Fiz. Nauk **163**, 35 (1993) (in Russian).
[12] D. B. Boercker, F. Rogers, and H. E. DeWitt, Phys. Rev. A **25**, 1623 (1982).
[13] V. M. Adamyan *et al.*, Teplofiz. Vys. Temp. **18**, 230 (1980) [High Temp. **18**, 186 (1980)].
[14] S. F. Edwards, Philos. Mag. **3**, 1020 (1958).
[15] S. Ichimaru, *Statistical Plasma Physics* (Addison-Wesley, Reading, MA, 1992), Vol. I.
[16] Z. Djurić, A. A. Mihajlov, V. A. Nastasyuk, M. Popović, and I. M. Tkachenko, Phys. Lett. A **155**, 415 (1991).
[17] A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinskii, *Quantum Field Methods in Statistical Physics* (GIFML, Moscow, 1962).
[18] I. M. Tkachenko, Europhys. Lett. **9**, 351 (1989).
[19] I. M. Tkachenko, P. Fernández de Córdoba, and M. Urrea, J. Phys. A **29**, 2599 (1996).
[20] G. S. Stringfellow, H. E. de Witt, and W. L. S. Slattery, Phys. Rev. A **41**, 1105 (1990).
[21] J. C. Kimball, Phys. Rev. A **7**, 1648 (1973); Phys. Rev. B **14**, 2371 (1976).
[22] N. R. Arista and W. Brandt, Phys. Rev. A **29**, 1471 (1983).
[23] L. Spitzer, Jr., *Physics of Fully Ionized Gases* (Interscience, New York, 1962).
[24] J. M. Ziman, *Theory of Solids* (Cambridge University Press, London, 1972).
[25] R. Redmer, Phys. Rep. **282**, 35 (1997).
[26] See, e.g., A. R. Hochstim, *Kinetic Processes in Gases and Plasma* (Academic, New York, 1969), Chap. 6.
[27] V. M. Adamyan, Z. Djurić, A. M. Ermolaev, A. A. Mihajlov, and I. M. Tkachenko, J. Phys. D **27**, 111 (1994).
[28] V. M. Adamyan, Z. Djurić, A. M. Ermolaev, A. A. Mihajlov , and I. M. Tkachenko, J. Phys. D **27**, 927 (1994).
[29] J. P. Hansen and I. R. McDonald, Phys. Rev. A **23**, 2041 (1981).
[30] S. V. Adamyan, I. M. Tkachenko, J. L. Muñoz-Cobo González, and G. Verdú Martín, Phys. Rev. E **48**, 2067 (1993).
[31] C. Deutsch, Phys. Lett. **60A**, 317 (1977); C. Deutsch, M. M. Gombert, and H. Minoo, *ibid.* **66A**, 381 (1978); **72A**, 481 (1979).
[32] R. Cauble and W. Rozmus, J. Plasma Phys. **37**, 405 (1987).
[33] G. A. Rinker, Phys. Rev. B **31**, 4207 (1985).
[34] S. Ichimaru, S. Mitake, S. Tanaka, and X.-Z. Yan, Phys. Rev. A **32**, 1768 (1985).
[35] R. L. Shepherd, D. R. Kania, and L. A. Jones, Phys. Rev. Lett. **61**, 1278 (1988).
[36] R. L. Shepherd *et al.*, in *Strongly Coupled Plasma Physics*, edited by S. Ichimaru (Yamada Science Foundation, 1990), p. 437.
[37] J. F. Benage *et al.*, *Strongly Coupled Plasma Physics* (Ref. [36]), p. 429.
[38] R. M. More, in *Physics of Laser Plasma*, edited by A. M. Rubenchik and S. Witkowski, Handbook of Plasma Physics Vol. 3 (Elsevier, Amsterdam, 1991), Chap. 2, p. 70; R. M. More, Adv. At. Mol. Phys. **21**, 305 (1985).
[39] K. S. Trainor, J. Appl. Phys. **54**, 2372 (1983).
[40] R. H. Williams and H. E. DeWitt, Phys. Fluids **12**, 2326 (1969).