Condensed Matter Physics, 2000, Vol. 3, No. 3(23), pp. 641–656

Linear static response of model plasmas and Yukhnovsky-Kelbg-Deutsch effective potential

V.M.Adamyan [1]*, I.M.Tkachenko [2]†

[1] Department of Theoretical Physics, University of Odesa, 65026 Odesa, Ukraine

[2] Department of Applied Mathematics, Polytechnic University of Valencia, 46071 Valencia, Spain

Received June 7, 2000

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 proposed approach is not connected directly with the kinetic equation. A comparison of the obtained results with the computer simulation data on the classical hydrogen-like plasmas macroscopic properties shows that using the Yukhnovsky-Kelbg-Deutsch effective pair potentials instead of the genuine Coulomb potentials can compensate, to a certain extent, inaccuracies related to the standard approximations of the quantum theory of Coulomb systems.

Key words: *hydrogen plasmas, transport coefficients, pair potentials*

PACS: *52.25.Fi, 52.25.Ub, 52.65.-y*

Dedicated to academician Igor Yukhnovsky on the occasion of his 75th birthday.

1. Introduction

The aim of this work is to bring together some results of the quantum statistical theory of the Coulomb systems transport properties with the results related to the completely ionized nearly classical hydrogen plasmas(HP). The "experimental" basis of this work is the computer simulation of the HP microscopic characteristics obtained in [1,2]. The molecular dynamics (MD) method used there was borrowed from the theory of classical liquids.

In order to avoid the Coulomb collapse while treating HP in the framework of the classical statistical mechanics, instead of bare Coulomb potentials the method of MD

*E-mail: vma@dtp.odessa.ua
†E-mail: imtk@mat.upv.es

employs *effective pair potentials,* which account, to a certain extent, for diffraction and symmetry effects.

Let Ψ_n and E_n be the eigenfunctions and eigenvalues of the complete Hamiltonian of the N electrons and N protons of HP, while $\{\vec{r}_a\}$ denotes the set of position vectors of all plasma particles, $r_{ab} = |\vec{r}_a - \vec{r}_b|$, and let $V\left(r_{ab}\right)$ be the effective (self-consistent) pair potential between particles a and b. Effective pair potentials can be in principle derived by transforming based on a reasonable approximation of the quantum-mechanical Slater sum

$$W\left(\{\vec{r}_a\}\right) = \sum_n \Psi_n^* \exp\left(-\beta E_n\right) \Psi_n \tag{1}$$

as

$$W \simeq \exp\left(-\beta \sum_{a<b} V\left(r_{ab}\right)\right). \tag{2}$$

reminding the classical Boltzmann factor [3]. In the classical (high-temperature) limit, $V\left(r_{ab}\right)$ should reduce to the bare Coulomb potential between the two particles, i.e.,

$$\lim_{T\to\infty} V\left(r_{ab}\right) = \frac{Z_a Z_b e^2}{r_{ab}}, \tag{3}$$

where $Z_a = +1$ (ions, $a = i$), or -1 (electrons, $a = e$). An effective potential determined this way is generally dependent both on temperature and density of the particles. Effective pair potentials appropriate to the low-density limit were first derived for the hydrogen plasma by Yukhnovsky [4], Kelbg, and Deutsch [5] and collaborators from an exact numerical computation of the two-particle Slater sum for electron-electron and electron-proton pairs. At sufficiently high temperatures ($k_{\mathrm{B}}T \gtrsim \mathrm{Ry}$), the contribution of bound states to the electron-proton Slater sum may be ignored. If, moreover, the scattering states are limited to s waves, and if the effects of permutative symmetry are neglected even for electron-electron pairs, the following very simple effective potentials can be derived:

$$V\left(r_{ab}\right) = \frac{Z_a Z_b e^2}{r_{ab}} \left[1 - \exp\left(\frac{-r_{ab}}{\lambda_{ab}}\right)\right], \tag{4}$$

where

$$\lambda_{ab} = \left[\frac{\hbar\beta}{2\pi}\left(m_a^{-1} + m_b^{-1}\right)\right]^{1/2}. \tag{5}$$

The fact that the potentials $V\left(r_{ab}\right)$ remain finite as $r_{ab} \to 0$ is a consequence of the uncertainty principle, which prevents the aforementioned Coulomb collapse. At the temperatures of interest, λ_{ii} is much smaller than the Wiegner-Seitz radius $d = (3/4\pi n)^{1/3}$, where $n = n_{\mathrm{e}} = n_i$ is the number density of the system particles. Thus the effective ion-ion interaction is virtually identical to the bare Coulomb potential at all separations.

An important approximation made in the MD simulations [2] is the neglect of the density dependence of the effective pair potentials, even at densities of the order of 10^{24} cm^{-3}, which is reasonable as long as $\lambda_{ab}/d \ll 1$, i.e., for a sufficiently nondegenerate plasma [3]. It was also implicitly assumed in [2] that the effective potentials of clusters of three or more particles are pairwise additive. Despite all these limitations, the results of [2] have not been surpassed in quality and precision: the character of collective properties of the plasma is dictated primarily by the long range part of the potential and therefore it is insensitive to the details of the short range behaviour. For the same reason, the numerical simulations were carried out in [2] without including the symmetry part of the electron-electron potential.

In this paper we study the electric conductivity of HP in the same near-classical region as in [2].

In the three sections that follow we outline the general theoretical approach to determining the strongly-coupled plasmas transport properties [6], based on the idea of independent particles walking randomly in the fluctuating internal self-consistent field. Thus first we obtain the expression for the plasma static conductivity using the two-particles Green functions calculated in the random–phase approximation (RPA). Then we improve this approximation taking into account the local field corrections (LFCs), which at the same time may be treated as those resulting from the substitution of the bare Coulomb potentials by the effective potentials according to Yukhnovsky-Deutsch. To compare our outcome with the simulation results the calculations [7] are carried out with the model effective potential of [5] employed in [2]. The corresponding data is summarized and discussed in section 5. It follows from this data that the substitution of the screened Coulomb potential in the quantum statistical expressions for the transport coefficients obtained in the LFC-corrected RPA by the screened Yukhnovsky-Deutsch potential brings results substantially closer to the experimental data. This fact deserves a further investigation.

The approach possesses no adjustable parameters, except for the Monte-Carlo one-component plasma equation of state [8], interpolated with the low-density expansion by Abe [9], see appendix 1.

From now on we use the following notations. The thermodynamic state of the system is characterized by the standard dimensionless parameters:

$\Gamma = \beta e^2(4\pi n/3)^{1/3}$ which measures the rate of Coulomb coupling in the system,

$D = \theta^{-1} = \beta E_{\mathrm{F}} = \beta\hbar^2 k_{\mathrm{F}}^2/2m$, measuring the plasma degeneracy rate, and

the Brückner parameter $r_{\mathrm{s}} = \Gamma\theta/0.543$.

As usual, $k_{\mathrm{F}} = (3\pi^2 n)^{1/3}$ is the Fermi wavevector, and E_{F} is the Fermi energy.

2. The Lorentz formula

The starting-point of the approach developed in [6] is the idea of self-consistent field: *each charge carrier of HP moves in a self-consistent field generated by all charges of the system.* The finite values of the transport coefficients then result from the electron's scattering on the self-consistent field fluctuations. This approach was prompted by the paper [10], which connects the Lorentz-model expression for the electrical conductivity with the Green's-function formalism for electrons in crystals with randomly distributed impurities as well as in metallic alloys and in conducting liquids.

We begin the calculation of the HP static conductivity with the general expression

$$\sigma = \frac{\partial}{\partial F} j_x(\vec{r},t)|_{F=0}, \tag{6}$$

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

$$\vec{F}(\vec{r},t) = (F,0,0)\exp(\delta\ t),\ \delta > 0,\ \delta \longrightarrow 0^+. \tag{7}$$

The specific time dependence of the field is introduced to avoid coherent currents induced at the switch-on moment $t = -\infty$. In the general quantum-mechanical expression

$$j_x(\vec{r},t) = \operatorname{Tr}\hat{\rho}(t)\{-\frac{\mathrm{i}\hbar e}{2m}[\Psi^+(\vec{r},-\infty)\frac{\partial}{\partial x}\Psi(\vec{r},-\infty) - \frac{\partial}{\partial x}\Psi^+(\vec{r},-\infty)\Psi(\vec{r},-\infty)]\}, \tag{8}$$

where $(-e)$ and m are the electronic charge and mass; only the density operator $\hat{\rho}(t)$ depends on the external field (7) through the interaction contribution

$$-eF\mathrm{e}^{-\delta t}\int_\Omega x\Psi^+(\vec{r},s)\Psi(\vec{r},s)\mathrm{d}\vec{r}$$

to the system Hamiltonian $H(t)$. Therefore

$$\left[\frac{\partial\hat{\rho}(t)}{\partial F}\right]_{F=0} = \frac{\mathrm{i}e}{\hbar}\int_0^\infty \mathrm{e}^{-\delta s}\mathrm{d}s\int_\Omega x[\Psi^+(\vec{r},s)\Psi(\vec{r},s),\hat{\rho}(-\infty)]\mathrm{d}\vec{r}, \tag{9}$$

where

$$\begin{aligned}\hat{\rho}(-\infty) &= \exp\{-\beta[H(-\infty)-\phi]\},\\ \exp(-\beta\phi) &= \operatorname{Tr}\exp[-\beta H(-\infty)],\end{aligned} \tag{10}$$

ϕ being the system free energy of Helmholtz and Ω the system volume, $\beta^{-1} = k_\mathrm{B}T$. Hence

$$\begin{aligned}\sigma = \frac{e^2}{2m}\Re\mathrm{e}\int_0^\infty \mathrm{e}^{-\delta s}\mathrm{d}s\int_\Omega \mathrm{d}\vec{r}\,'x'\operatorname{Tr}\hat{\rho}(-\infty)\\ \times\left[\Psi^+(\vec{r},-\infty)\frac{\partial}{\partial x}\Psi(\vec{r},-\infty) - \frac{\partial}{\partial x}\Psi^+(\vec{r},-\infty)\Psi(\vec{r},-\infty),\Psi^+(\vec{r}\,',s)\Psi(\vec{r}\,',s)\right].\end{aligned} \tag{11}$$

The second-quantized wave function $\Psi(\vec{r},t)$ in (11) is expressible in terms of the one-electron normalized eigenfunctions $\psi_\nu(\vec{r})$ of the one-electron free Hamiltonian $\widehat{h}_0$,

$$\widehat{h}_0\psi_\nu(\vec{r}) = \varepsilon_\nu\psi_\nu(\vec{r}), \tag{12}$$

$$\Psi(\vec{r},s) = \sum_\nu a_\nu\exp\left(-\frac{\mathrm{i}}{\hbar}\varepsilon_\nu s\right)\psi_\nu(\vec{r}), \tag{13}$$

a_ν being the corresponding annihilation operator.

For the averaged commutator $[a^+_{\mu'}a_\mu, a^+_{\nu'}a_\nu]$ we have

$$\mathrm{Tr}\,\hat{\rho}(-\infty)[a^+_{\mu'}a_\mu, a^+_{\nu'}a_\nu] = \delta_{\mu\nu'}\delta_{\mu'\nu}[w_\nu - w_\mu], \tag{14}$$

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. Using (14) in (11) yields

$$\begin{aligned}\sigma \;=\; & \frac{e^2}{2m}\Re\mathrm{e}\int_0^\infty\int_0^\infty \mathrm{d}\varepsilon_1\mathrm{d}\varepsilon_2\int_\Omega \mathrm{d}\vec{r}\,'x'\left\langle G(\vec{r},\vec{r}\,';\varepsilon_1)\frac{\partial}{\partial x}G(\vec{r},\vec{r}\,';\varepsilon_2)\right.\\ & \left. - G(\vec{r},\vec{r}\,';\varepsilon_2)\frac{\partial}{\partial x}G(\vec{r},\vec{r}\,';\varepsilon_1)\right\rangle \frac{\hbar[w(\varepsilon_1) - w(\varepsilon_2)]}{\mathrm{i}(\varepsilon_1 - \varepsilon_2 - \mathrm{i}\hbar\delta)},\end{aligned} \tag{15}$$

where

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

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

$$\begin{gathered}-\frac{\hbar^2}{2m}\Delta G + eV(\vec{r})G = \varepsilon G + \delta(\vec{r} - \vec{r}\,),\\ G(\vec{r},\vec{r}\,';\varepsilon) = G(\vec{r}\,',\vec{r};\varepsilon).\end{gathered} \tag{16}$$

The symmetry properties of the Green's function lead to

$$\sigma = \frac{\pi e^2\hbar^3}{m^2}\Re\mathrm{e}\int_0^\infty \mathrm{d}\varepsilon\frac{\mathrm{d}\omega(\varepsilon)}{\mathrm{d}\varepsilon}\int_\Omega \mathrm{d}\vec{r}\,'\left\langle\frac{\partial G(\vec{r}\,',\vec{r};\varepsilon)}{\partial x'}\cdot\frac{\partial G(\vec{r},\vec{r}\,';\varepsilon)}{\partial x}\right\rangle. \tag{17}$$

Averaging in equation (15) is to be carried out over the self-consistent field fluctuations.

An important advantage of formula (17) for σ is that the diagrammatic technique of perturbation theory can be directly applied to calculate its right-hand side. In addition, the present problem lacks the divergence difficulties characteristic of quantum electrodynamics and the expression (17) permits one to carry out the averaging over the fluctuations of the self-consistent field before the coordinate integration. Applying a diagrammatic technique analogous to that of the quantum field theory to the calculation of the electron conductivity in crystals with randomly distributed defects, Edwards [10] established that the averaging of the product of the Green functions in (17) and subsequent coordinate integration yields the Lorentz formula

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

where $\rho(E) = (2m^3E)^{1/2}/2\pi^2\hbar^3$ is the density of one-electron states in the energy space and $\tau(E)$ is the mean relaxation time.

Under certain approximations and in the case of finite conductivity conditioned by the scattering on point defects, the mean relaxation time $\tau(E)$ in (18) can be expressed through the exact scattering cross-section of electron scattering on a single defect and the pair correlation functions of defects [10]. Using arguments similar to those of [10], it was shown in [6] that formula (18) is also true for strongly correlated plasmas of high density and, in particular, for dense HP. However, the finite values of the mean relaxation time for electrons in plasmas are due to the electron scattering on thermal fluctuations of the self-consistent electric field formed by all charged particles of a plasma.

3. Calculation of conductivity

According to the results obtained in [6] as a modification of the approach developed in [10], the main contribution to the expressions for the averaged one-electron Green's function $\langle G\rangle$ and the averaged product $\langle GG\rangle$ in dense fully ionized plasmas produces an infinite sum of a certain subclass of diagrams of the formal perturbation series in the powers of the fluctuations of the self-consistent field potential. These diagrams are actually those appearing in the H.Brückner method. Their summation leads, in particular, to the following expression for the inverse mean relaxation time in terms of the self-consistent field correlation function

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

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

$$\hat{V}_\mathrm{s}(\vec{q},\omega) = \frac{4\pi e}{q^2\varepsilon(q,\omega)} \sum_{a=e,i} Z_a \ \hat{\rho}_a(\vec{q},\omega) \tag{20}$$

is the screened field potential operator complete Fourier transform, $\hat{\rho}_a(\vec{q},\omega)$ being the a-species density operator in the $(\vec{q},\omega)$-space, and $\varepsilon^{-1}(q,\omega)$ – the plasma dynamic screening function. The field potential correlation function thus equals

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

The dynamic structure factor of the species a and b,

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

is related, by the fluctuation dissipation theorem

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

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

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

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

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

$$\varepsilon(q,\omega) = 1 + \frac{4\pi e^2}{q^2}\sum_{a=e,i} Z_a^2 \Pi_a(q,\omega). \tag{26}$$

Substitution of equations (21)–(25) into equation (19) and integration [11], yields

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

Here the l-summation is spread over the poles

$$\Omega_l = 2\pi l/\beta\hbar \quad (l = 0, \pm 1, \pm 2, \ldots) \tag{28}$$

of $\coth(\beta\hbar z/2)$ on the imaginary z-axis, i.e., over the Matsubara frequencies [12] and $\Pi_a(q,l)$ are the real parts of the $\Pi_a(q,\omega)$ operators at $\omega = \mathrm{i}\Omega_l$. Equation (27), together with equation (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, see appendix 1.

Observe that the expression obtained for the relaxation time coincides with that calculated in the Born approximation for an extraneous particle having the electron mass and charge and scattering on the fluctuating internal field of HP.

4. Limiting cases

Despite the approximations made to obtain equation (27) 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 equation (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 equation (27) becomes a constant βn. If we further presume E to be equal to the mean kinetic energy of an electron, we retrieve from equation (27) the Coulomb logarithm, and equation (18) with $w(E)$ substituted by the Boltzmann distribution takes the form of the Spitzer formula without corrections due to electron-electron interactions [13].

On the other hand, if we consider the low-temperature limiting case ($\beta^{-1} \to 0$), the Fermi-Dirac distribution derivative in equation (18) turns into $-\delta(E - E_{\mathrm{F}})$ and

Table 1. σ^*_{L} are the results of the extrapolation procedure according to equation (31) and σ^*_{D} were calculated in terms of the diffusion coefficients as explained. σ^*_{Cp} are the results of the present work computed using the Coulomb potential, and σ^*_{ep} represent our results; σ^*_{BRD} stands for the results of [15]

$n_{\mathrm{e}} \times 10^{-24}(\mathrm{cm}^{-3})$	$T \times 10^{-5}(\mathrm{K})$	Γ	r_{s}	σ^*_{L}	σ^*_{D}	σ^*_{Cp}	σ^*_{ep}	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

Q becomes equal to $2k_{\mathrm{F}}$, so that we immediately regain the Ziman specific resistance formula [14].

Notice that no special effort was done *ab initio* to guarantee the correct limiting behaviour of our model. Nevertheless, further studies of the limiting behaviour of our model and a comparison with other general expressions for the collision frequency (e.g., [15]) or for the conductivity itself (see [16]) are to be carried out.

In general, the difference between our expression and that of Ziman (widely used lately to calculate conductivity [17–19]) is that we include the energy-dependent relaxation time [equation (27)], and the Ziman formula takes it at $E = E_{\mathrm{F}}$. In addition, we have the electron-electron interaction included explicitly via the structure factor $S_{\mathrm{ee}}(q, \omega)$.

As it is well known, the $\sigma(T)$ dependence at a constant density is characterized by a minimum corresponding to a transition from the low-temperature regime with decreasing (with growing T) conductivity characteristic of metals and liquid metals (Ziman regime) to that of increasing conductivity at higher temperatures, characteristic of dilute plasmas (Spitzer regime) with $\sigma_{\mathrm{Sp}}(T) \propto T^{3/2}$.

5. Results and conclusions

Here we report our results on the conductivity computation obtained for the conditions corresponding to model Coulomb plasmas [2]. Other results, including those for the thermal conductivity (see appendix 2), can be found elsewhere [20,7].

The *dynamical* results of [2] were successfully considered in [21].

A reasonable agreement with the conductivity results of [2] was obtained in [15] (see table 1, where the results are presented for the dimensionless conductivity $\sigma^* = \sigma/\omega_p$, $\omega_p = (4\pi n e^2/m)^{1/2}$ being the electronic plasma frequency).

The static conductivity of model plasmas was obtained in [2] based on the Nernst-Einstein law in terms of electronic and ionic diffusion coefficients directly estimated by MD simulations:

$$\sigma_{\mathrm{D}} = \beta n_{\mathrm{e}} e^2 (D_{\mathrm{i}} + D_{\mathrm{e}}). \tag{29}$$

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

Notice that the simulation data for $\Gamma = 2$ and $r_\mathrm{s} = 1$ were obtained in [2] by MD calculations; in this case the value σ^*_D was calculated as

$$\sigma^*_\mathrm{D} = \frac{3\Gamma}{4\pi}\left(\frac{m}{M}\right) D^*_\mathrm{i} + D^*_\mathrm{e}, \tag{30}$$

where M is the proton mass, D^*_e and D^*_i being the dimensionless diffusion coefficients determined in [2]. Other results were found in [2] by extrapolation. In these cases D^*_i was set equal to zero (not determined in [2]).

The value of σ^*_L was obtained in [2] by a limiting procedure over the dynamic conductivity $\sigma(k,\omega)$,

$$\sigma_\mathrm{L} = \lim_{\omega\to 0}\lim_{k\to 0} \Re\mathrm{e}\,\sigma(k,\omega)\ , \tag{31}$$

and thus related via the fluctuation-dissipation theorem to the dynamic *charge-charge* structure factor. The limiting value of equation (31) could be found in [2] only by extrapolation of long-wavelength MD data (see table IV of [2]). The point with $\Gamma = 2.0$ was the only point really simulated in [2]. The other two points were obtained in this work using an extrapolation procedure, its precision is not known to us. We would rather not consider $\sigma^*_\mathrm{L} = \sigma_\mathrm{L}/\omega_\mathrm{pe}$ (characterized in [2] 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 [2]. The calculations were carried out for both the Coulomb interaction and the effective potential of [5], and employed in [2]. In the case of Coulomb interactions the relaxation time was calculated according to equation (27) with $Z_a^2 = 1, a = e, i$; see the σ^*_Cp data in table 1.

The effective potential of [5] is determined by charge numbers of the interacting particles and by their reduced masses. The species form factors cannot be introduced, so that equation (21) should be modified:

$$\left\langle |\hat{V}(\vec{q},\omega)|^2 \right\rangle = \left(\frac{4\pi e}{q^2\varepsilon(q,\omega)}\right)^2 \sum_{a,b} Y_{ab}(q) S_{ab}(\vec{q},\omega), \tag{32}$$

where

$$Y_{ab}(q) = Y_{ba}(q) = Z_a Z_b \left[1 + (q\lambda_{ab})^2\right]^{-1}, \tag{33}$$

$$\varepsilon(q,\omega) = 1 + \varphi(q) \sum_a Y^2_{aa}(q) \Pi_a(q,\omega); \tag{34}$$

$$\varphi(q) = \frac{4\pi e^2}{q^2}. \tag{35}$$

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

$$\tau^{-1}_\mathrm{pp}(E) = \frac{4\pi m e^4}{\beta(2mE)^{3/2}} \int_0^Q \frac{\mathrm{d}q}{q} \sum_l \frac{Y^2_\mathrm{ee}\Pi_\mathrm{e} + Y^2_\mathrm{ii}\Pi_\mathrm{i} + 2\varphi(q)\left(Y_\mathrm{ee}Y_\mathrm{ii} - Y^2_\mathrm{ei}\right)\Pi_\mathrm{e}\Pi_\mathrm{i}}{\varepsilon^3(q,l)}. \tag{36}$$

The results of our computations with all these changes included, labelled σ^*_{ep}, are also provided in table 1. We cannot overestimate the fact that σ^*_{ep} 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 behaviour of the classical pseudoparticles with the effective potential of [4,5] imitates the behaviour of the true quantum system. We conclude that overall satisfactory agreement with the plasma-simulation data available is achieved.

It is worth mentioning that all Y_{ab} appearing in (36) on the other hand can also be treated as factors improving the LFC-corrected RPA expressions for the polarization operators $\Pi_a(q,\omega)$ and the vertex operator.

In conclusion, notice that the proposed self-consistent field theory of plasma transport properties 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 [15] that takes into account the 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.

6. Acknowledgements

The authors are grateful to W.Ebeling, J.Ortner, and A.A.Mihajlov for valuable discussions, and to P.Fernández de Córdoba and J.Alcober for their aid in numerical calculations.

A. Static structural characteristics

A natural approach to the investigation of static correlations in strongly coupled plasmas, is based on the separation of electronic and ionic components of the system, so that the interionic interactions are assumed to be screened by the electronic static dielectric function $\varepsilon_{\mathrm{e}}(k)$. In dense systems the latter should be treated beyond the RPA, i.e., the calculation of $\varepsilon_{\mathrm{e}}(k)$ involves the electronic static local field correction (LFC) $G_{\mathrm{e}}(k)$.

There exists a number of various approaches to the computation of the LFC $G_{\mathrm{e}}(k)$ (see, e.g. [22]), but mostly they are applicable in specific realms of the system phase diagram. In our calculations we used a simple alternative model [23] which is to also serve as a basis for future studies of various properties of strongly coupled systems.

The interpolating formula for the electronic LFC suggested and tested in [23],

$$G_{\mathrm{e}}(z) = \left(b + a/4z^2\right)^{-1} \quad z = k/2k_{\mathrm{F}}, \tag{37}$$

incorporates both long and short wavelength asymptotic values of $G_{\mathrm{e}}(k)$. In particular,

$$b^{-1} = \lim_{k\to\infty} G_{\mathrm{e}}(k). \tag{38}$$

The short-range behaviour of $G_e(k)$ in the low-temperature limit has been studied in the papers of Shaw [24] and Kimball [25]. Namely, it has been shown that if $T \to 0$ in hydrogen-like systems,

$$b^{-1} = 1 - g_e(0), \tag{39}$$

$g_e(r)$ being the usual electronic radial distribution function. This result is based on the "cusp" condition which can be obtained from the s-solution of the two-particle Schrödinger equation at r=0 (see, e.g.[25]).

On the other hand, since $G_e(k \to \infty)$ involves only the short-range properties of the system, one expects the asymptotic value of equation (38) to be finite and the relation (39) to hold at arbitrary values of temperature T.

One can further notice that the long-wavelength behaviour of $G_e(k \to 0) \approx a^{-1}(k/k_F)^2$ is responsible for the screening of a static impurity in the plasma. On the other hand, the parameter a is determined by the system thermodynamic properties via the compressibility sum rule:

$$a = -\frac{(12/\pi)^{2/3}\Gamma}{f(\Gamma) + \Gamma f'(\Gamma)/3}. \tag{40}$$

Since the best Monte-Carlo (MC) fit [8] for the dimensionless excess interaction energy $f(\Gamma)$ in equation (40),

$$f_{\mathrm{MC}}(\Gamma) = A\Gamma + B + C\Gamma^{-1/3} + D\Gamma^{1/3}, \tag{41}$$

where

$$\begin{aligned} A &= -0.8993749, \qquad B = -0.2244699, \\ C &= -0.0178747, \qquad D = 0.5175753, \end{aligned} \tag{42}$$

is valid only for $\Gamma \geqslant 1$, we sought a smooth interpolation between equation (41) and the Abe low-Γ expansion [9]

$$f_{\mathrm{Abe}}(\Gamma) = -\frac{\sqrt{3}}{2}\Gamma^{3/2} - 3\Gamma^3\left[\frac{3}{8}\ln(3\Gamma) + \frac{\gamma}{2} - \frac{1}{3}\right], \tag{43}$$

$\gamma = 0.577215665$ being the Euler's constant, applicable for $\Gamma < 0.1$. We used a four-parameter interpolation

$$F(\Gamma) = \frac{s + \Gamma^{\sigma}}{t + \Gamma^{\tau}}, \tag{44}$$

to satisfy the conditions of continuity and smoothness between the functions equations (41) and (43) at the points $\Gamma = 0.1$ and $\Gamma = 1$. The resulting values of the parameters are

$$\begin{aligned} s &= -1.800549291, \qquad t = 0.2826351523, \\ \sigma &= 0.02932213806, \qquad \tau = -1.528433658. \end{aligned} \tag{45}$$

Thus in our computations we used

$$f(\Gamma) = \begin{cases} f_{\mathrm{Abe}}(\Gamma), & \Gamma < 0.1; \\ F(\Gamma), & 0.1 \leqslant \Gamma \leqslant 1; \\ f_{\mathrm{MC}}(\Gamma), & \Gamma > 1. \end{cases} \tag{46}$$

It remains to be seen how our results would be modified if instead of equation (46) other interpolations [26] were used.

No quantum effects are included in the EOS (5) and, hence, there is a discrepancy between (40) (and, thus, equation (37) as well) and our desire to apply it to electron liquids under "quantum" thermodynamic conditions.

To diminish the influence of this inconsistency, electronic radial distribution function $g_{\mathrm{e}}(r)$ and its zero separation value $g_{\mathrm{e}}(0)$ (and b of equation (37)) were determined by a self-consistent procedure. In effect, the value of $g_{\mathrm{e}}(r)$ was computed via a simultaneous solution of two integral equations,

$$S_{\mathrm{e}}(z) = \sum_{l=-l_1}^{l_1} \frac{P_{\mathrm{e}}(z,l)}{\varepsilon_{\mathrm{e}}(z,l)}, \tag{47}$$

$$g_{\mathrm{e}}(r) = 1 + \frac{6}{rk_{\mathrm{F}}} \int_0^\infty z \sin(2k_{\mathrm{F}} rz)\, \left(S_{\mathrm{e}}(z) - 1\right) \mathrm{d}z. \tag{48}$$

In equation (47) the summation is over the Matsubara frequencies $v_l{=}(\pi\theta l)/(2z)$, and

$$\varepsilon_{\mathrm{e}}(z,l) = 1 + \frac{\Gamma}{(12\pi^2)^{1/3}} \frac{P_{\mathrm{e}}(z,l)}{z^2}; \tag{49}$$

the l_1-parameter was determined by the numerical precision. $P_{\mathrm{e}}(z,l)$ in equation (47) is the dimensionless polarization operator $\Pi_{\mathrm{e}}(k,\omega)$ with the LFC, included,

$$P_{\mathrm{e}}(z,l) = P_{\mathrm{e}}^0(z,l) \left(1 - \frac{\Gamma}{(12\pi^2)^{\frac{1}{3}}} \frac{G_{\mathrm{e}}(z) P_{\mathrm{e}}^0(z,l)}{z^2}\right)^{-1}, \tag{50}$$

The RPA dimensionless polarization operator $P_{\mathrm{e}}^0(z,l)$ can be calculated (for each value of density and temperature, z and l) by simple integration [27],

$$P_{\mathrm{e}}^0(z,l) = \frac{3\theta}{4z} \int_0^\infty \frac{y\,\mathrm{d}y}{\mathrm{e}^{y^2/\theta-\eta}+1} \ln\left|\frac{z+y+\mathrm{i}v_l}{z-y+\mathrm{i}v_l}\right|, \tag{51}$$

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

$$\int_0^\infty \frac{t^{1/2}\mathrm{d}t}{\mathrm{e}^{(t-\eta)}+1} = \frac{2}{3}\theta^{-3/2}\ . \tag{52}$$

Thus we used in equation (27)

$$\Pi_{\mathrm{e}}(q,l) = n_{\mathrm{e}}\beta P_{\mathrm{e}}^0(z,l) \tag{53}$$

Table 2. The excess Coulomb interaction energy density (normalized to temperature) $f(\Gamma)$, and the results of the electronic liquid MC-simulation, equation (41).

$n_e(10^{24}\text{cm}^{-3})$	$T(10^5\text{K})$	Γ	θ	$f(\Gamma)$	$f_{\text{MC}}(\Gamma)$
0.258	1.715	1.00	1.00	–0.54	–0.62
1.610	6.315	0.5	1.09	–0.24	–0.29
1.611	1.579	2.0	0.27	–1.11	–1.38
$2.579 \cdot 10^5$	$1.715 \cdot 10^3$	0.10	0.10	–0.044	–0.11

for the electronic polarization operator and [22]

$$\Pi_i(z,l) = \beta n_i \delta_{l,0} \left(1 - \frac{\Gamma}{(12\pi^2)^{1/3}} \frac{G_i(z)}{z^2}\right)^{-1} \tag{54}$$

with

$$G_i(z) = \left\{b\left[\varepsilon_e(z,l)\right] + a/(2z)^2\right\}^{-1}, \tag{55}$$

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.

Using our data for the radial distribution function we calculated the excess Coulomb interaction energy density normalized to β, $f(\Gamma)$:

$$f(\Gamma) = \frac{1}{8}\frac{k_D^2}{k_F^2}\int_0^\infty (g_e(r) - 1)\; r\; dr \tag{56}$$

with $k_D^2 = 4\pi n e^2 \beta$. The results are given in table 2, where we also provided the corresponding values of $f_{\text{MC}}(\Gamma)$ of equation (41). Both estimates are closer in less degenerate electronic liquids.

Further studies of $g_e(0)$ should be carried out to include low-temperature and dynamic effects.

In addition, to improve the physical self-consistency of our approach, one needs the quantal EOS, either theoretical or numerical (obtained, e.g. within a quantum-statistical variant of the MC method), see, e.g. [28].

B. 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 [29]

$$\vec{J} = e^2 K_0 \vec{F} + T^{-1} e K_1 (-\vec{\nabla} T), \tag{57}$$

$$\vec{Q} = e K_1 \vec{F} + T^{-1} K_2 (-\vec{\nabla} T). \tag{58}$$

T is the plasma temperature and no magnetic effects are taken into account. The transport coefficients K_i $(i = 0, 1, 2)$ in equations (57) and (58) satisfy the Onsager relations [29] and within the same approximation instead of equation (18) we have

$$K_i = -\frac{4}{3m}\int_0^\infty E\rho(E)\tau(E)\frac{\mathrm{d}w(E)}{\mathrm{d}E}(E-\mu)^i\mathrm{d}E\ , \tag{59}$$

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

$$\sigma = e^2 K_0\ , \tag{60}$$

while the static thermal conductivity

$$\kappa = \frac{1}{T}(K_2 - K_1^2/K_0), \tag{61}$$

and the thermal electromotive potential

$$\alpha = K_1(eTK_0)^{-1}. \tag{62}$$

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

$$\frac{\kappa}{\sigma} = \frac{\pi^2}{3}\left(\frac{k_\mathrm{B}}{e}\right)^2 T. \tag{63}$$

If the degeneracy is incomplete, like in our case, there appear temperature-dependent corrections to equation (63). Nevertheless, these corrections under the conditions we consider are quite small [20].

References

1. Hansen J.P., McDonald I.R. Theory of Simple Liquids. London, Academic Press, 1976.
2. Hansen J.P., McDonald I.R. // Phys. Rev. A, 1981, vol. 23, p. 2041.
3. Dunn T., Broyles A.A. // Phys. Rev., 1967, vol. 157, p. 156; Pokrant M.A., Broyles A.A., Dunn T. // Phys. Rev. A, 1974, vol. 10, p. 379.
4. Yukhnovsky Yu.R. // Zh. Eksp. Teor. Fiz., 1958, vol. 34, p. 379 [Sov. Phys. JETP, 1958, vol. 34, p. 263] (and references therein).
5. Deutsch C. // Phys. Lett., 1977, vol. 60A, p. 317; Deutsch C., Gombert M.M., Minoo H. // Phys. Lett., 1978, vol. 66A, p. 381; 1977, vol. 72A, p. 481.
6. Adamyan V.M. et al. // Teplofiz. Vys. Temp., 1980, vol. 18, p. 241; Adamyan V.M., Tkachenko I.M. – In: Rep. II All-Union Conference "Electric Discharge in Liquids and its Applications", Kiev, Naukova Dumka, 1980, p. 72; Djuric Z. et al. // Phys. Lett., 1991, vol. 155A, p. 415; Adamyan V.M. et al. // J. Phys. D, 1994, vol. 27, p. 111; Adamyan V.M. et al. // J. Phys. D, 1994, vol. 27, p. 927; Tkachenko I.M., Fernández de Córdoba P. // Phys. Rev. E, 1998, vol. 57, p. 2222.
7. Tkachenko I.M., Fernández de Córdoba P. // Contrib. Plasma Phys., 1999, vol. 39, p. 131.

8. Stringfellow G.S., DeWitt H.E., Slattery W.L.S. // Phys. Rev. A, 1977, vol. 60A, p. 317.
9. Abe R. // Progr. Theor. Phys., 1959, vol. 21, p. 475.
10. Edwards S.F. // Philos. Mag. 1977, vol. 3, p. 1020.
11. Ichimaru S. // Statistical Plasma Physics. Vol. I. Addison-Wesley, Reading, MA, 1991.
12. Abrikosov A.A., Gor'kov L.P., Dzyaloshinskii I.E. Quantum Field Methods in Statistical Physics. Moscow, GIFML, 1962 (in Russian).
13. Spitzer L. Jr. Physics of Fully Ionized Gases. New York, Interscience, 1962.
14. Ziman J.M. Theory of Solids. London, Cambridge University Press, 1972.
15. Boercker D.B., Rogers F., DeWitt H.E. // Phys. Rev. A, 1959, vol. 25, p. 1623.
16. Redmer R. // Phys. Rep., 1997, vol. 282, p. 35.
17. Yuan J.K., Sun Y.S., Zhang S.T. // Phys. Rev. E., 1996, vol. 53, p. 1059.
18. Nardi E. // Phys. Rev. E, 1996, vol. 54, p. 1899.
19. Reinholz H., Redmer R., Nagel S. // Phys. Rev. E, 1995, vol. 52, p. 5368.
20. Tkachenko I.M., Fernández de Córdoba P., Solís B., Zubía P. – In: 24th EPS Conf. on Contr. Fusion and Plasma Phys., Berchtesgaden, Germany, 1997. Europhysics Conference Abstracts, 1997, vol. 21a, part III, p. 1377; Tkachenko I.M., Fernández de Córdoba P. – In: Strongly Coupled Coulomb Systems. Edited by G.J. Kalman, J.M. Rommel, and K.Blagoev, New York, Plenum Press, p. 561.
21. Adamyan S.V., Tkachenko I.M., Muñoz-Cobo González J.L., Verdú Martín G. // Phys. Rev. E, 1993, vol. 48, p. 2067.
22. Ichimaru S. Statistical Plasma Physics. Vol. II: Condensed Plasmas. Addison-Wesley, 1994.
23. Tkachenko I.M. // Europhys. Lett., 1989, vol. 9, p. 351; Tkachenko I.M., Fernández de Córdoba P., Urrea M. // J. Phys. A., 1996, vol. 29, p. 2599; Tkachenko I.M, Fernández de Córdoba P., Belda J.M. – In: Strongly Coupled Coulomb Systems. Edited by G.J. Kalman, J.M. Rommel, and K. Blagoev, New York, Plenum Press, p. 479; Tkachenko I.M., Alcober J., Fernández de Córdoba P. // J. Physique, 2000, vol. 10, p. Pr5-199.
24. Shaw R.W. // J. Phys. C, 1970, vol. 3, p. 1140.
25. Kimball J.C. // Phys. Rev. A, 1973, vol. 7, p. 1648; Phys. Rev. B, 1976, vol. 14, p. 2371.
26. Chabrier G., Potekhin A.Y. // Phys. Rev. E, 1998, vol. 58, p. 4941.
27. Arista N.R., Brandt W. // Phys. Rev. A, 1981, vol. 29, p. 1471.
28. Stolzmann W., Blöcker T. // Phys. Lett. A, 1996, vol. 221, p. 99; Astron. Astrophys., 1996, vol. 314, p. 1024; Stolzmann W., Rösler M. Physics of Strongly Coupled Plasmas. eds. W.D. Kraeft, M. Schlanges, Singapore, World Scientific, 1996, p. 87; Rösler M., Stolzmann W. Physics of Strongly Coupled Plasmas. eds. W.D. Kraeft, M. Schlanges, Singapore, World Scientific, 1996, p. 91.
29. Hochstim A.R. Kinetic Processes in Gases and Plasma. New York, Academic, 1969, chap. 6.

Лінійний статичний відгук модельної плазми та ефективний потенціал Юхновського-Кельбга-Дойча

В.М.Адамян [1], І.М.Ткаченко [2]

[1] Одеський державний університет, кафедра теоретичної фізики, 65026 Одеса

[2] Валенсійський політехнічний університет, кафедра прикладної математики, 46071 Валенсія, Іспанія

Отримано 7 червня 2000 р.

На основі уявлень про самоузгоджене внутрішньоплазмове поле пропонується методика обчислення коефіцієнтів переносу у повністю іонізованій густій плазмі. Ця методика прямо не використовує ані кінетичне рівняння, ані параметри підгонки. Порівняння отриманих результатів з даними комп'ютерного моделювання параметрів густої майже класичної воднево-подібної плазми показує, що використання з самого початку ефективного парного потенціалу Юхновського-Кельбга-Дойча замість кулонівського може до певної межі компенсувати похибки простіших стандартних наближень квантової теорії багатьох заряджених частинок.

Ключові слова: *воднева плазма, транспортні коефіцієнти, парні потенціали*

PACS: *52.25.Fi, 52.25.Ub, 52.65.-y*