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Linear electronic transport in dense plasmas. I. Specific features of Boltzmann-Ziman formalism within the Lorentzian approximation

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Résumé. — Cet article est le premier d'une série consacrée à l'étude systématique du transport électronique linéaire dans les plasmas denses fortement couplés, comportant plusieurs espèces ioniques classiques plongées dans un jellium électronique fortement dégénéré. Le formalisme retenu, spécialisé ici au cas des coefficients thermoélectroniques et du transport mécanique (viscosité), repose pour l'essentiel sur l'extension de la théorie de Boltzmann-Ziman, dans le cadre de l'approximation Lorentzienne. Les conditions de validité de cette dernière sont largement développées, et l'accent mis sur les corrections de température finies et les corrections inélastiques. Les coefficients de transport sont exprimés analytiquement sous forme de quantités réduites, à la fois dans le cas élastique et inélastique, respectivement au moyen des solutions exactes et variationnelles de l'équation de transport. Ceci permet un calcul simplifié des corrections précédemment mentionnées, calcul qui sera détaillé dans l'article II de cette série. Finalement, nous démontrons la validité de la méthode en reproduisant, dans les limites appropriées, les formules de Ziman et d'Edwards pour la résistivité, ainsi que d'autres résultats bien connus.

Abstract. — This is the first paper in a series devoted to a systematic investigation of linear electronic transport properties in strongly coupled plasmas consisting of a multicomponent and classical ionic mixture embedded in a highly degenerate electron jellium. The basic formalism rests upon suitable extensions of the Boltzmann-Ziman theory as explained in this work. It is hereafter specialized in a thorough investigation of thermoelectronic and mechanical transport coefficients. Validity conditions for the Lorentzian approximation are first carefully examined. High temperature and inelastic corrections are emphasized. Basic transport quantities are expressed under an analytic and compact form both in the elastic and inelastic cases, through exact and variational solutions of the transport equation, respectively. This allows for an easy algebraic treatment of finite degeneracy and inelastic corrections, to be given in the next paper II in this series. Finally, the validity of the method is demonstrated by recovering Ziman's and Edwards' resistivity formula, and other well-known results, in the appropriate limits.

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1. Introduction.

Equilibrium and transport properties in very dense and strongly coupled plasmas consisting of a fully or partially ionized multicomponent ionic mixture interacting through the (screened) Coulomb potential and embedded in a highly degenerate electron jellium, play a central role in several areas of Statistical Mechanics [1], Astrophysics [2, 3] and Liquid Metals Theory [4]. As a particular and very important example, let us mention the determination of equation of state and transport properties of the strongly coupled hydrogenic binary ionic mixture H⁺-He²⁺ retained to model the Jovian planets interior [2, 3]. Recently, we have already investigated [1] the critical demixing properties of such systems, which were assumed in this case to be in thermodynamical equilibrium. Basically, the key parameters in such analysis are the classical ion plasma parameter Γ , and the degenerate electron jellium parameter r_{s} . This paper is devoted to a systematic investigation of linear and electronic transport properties within a Lorentzian framework. This one is especially well-suited to a modelling of the interaction between a nearly fully degenerate electron jellium and ion density fluctuations. This interaction constitutes the very basis for the evaluation of all transport quantities. Moreover the superposition of a fully degenerate electron gas to a strongly coupled ion fluid is also central to building up the so called Binary Ionic Mixture model (BIM) [5] where the dynamic and static properties of the classical ion plasma are decoupled from a mechanically rigid and neutralizing electron background. Focusing attention on the electron component, let us notice that its complete degeneracy allows a safe neglect of the electron-electron interaction. This allows a simplified but accurate treatment of transport properties within a Lorentzian approximation to the Boltzmann equation [6] which has already been extensively applied to the one component plasma (OCP) model [7a, b]. The main formal characteristics of this Boltzmann-Ziman (BZ) formalism relies upon simple expressions for time-independent transport quantities. These simple expressions essentially consist of single quadratures of electron-ion effective interactions factorized out by ion structure factors. The latter are generally deduced from the nonlinear hypernetted chain (HNC) scheme extensively used in the study of static and transport properties [1, 5, 7b].

Having in mind a thorough investigation of finite temperature and inelastic contributions (Paper II) to the standard elastic scattering at T = 0, we detail at length in section 2 the various parameters used in this analysis. Finite degeneracy and inelastic effects, parametrized respectively with $\alpha = T/T_F$ (T_F , Fermi temperature) and $\tilde{\omega} = \beta \hbar \omega$ ($\beta = 1/k_B T$), are shown to act significantly in well-decoupled domains A and B of the Γ - r_s plane, which will allow a further separate analysis of the previously mentioned contributions. In section 3, we review the standard BZ formalism [6], hereafter specialized to a Lorentz gas interacting weakly with a multicomponent ionic mixture. The investigated transport quantities include electric and thermal conductivities, as well as the corresponding thermopower and the (mechanical) shear viscosity. The bulk viscosity is seen to have an identically zero value in a Lorentz gas.

Section 4 is devoted to a thorough dimensional investigation of the various transport quantities of present concern. The latter are expressed in terms of basic reduced quadratures, both in the purely elastic case (Sect. 4.2) where exact solutions of the transport equation are available, and in the inelastic case (Sect. 4.3) where only approximate solutions may be derived from the variational principle [6]. The significant contribution played by a number of suitable Γ - r_s -dependent prefactors is emphasized. In both elastic and inelastic situations, we consider briefly the limiting $\alpha \ll 1$ and $\tilde{\omega} \ll 1$ cases, in view of evaluating finite degeneracy and inelastic corrections to electron transport in terms of α^2 and $\tilde{\omega}^2$ expansions respectively (Paper II). The latter necessitates the underlying calculation of dimensionless quadratures $\langle \hat{\eta}^n \rangle_0$ and $\langle \hat{\eta}'^n \rangle_1$ explained in this work. Our methodology is applied in section 4.2.2 to the simultaneous $\alpha \to 0$ and $\tilde{\omega} \to 0$ limits, giving back straightforwardly the well-known Ziman resistivity formula [6], the standard Lorentz number as well as classical thermopower and shear viscosity expressions. Finally (Sect. 4.3.3), we intend to make a connection between the variational approach and exact elastic transport calculations. For that purpose, we focus our attention on some variational transport quantities computed with monomial trial functions in the appropriate $\tilde{\omega} \to 0$ limit. We show that Edwards' resistivity formula [8] as well as some other transport expressions, belong to that specific class of solutions.

2. The Lorentz model.

2.1 NOTATIONS. — We consider a multicomponent mixture built of degenerate electrons and ν_s ion species subindexed with ν , enclosed in the total volume V of a connex domain. Each ion species is assumed to be fully or only partially ionized and endowed with atomic number Z_{ν}^{A} , effective charge $-Z_{\nu}e$ (e denotes the electron charge), mass M_{ν} and particle number N_{ν} . Conventionally, $\nu = 1$ refers to the smallest charge. The neutralizing background is of opposite sign and contains N_e nearly free electrons. Electroneutrality thus reads as $N_e = \bar{Z}N_i$ where $N_i = \sum_{\nu} N_{\nu}$ and $\bar{Z} = \sum_{\nu} c_{\nu} Z_{\nu}$ is the mean valence. More generally, the

average by concentration number of a given quantity X will be defined as

$$\overline{X^{\mathrm{m}}} = \sum_{\nu} c_{\nu} X^{\mathrm{m}}_{\nu} .$$
(2.1)

The ionic component is characterized by the densities $n_i = \lim_{V \to \infty} N_i/V$ and $n_v = \lim_{V \to \infty} N_v/V$. The partial concentration numbers are $c_v = N_v/N_i$ and fulfill the constraint $\sum_{v} c_v = 1$. We choose the ion sphere radius $a_i = [3/(4 \pi n_i)]^{1/3}$ as a convenient unit of length and we define the classical plasma parameter as $\Gamma = \beta e^2/a_i$. The quantum jellium, endowed with electron density $n_e = \lim_{v \to \infty} N_e/V$, is parametrized with $r_s = a_e/a_0$ where a_0 is the Bohr radius and

 $a_{\rm e} = [3/(4 \pi n_{\rm e})]^{1/3} \equiv a_{\rm i}/\bar{Z}^{1/3}$ is the electron sphere radius. This unit of length allows to define $\Gamma' = \beta e^2/a_{\rm e}$ as another plasma parameter. The effective strength of the plasma coupling is measured by $\Gamma_{\rm eff} = \Gamma Z_{\rm eff}^2$. By reference to the ion-sphere model of Salpeter [9], the effective quadratic charge $Z_{\rm eff}^2$ can be chosen as (Ref. [10]) $Z_{\rm eff}^2 = \bar{Z}^{1/3} \overline{Z}^{5/3}$.

Throughout this paper, λ will stand for the numerical constant $(9 \pi/4)^{1/3}$. We will denote by $z_{\nu} = Z_{\nu}/\bar{Z}$ a reduced charge number. Also, it will prove convenient to deal with the variables :

$$\hat{\alpha} = \pi \alpha / 2, \quad \hat{\omega} = \tilde{\omega} / 2 \pi, \quad \hat{\eta} = \eta / \pi, \quad \hat{\eta}' = \hat{\eta} - \hat{\omega}, \quad (2.2)$$

which will be detailed in the sequel. Transport quantities investigated in this work will be measured in atomic unit (a.u.), namely $\sigma_0 = e^2/a_0 \hbar = 4.60 \times 10^4 \Omega^{-1} \mathrm{cm}^{-1}$ and $\eta_0 = \hbar/a_0^3 = 7.12 \times 10^{-3}$ poise, for electrical conductivity and viscosity respectively.

2.2 VALIDITY CRITERIA FOR THE LORENTZIAN APPROXIMATION. — As previously stated, we restrict ourselves to the case of a classical and strongly coupled ionic component

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interacting weakly with a highly degenerate electron jellium. The latter assumption is written in terms of the degeneracy parameter α as

$$\alpha \equiv \frac{k_{\rm B} T}{E_{\rm F}} = \frac{2}{\lambda^2} \frac{r_{\rm s}}{\Gamma'} \equiv 0.54 \frac{r_{\rm s}}{\Gamma'} \ll 1 , \qquad (2.3)$$

so that $T(\mathbf{K}) \ll 6 \times 10^5 r_s^{-2}$. E_F stands for the Fermi energy of the jellium which can be treated nonrelativistically as long as $E_F/m_e c^2 \ll 1$, i.e., $r_s \gg 10^{-2}$ (m_e , electron mass).

The weak coupling hypothesis (WCH) is ensured when $E_{\rm F}$ remains larger than the (absolute) coulombic e⁻-ion energy. This can be readily expressed by evaluating the latter for each ion-species in a neutral sphere of radius $a'_{\nu} = [3 Z_{\nu}/(4 \pi n_{\rm e})]^{1/3}$ and next performing the c_{ν} average according to (2.1). This yields :

$$\frac{3}{2}\overline{Z_{\nu} e^2/a'_{\nu}} \le E_{\rm F} \Rightarrow r_{\rm s} \le \frac{\lambda^2}{3} \overline{Z}^{-2/3} = 1.23 \ \overline{Z}^{-2/3} \tag{2.4}$$

which typically restricts r_s to be lower than unity in the hydrogen-helium mixture. Alternatively, the WCH can be implemented as an adequate criterion validating the first Born approximation in the calculation of the e⁻-ion scattering cross-section. For our purpose, and following Stevenson and Ashcroft [11], we write it in the form $\sigma_{app}/4 \pi a^2 \leq 1$, where the « geometrical » cross-section $4 \pi a^2$ is evaluated with the characteristic Thomas-Fermi screening length $\lambda_{TF} = (6 \pi n_e e^2/E_F)^{-1/2}$ while σ_{app} , the apparent cross-section per ion, is defined by the identity :

$$n_i \sigma_{app} v_F \tau \equiv 1 \quad (v_F = \text{Fermi velocity}).$$
 (2.5)

An obvious estimate for the time relaxation τ is provided by the standard expression $\sigma = n_e e^2 \tau / m_e$ for the electric conductivity. We thus arrive at $\sigma / \sigma_0 \ge \overline{Z} / \pi^2$, i.e., just a lower bound for σ . A more suitable conclusion can however be reached, by making use of the following reduced expression for the well-known Ziman resistivity formula *including the Born approximation*, detailed in section 4:

$$\rho / \rho_0 = \frac{16}{9} r_s^3 \bar{Z} I_1^0 \text{ with } \rho_0 = \sigma_0^{-1}.$$
 (2.6)

This yields

$$r_{\rm s} \leq \left(\frac{9\pi^2}{16}\right)^{1/3} (I_1^0)^{-1/3} \bar{Z}^{-2/3} = \frac{1.77}{\bar{Z}^{2/3}} (I_1^0)^{-1/3}, \qquad (2.7)$$

which *formally* corresponds to inequality (2.4). As we shall see, this assertion is corroborated by the fact that the basic dimensionless quadrature I_1^0 entering in Ziman's formula (2.6), a) remains close to unity, b) only involves ion charges under their reduced form z_{α} and c) also exhibits a *smooth* r_s variation (¹). Moreover, additional constraints such as a) the electron

^{(&}lt;sup>1</sup>) An upper-bound for I_1^0 can be crudely derived with $V(x) = (x^2 + 0.166 r_s)^{-1}$, the Thomas-Fermi potential, and $S(x) = \overline{Z}^2$, the asymptotic limit of structure factor S(x). This provides $I_1^0 \ge (\overline{Z}^2/2) \ln (1 + 6.02/r_s)$ which varies only from 2.86 to 0.40 times \overline{z}^2 within the full range $0.02 \le r_s \le 5$.

jellium remains only weakly polarized by ion density fluctuations, namely $\lambda_{TF} \ge \overline{a_{\nu}}$, and b) the electron mean free path $\lambda_e = v_F \tau$ is large in comparison with a_i , also agree with (2.4) or (2.7) endowed with a $\overline{Z}^{-2/3}$ factor. We are thus led to conclude that in addition to the previous (2.3), inequality (2.7) provides *a correct criterion* for the Lorentzian approximation, including the Born one.

Looking at the thermodynamical coherence of the Lorentz model through the requirement $p \simeq p_e + p_i \ge 0$ also provides another upper-bound for r_s (Ref. [1b]), which amounts to $r_s \le (0.206 + 0.405 \ \overline{Z^{5/3}}/\overline{Z})^{-1}$, i.e., $r_s \le 1.6$ for pure H and $r_s \le 1.2$ for pure He. Negative pressure for non-negligible jellium correlations (typically $r_s \sim 1.5$) can thus arise at large He concentration. This is a warning that a polarized background should be introduced within the so-called polarized BIM model (PBIM) (Ref. [1]) in lieu of the rigid BIM one.

The conditions derived above form the very basis for the Lorentz model under investigation. It should be appreciated however that they do not match the condition that atomic nuclei get completely stripped of their orbital electrons, especially at large Z values. The latter requirement can be roughly derived by demanding the electronic pressure $p_e \sim 2/5 n_e E_F$ to be large enough for pressure ionization to hold:

$$p_{\rm e}(a_0/Z_{\nu})^3 \ge Z_{\nu}^2 e^2/2 a_0 \Rightarrow r_{\rm s} \le \left(\frac{2}{15 \pi^2}\right)^{1/5} \frac{\lambda}{Z_{\nu}} = 0.81/Z_{\nu} .$$
 (2.8)

Even in the deep fluid interior of giant planets such as, say Jupiter, where (Ref. [12]) $r_s \approx 0.85$, $\Gamma_{\text{eff}} \approx 45$ and $c_1 \approx 0.9$, condition (2.8) indicates that the heaviest (helium) component may be only partially ionized.

Turning to the ion component properties, we inquire for ion departure from their classical behaviour, a feature which plays an important role within the BZ transport formalism, due to the enhancement of inelastic electron-ion scattering processes at the Fermi surface. The latter are usually measured by

$$y = \frac{\beta \hbar^2 k_{\rm F}^2}{2 \bar{M}} \equiv \frac{\lambda^2}{4 \pi} \overline{Z^{2/3}} \,\delta^2 \equiv \alpha^{-1} \frac{m_{\rm e}}{\bar{M}}, \qquad (2.9)$$

where $k_{\rm F} = (2 \, m_{\rm e} \, E_{\rm F})^{1/2} / \hbar$ is the Fermi wavevector while $\delta = \Lambda / a_{\rm i}$ defines a « one-fluid » parameter with $\Lambda = [\beta h^2 / (2 \pi \overline{M})]^{1/2}$, the average thermal De Broglie wavelength. A detailed analysis (Paper II) shows that inelastic scattering contributions to the BZ formalism are to be measured in $\Gamma y / 10$ units. For our purpose, the classical ion range is thus well-characterized by $y \ll 1$ for $\Gamma < 10$ and $y \ll 10/\Gamma$ for $\Gamma \ge 10$. Finally, the OCP fluid-solid transition [13] also provides the upper bound $\Gamma_{\rm eff} \le 171$, i.e., $\Gamma \le 171$ for pure H and $\Gamma \le 42.75$ for pure He.

The various Γ - r_s domains featuring the overall inequalities described above are pictured in figure 1, in the case of a 90 % H-10 % He mixture corresponding to Jupiter's deep interior. Inelastic contributions are expected to act significantly in domain B. Hopefully, this latter appears well-decoupled from domain A where finite degeneracy (α -dependent) corrections to the T = 0 jellium play an important role. This decoupling is the most conspicuous by-product of the present analysis. It allows us to treat the corresponding transport formalism separately, with a significant simplification of the required algebras. Those are explained in section 4 of this paper and will be worked out in the following paper II in this series.



Fig. 1. — Γ - r_s plane for the H⁺-He²⁺ mixture at $c_2 = 0.1$ (10 % He), corresponding to the deep-fluid interior of Jupiter. Finite degeneracy and inelastic electron-ion scattering effects get significantly enhanced in domains A and B respectively.

3. Boltzmann-Ziman transport theory.

Let us consider a jellium fluid submitted to an external electric field & and a thermal gradient ∇T . We also introduce the local and macroscopic velocity $\mathbf{v}(\mathbf{r}, t)$ of the ionic component with respect to the observer in order to account for viscosity effects $\sim \nabla \mathbf{v}$. The $\mathbf{v} \to 0$ limit taken at the end will ensure that we get the correct limit for transport coefficients in a frame where the ions are at rest. In agreement with the Lorentzian approach, nearly-free electron states are represented by plane waves of energy $E_k = \hbar^2 k^2/(2m_e)$ and velocity $\mathbf{v}_k = \hbar k/m_e$. Then, electron transport can be worked out through the linearized Boltzmann equation :

$$-\frac{\partial f_{e}^{0}}{\partial E_{k}}\left(\left(E_{k}-\mu_{e}\right)\mathbf{v}_{k}\cdot\frac{\nabla T}{T}-e\mathbf{v}_{k}\cdot\mathbf{E}+m_{e}(\mathbf{v}_{k}\mathbf{v}_{k}):\overline{\mathbf{\Lambda}}\right)=\mathfrak{I}_{\mathrm{lin}}(\boldsymbol{\Phi}(\mathbf{k})),\qquad(3.1a)$$

$$\mathfrak{J}_{\mathrm{lin}}(\boldsymbol{\Phi}(\mathbf{k})) = \boldsymbol{\beta} \sum_{\mathbf{p}} \left[\boldsymbol{\Phi}(\mathbf{p}) - \boldsymbol{\Phi}(\mathbf{k}) \right] \boldsymbol{\Gamma}_{0}(\mathbf{k} \to \mathbf{p}), \qquad (3.1b)$$

$$\Gamma_0(\mathbf{k} \to \mathbf{p}) \equiv f_{e}^0(k) [1 - f_{e}^0(p)] F(\mathbf{k} \to \mathbf{p}).$$
(3.1c)

Function $\Phi(\mathbf{k})$ within the collision term provides a standard linear estimate $f_e \approx f_e^0 - \Phi(\mathbf{k})(\partial f_e^0/\partial E_k)$ for the true electronic distribution f_e in terms of the Fermi function f_e^0 .

The e⁻-ion transition probability per unit time $F(\mathbf{k} \rightarrow \mathbf{p})$ computed in the first Born approximation can be written in a convenient compact form $(q = |\mathbf{k} - \mathbf{p}|)$:

$$F(\mathbf{k} \to \mathbf{p}) = \frac{2 \pi}{N_{\rm i} \hbar} \int_{-\infty}^{+\infty} \mathrm{d}\omega \,\,\delta\left(E_k - E_p - \hbar\omega\right) \,\hat{V}^2(q) \,S(q,\,\omega)\,. \tag{3.2}$$

Here we define $\hat{V}(q)$ as an obvious linear combination

$$\hat{V}(q) = \sum_{\nu=1}^{\nu_{s}} c_{\nu} \, \hat{V}_{\nu}(q) \,, \qquad (3.3)$$

of the screened electron-ion pseudopotentials $\hat{V}_{\nu}(q) \equiv \hat{U}_{\nu}(q)/\varepsilon(q)$ (Ref. [4]), including a static limit of the jellium dielectric function $\varepsilon(q) = \lim_{\omega \to 0} \varepsilon(q, \omega)$. Hence the «one-fluid »

structure factor $S(q, \omega)$ reads as :

$$\hat{V}^{2}(q) S(q, \omega) = \sum_{\mu\nu=1}^{s} (c_{\mu} c_{\nu})^{1/2} \hat{V}_{\mu}(q) \hat{V}_{\nu}(q) S_{\mu\nu}(q, \omega).$$
(3.4)

The $S_{\mu\nu}$'s stand for partial ion-ion structure factors which are double Fourier transforms of *t*-dependent correlation functions [10]. The physical meaning of definitions (3.3) and (3.4) becomes clear in the coulombic case where the ν -dependence is only contained within the charge number Z_{ν} . This yields

$$\hat{V}(q) = -\frac{4\pi \bar{Z}e^2 n_{\rm i}}{q^2 \varepsilon(q)}$$
(3.5)

and

$$S(q, \omega) \equiv S_{zz}(q, \omega) = \sum_{\mu\nu=1}^{\nu_s} (c_{\mu} c_{\nu})^{1/2} z_{\mu} z_{\nu} S_{\mu\nu}(q, \omega).$$
(3.6)

 $S_{zz}(q, \omega)$ corresponds to the reduced charge density-charge density structure factor with the emergence of reduced valences $z_{\nu} = Z_{\nu}/\bar{Z}$, previously defined in section 2.1.

The neglect of e^-e^- collisions within $F(\mathbf{k} \to \mathbf{p})$ (Eq. (3.2)) has obviously no practical incidence in the calculation of electric conductivity. However, turning to the thermal conductivity, we already know from Lampe's analysis [15] that electronic interactions within a partially degenerate electron-jellium could lower it by an amount of 25-50 %! This is a warning that linear transport theory within a Lorentzian framework has to be *strictly* restricted to its range of applicability, delineated by inequalities (2.3) and (2.7).

Linearized transport equation (3.1) plays a fundamental role in assessing thermoelectronic and viscosity transport. $\mathbf{E} = \delta - \nabla \mu_{e}/e$ behaves like an effective electric field. Another possible choice, among others, reads as (Ref. [14b], Sect. 3.2) $\mathbf{E}' = \delta - (\nabla \mu_{e})_{T}/e$ where the gradient operator is taken at constant temperature. Then μ_{e} within equation (3.1a) has to be replaced by h_{e} , enthalpy per electron. $\overline{\Lambda}$ corresponds to the *symmetrical* and *traceless* part in $\nabla \mathbf{v}$. As in the classical case [14], the viscosity term does not exhibit an independent contribution ~ div v. Consequently, the bulk viscosity [16] is seen to have an identically zero value to all orders in the degeneracy parameter. This result can be proved on a rigorous basis [1b] through a Chapman-Enskog-like treatment of the transport equation (3.1) belonging to quantum Lorentz gases. It extends a previous and similar conclusion already obtained by Abrikosov and Khalatnikov [17] at order $\alpha = 0$ within the context of the Landau theory for quantum liquids, and it agrees with the neglect of e^-e^- interactions.

Entropy production arising from all processes dissipating energy is readily deduced by factorizing out (3.1a) with $-\Phi(\mathbf{k})$ and next performing the sum on \mathbf{k} (Ref. [6]). One gets

$$\sigma_{s} = \frac{\beta}{2 T V} \sum_{\mathbf{k}} \left[\boldsymbol{\Phi}(\mathbf{k}) - \boldsymbol{\Phi}(\mathbf{p}) \right]^{2} \Gamma_{0}(\mathbf{k} \to \mathbf{p}) = \frac{\mathbf{J} \cdot \mathbf{E}}{T} + \mathbf{U} \cdot \nabla \frac{1}{T} - \frac{\mathbf{\bar{\Pi}}}{T} : \mathbf{\Lambda} , \qquad (3.7)$$

with

$$\mathbf{J} = \frac{e}{V} \sum_{\mathbf{k}} \mathbf{v}_{k} \left(-\frac{\partial f_{e}^{0}}{\partial E_{k}} \right) \boldsymbol{\Phi}(\mathbf{k}), \qquad (3.8a)$$

$$\mathbf{U} = \frac{1}{V} \sum_{\mathbf{k}} \mathbf{v}_k (E_k - \boldsymbol{\mu}_e) \left(-\frac{\partial f_e^0}{\partial E_k} \right) \boldsymbol{\Phi}(\mathbf{k}), \qquad (3.8b)$$

$$\overline{\overline{\Pi}} = \frac{m_{\rm e}}{V} \sum_{\mathbf{k}} \left(\mathbf{v}_k \, \mathbf{v}_k - \frac{1}{3} \, \mathbf{v}_k^2 \, \mathbf{I} \right) \left(-\frac{\partial f_{\rm e}^0}{\partial E_k} \right) \, \boldsymbol{\Phi}(\mathbf{k}) \,. \tag{3.8c}$$

Equations (3.8) provide the required microscopic expressions for electric and heat-flux currents and the stress tensor, respectively. Supplementing transport equation (3.1a), they will allow us to determine thermoelectronic coefficients and the shear viscosity. This is achieved by comparing them with their phenomenological homologues detailed in the next section.

4. Basic transport quantities.

4.1 GENERAL. — Linear transport coefficients are defined by [6, 16]

$$\mathbf{J} = L_{\mathrm{EE}} \,\mathbf{E} + L_{\mathrm{ET}} \,\nabla T \,, \tag{4.1a}$$

$$\mathbf{U} = L_{\mathrm{TE}} \mathbf{E} + L_{\mathrm{TT}} \nabla T, \qquad (4.1b)$$

$$\bar{\Pi} = -2 \eta_s \bar{\Lambda} \qquad \eta_s = \text{shear viscosity}, \qquad (4.1c)$$

 $L_{ee} \equiv \sigma$ corresponds to the electric conductivity at constant temperature while the thermal conductivity is defined by $\mathbf{U} = -K\nabla T$ with $\mathbf{J} = 0$, which implies $K = -(L_{\text{TT}} - L_{\text{TE}} L_{\text{ET}}/L_{\text{EE}})$. Crossed quantities L_{TE} and L_{ET} fulfill Onsager's relation [14b], $L_{\text{TE}} = -TL_{\text{ET}}$. The Lorentz number \mathfrak{L} relates the thermal and electrical conductivities through $K = \mathfrak{L}T\sigma$. Finally, the thermopower is defined as $Q = -L_{\text{ET}}/L_{\text{EE}}$.

Phenomenological equations (4.1a-b) hold for the effective electric field $\mathbf{E} = \delta - \nabla \mu_e/e$ retained throughout this work. With the alternative definition $\mathbf{E}' = \delta - (\nabla \mu_e)_T/e$, the thermal current (4.1b) contains an additional term $(\mathbf{J}/e)(Ts_e)$ with s_e , entropy per electron; thus σ and K remain unchanged but Q must be replaced by $Q' = Q - (s_e/e)$.

4.2 LINEAR TRANSPORT IN THE ELASTIC CASE. — We intend to solve linearized transport equation (3.1a) in the standard limit where electrons are elastically scattered by ionic density fluctuations. The actual content of elastic diffusion is the following: through successive collisions, the electron absorbs as much energy as it reemits. It is then sufficient to put $\tilde{\omega} = \beta \hbar \omega \rightarrow 0$, in agreement with the electron-ion cross section proportional to $S(q, \omega)$ (Eq. (3.4)). Also, it should be kept in mind that in the $\tilde{\omega} \rightarrow 0$ limit, $S(q, \omega)$ as well as the $S_{\mu\nu}(q, \omega)$'s remain symmetric under $\omega \rightarrow -\omega$, in agreement with the principle of detailed balancing. As a consequence, emission or absorption of a quantum $\hbar \omega$ is equally likely to occur. With these premises taken into account, one gets

$$\lim_{\tilde{\omega} \to 0} \Gamma_0(\mathbf{k} \to \mathbf{p}) = -\frac{\partial f_e^0}{\partial E_k} \frac{2 \pi}{N_i \hbar \beta} \,\delta\left(E_k - E_p\right) \,\hat{V}^2(q) \,S(q) \,, \tag{4.2}$$

for the basic $\Gamma_0(\mathbf{k} \to \mathbf{p})$ expression which actually depends on the static (classical) « one fluid » structure factor :

$$S(q) = \int_{-\infty}^{+\infty} d\omega \ S(q, \omega) .$$
 (4.3)

Equation (3.1a) also shows how intertwined the vectorial thermoelectronic coefficients are with the order 2 tensorial shear viscosity. So, one is entitled to write $\Phi(\mathbf{k}) = \Phi_1(\mathbf{k}) + \Phi_2(\mathbf{k})$ where functions $\Phi_1(\mathbf{k})$ and $\Phi_2(\mathbf{k})$ correspond to separate solutions for thermoelectric and mechanical transport respectively. Within the elastic limit, those can be derived exactly because collision term (4.2) relates only **p** states located on k sphere. Therefore $\Phi_1(\mathbf{k})$ and $\Phi_2(\mathbf{k})$ may be written as

$$\boldsymbol{\Phi}_{1}(\mathbf{k}) = -\tau_{1}(k) \left(\left(E_{k} - \boldsymbol{\mu}_{e} \right) \mathbf{v}_{k} \cdot \frac{\nabla T}{T} - e \mathbf{v}_{k} \cdot \mathbf{E} \right), \qquad (4.4a)$$

$$\boldsymbol{\Phi}_{2}(\mathbf{k}) = -\tau_{2}(k) \left(m_{\mathrm{e}} \, \mathbf{v}_{k} \, \mathbf{v}_{k} : \overline{\mathbf{\Lambda}} \right), \tag{4.4b}$$

with generalized relaxation times $\tau_1(k)$ and $\tau_2(k)$ depending only on k. There is no need for two distinct relaxation times in E and ∇T respectively, because $(E_k - \mu_e)$ remains constant on k sphere. A similar reasoning would have easily convinced us that a hypothetical bulk viscosity term $\sim f(E_k - \mu_e)$ div v, where f is a given scalar function, should lead to a vanishing elastic contribution.

Upon replacing formal solutions (4.4) in equation (3.1a) yields after straightforward identifications:

$$\tau_1^{-1}(k) = \frac{4 m_{\rm e} k}{\pi n_{\rm i} \hbar^3} \int_0^{2k} \frac{\mathrm{d}q}{2k} \left(\frac{q}{2k}\right)^3 \hat{V}^2(q) S(q) , \qquad (4.5a)$$

$$\tau_2^{-1}(k) = \frac{4 m_{\rm e} k}{\pi n_{\rm i} \hbar^3} \int_0^{2k} \frac{\mathrm{d}q}{2k} \left(\frac{q}{2k}\right)^3 \left[3 - 3\left(\frac{q}{2k}\right)^2\right] \hat{V}^2(q) S(q) , \qquad (4.5b)$$

 $\tau_1^{-1}(k)$ is nothing but the well-known Ziman-like [6] integrant extending to a running upper bound, while $\tau_2^{-1}(k)$ taken in the $k \to k_F$ limit does the same for Baym's viscosity formula [18] in the elastic case.

4.2.1 Reduced quantities and methodology. — Bearing in mind a thorough investigation of α dependent contributions to the electronic transport (domain A of Fig. 1), it appears useful at this stage to re-express (4.4) and (4.5) in a reduced form especially well suited for further algebraic analysis and numerical integration. This will also prove convenient for investigating inelastic corrections, as is detailed in section 4.3. First, let us introduce the dimensionless variables

$$x = \frac{q}{2k_{\rm F}}, \quad t = \frac{k}{k_{\rm F}}, \quad \eta = \beta \ (E_k - \mu_{\rm e}) \ . \tag{4.6}$$

t has to be taken as a function of η and $\alpha = T/T_{\rm F}$

$$t \equiv (\eta \alpha + \gamma)^{1/2}$$
 with $\gamma \equiv \mu_e/E_F$. (4.7)

With the help of the dimensionless variable x, the effective interaction $\hat{V}(q)$ (Eqs. (3.3) and (3.5)) now reads as

$$\hat{V}(q) = -\frac{3}{4\lambda^2} \frac{e^2}{a_0} \frac{1}{r_s} V(x) .$$
(4.8)

The jellium dielectric function $\varepsilon(x)$ within V(x) depends solely on x. Also, the structure factor $S(q = 2k_F x)$ is now simply denoted as S(x).

Electric conductivity and shear viscosity are respectively measured in a.u. (see Sect. 2.1). We will also introduce the corresponding time unit

$$\tau_0 = \frac{3 \pi}{4 \bar{Z}} \frac{a_0 \hbar}{e^2} \,. \tag{4.9}$$

Generalized relaxation times $\tau_1(k)$ and $\tau_2(k)$ thus read as

$$\frac{1}{\tau_1(k)} = \frac{1}{\tau_0} t L_1(t) , \quad \frac{1}{\tau_2(k)} = \frac{3}{\tau_0} t L_2(t) , \qquad (4.10)$$

with

$$L_1(t) = \int_0^1 \mathrm{d}x \, x^3 \, V^2(xt) \, S(xt) \,, \tag{4.11a}$$

$$L_2(t) = \int_0^1 \mathrm{d}x \, x^3(1-x^2) \, V^2(xt) \, S(xt) \,. \tag{4.11b}$$

Next, one introduces quadratures $K_{n,m}^{(i)}$ such as

$$K_{n,m}^{(i)} = \int_{-\beta\mu_e}^{+\infty} \mathrm{d}\eta \left(-\frac{\partial f_e^0}{\partial \eta}\right) \eta^n \frac{t^{2+m}}{L_i(t)} \quad (i=1,2), \qquad (4.12)$$

from which one derives

$$\sigma = L_{\rm EE} = \frac{\sigma_0}{\frac{16}{9} r_s^3 \bar{Z}} K_{0,0}^{(1)}, \qquad (4.13a)$$

$$Q = -\frac{L_{\rm ET}}{L_{\rm EE}} = \frac{k_{\rm B}}{e} \frac{K_{\rm I,0}^{(1)}}{K_{0,0}^{(1)}},$$
(4.13b)

$$K = \Omega T \sigma \quad \text{where} \quad \Omega = \left(\frac{k_{\rm B}}{e} \right)^2 \left[\frac{K_{2,0}^{(1)}}{K_{0,0}^{(1)}} - \left(\frac{K_{1,0}^{(1)}}{K_{0,0}^{(1)}} \right)^2 \right], \tag{4.13c}$$

and

$$\eta_{s} = \frac{3}{80} \frac{\lambda^{2}}{r_{s}^{5} \bar{Z}} \eta_{0} K_{0,2}^{(2)}, \quad \text{with} \quad \lambda = (9 \pi/4)^{1/3}.$$
(4.13d)

Equations (4.13) pertain to exact solutions of the transport equation at any temperature, in the elastic limit. Numerical exploration would require a tabulation of $L_1(t)$ and $L_2(t)$ deduced from V(x), for a given $\varepsilon(x)$ suitably chosen in the temperature-density domain of interest. In a forthcoming work, we shall give specific attention to the temperature extension of the Lindhard dielectric function [19], worked out by Gouedard-Deutsch [20]. These functions hereafter referred to as L and GD respectively, will play a central role in evaluating $L_1(t)$ and $L_2(t)$, looking for an α^2 expansion of transport quantities of present concern within the range $r_s \leq 1$ and $\Gamma \geq 1$.

Anticipating the main analysis displayed there, let us notice that an *algebraic* α *expansion* of solutions (4.13) obviously necessitates an underlying expansion of the *t*-dependent part in the integrant of quadrature $K_{n,m}^{(i)}$:

$$K_{n,m}^{(i)} = \sum_{\ell=0}^{+\infty} \int_{-\infty}^{+\infty} \mathrm{d}\eta \left(-\frac{\partial f_{e}^{0}}{\partial \eta}\right) \eta^{n} \frac{(t-1)^{\ell}}{\ell!} \left(\frac{\mathrm{d}^{\ell}}{\mathrm{d}t^{\ell}} \frac{t^{2+m}}{L_{i}(t)}\right)_{t=1}.$$
 (4.14)

This in turns brings about a simultaneous expansion of $t(\eta, \alpha)$ with respect to η leaving us with the evaluation of quadratures such as $\binom{2}{2}$

$$\langle \hat{\eta}^n \rangle_0 = \int_{-\infty}^{+\infty} \mathrm{d}\eta \left(-\frac{\partial f_e^0}{\partial \eta} \right) \hat{\eta}^n,$$
 (4.15)

where notation (2.2) has been used. Those quadratures are identically zero for n odd or expressed analytically in terms of Bernoulli numbers in other cases [21], with the simplest results :

$$\langle \hat{\eta}^0 \rangle_0 = 1$$
, $\langle \hat{\eta}^2 \rangle_0 = 2/3$, $\langle \hat{\eta}^4 \rangle_0 = 4/15$. (4.16)

The scheme described above constitutes the very basis of our methodology for evaluating finite degeneracy corrections. It is straightforwardly applied in the sequel to the simple $\alpha \rightarrow 0$ limiting case. Let us emphasis however that the calculation of higher order terms in expansion (4.14) is not an obvious matter. When dealing with L and GD dielectric functions for exemple, this requires first a highly non trivial analysis of the singularities contained in the derivatives of these functions at x = 1 (i.e., $q = 2k_F$). The net contributions of these singularities have next to be resumed in order to get the correct T-dependence of transport quantities, even at lowest α^2 order.

4.2.2 Linear transport in the $\alpha \to 0$ limit. — At the lowest order, α expansion of $K_{n,m}^{(i)}$ yields at once

$$\lim_{\alpha \to 0} K_{0,0}^{(1)} = \lim_{\alpha \to 0} \frac{3}{\pi^2} K_{2,0}^{(1)} = 1/L_1(t=1) \equiv \tau_1(k_{\rm F})/\tau_0, \qquad (4.17a)$$

$$\lim_{\alpha \to 0} K_{1,0}^{(1)} = \frac{\pi^2 \alpha}{6} \left(\frac{\mathrm{d}}{\mathrm{d}t} \frac{t^2}{L_1(t)} \right)_{t=1} = \frac{\pi^2 \alpha}{3} \left(\frac{3}{L_1(t=1)} - \frac{S(x=1) V^2(x=1)}{2 L_1^2(t=1)} \right), \quad (4.17b)$$

$$\lim_{\alpha \to 0} K_{0,2}^{(2)} = 1/L_2(t=1) = 3 \tau_2(k_{\rm F})/\tau_0.$$
(4.17c)

Upon introducing these results into equations (4.13a-d), we obtain the required expressions for the linear transport coefficients in the $T \rightarrow 0$ limit. In order to avoid the repetition of lengthy expressions, it appears useful to introduce the following notations

$$\left\langle \varphi\left(x\right)\right\rangle_{x} = \int_{0}^{1} \mathrm{d}x \, x^{3} \, V^{2}(x) \, \varphi\left(x\right), \qquad (4.18)$$

^{(&}lt;sup>2</sup>) For $\alpha \ll 1$, quadratures (4.15) are simplified, replacing their lower bound $-\beta \mu_e$ by $-\infty$. This is equivalent to neglecting terms $\sim \exp(-\beta \mu_e) \approx \exp(-1/\alpha)$ arising from $(-\partial f_e^0/\partial \eta)$.

and

$$I_1^0 = \langle S(x) \rangle_x, \quad \tilde{I}_1^0 = \langle (1 - x^2) S(x) \rangle_x$$
 (4.19a)

$$\zeta^{0} = \left[3 - \frac{\langle \delta(x-1) S(x) \rangle_{x}}{2 I_{1}^{0}}\right], \quad (\delta = \text{Dirac distribution}). \tag{4.19b}$$

Then, one finally gets

$$(\sigma^{0})^{-1} = \lim_{\alpha \to 0} \sigma^{-1} \equiv \rho^{0} = \frac{16}{9} r_{s}^{3} \bar{Z} \rho_{0} I_{1}^{0} \quad (\rho_{0} = 1/\sigma_{0}) , \qquad (4.20a)$$

$$Q^{0} = \lim_{\alpha \to 0} Q = \frac{\pi^{2} k_{\rm B}}{3 e} \alpha \zeta^{0} \quad (e = \text{electron charge}), \qquad (4.20b)$$

$$K^{0} = \lim_{\alpha \to 0} K = \mathcal{L}^{0} T \lim_{\alpha \to 0} \sigma \quad \text{with} \quad \mathcal{L}^{0} = \lim_{\alpha \to 0} \mathcal{L} = \frac{\pi^{2}}{3} \left(\frac{k_{\rm B}}{e}\right)^{2}, \tag{4.20c}$$

$$(\eta_s^0)^{-1} = \lim_{\alpha \to 0} \eta_s^{-1} = \eta_0^{-1} \frac{80}{3} \frac{r_s^5 Z}{\lambda^2} \tilde{I}_1^0.$$
(4.20d)

which provide standard expressions for thermoelectronic coefficients σ^0 , K^0 and Q^0 as well as for the shear viscosity η_s^0 , expressed in a reduce form. It should be noticed that superscript 0 in our notation refers specifically to the *simultaneous* $\tilde{\omega} \to 0$ and $\alpha \to 0$ limits. (Lowerscript 0 on the other hand, refers to a.u.). It should also be appreciated that equation (4.20a) yields back the well-known Ziman expression for electrical resistivity :

$$\rho^{0} = \frac{12 \pi}{\hbar e^{2} v_{\rm F}^{2} n_{\rm i}} \int_{0}^{2k_{\rm F}} \frac{\mathrm{d}q}{2k_{\rm F}} \left(\frac{q}{2k_{\rm F}}\right)^{3} \hat{V}^{2}(q) S(q) , \qquad (4.21)$$

 Q^0 is at least of order α , in agreement with a term of order η arising from $K_{1,0}^{(1)}$. In this case, the first non-zero contribution in expansion (4.14) behaves as (t-1). Moreover, in the $\alpha \ll 1$ limit, the Lorentz number retrieves its Wiedmann-Franz value $\Omega^0 = (\pi^2/3)(k_{\rm B}/e)^2$. Finally, transport coefficients in the elastic limit at T = 0 are derived from the structure factor S(q) and the mean potential $\hat{V}(q)$ through I_1^0 , \tilde{I}_1^0 and the local parameter ζ^0 . Physics thus lies in those dimensionless quantities. As we will show in a forthcoming work, a salient feature is that pre-factors contained in expressions (4.20) contribute mainly to the net behavior of the corresponding transport coefficients, through their Γ and $r_{\rm s}$ dependence (see previous footnote 1). This explains the interest of introducing scaled expressions like (4.20) when studying analytical properties of those linear transport quantities.

4.3 LINEAR TRANSPORT IN THE INELASTIC CASE. — We now turn to solve equation (3.1a) in the more general case where inelastic collisions between electrons and the ionic component cannot be neglected. As already stressed, this feature arises in domain B of figure 1. In contradistinction with the elastic case, only approximate solutions to the linear transport equation can actually be derived, with the help of a well known variational method [6] which we first outline in section 4.3.1. Next we display an « inelastic methodology » extending previous results derived in section 4.2.2. Finally, we applied the latter formalism to the specific case of variational transport taken in the elastic limit, with simple monomial trial

functions. A few well known transport expressions such as Edwards' resistivity formula [8] are shown to belong to this class of solutions.

4.3.1 Standard variational method. — Let us consider transport equation (3.1a) written in the compact form $X(\mathbf{k}) = P\Phi(\mathbf{k})$ where $P\Phi(\mathbf{k}) = -\mathfrak{I}_{\text{lin}}(\Phi(\mathbf{k}))$ defines a linear, definite positive and self-adjoint operator acting on a class of real trial functions $\Phi(\mathbf{k}) = \sum_{i} \gamma_i \Phi_i(\mathbf{k})$. Entropy balance (3.7) reads as :

$$\langle \Phi(\mathbf{k}), X(\mathbf{k}) \rangle = \langle \Phi(\mathbf{k}), P \Phi(\mathbf{k}) \rangle.$$
 (4.22)

where brackets $\langle ... \rangle$ refer here to the scalar product $(1/V) \sum_{k} (...)$. The variational principle

states that amongst all $\Phi(\mathbf{k})$ fulfilling equation (4.22), the exact solution of transport equation optimizes the system entropy $\langle \Phi(\mathbf{k}), P\Phi(\mathbf{k}) \rangle$ whereas the applied external fields are kept constant. The scalar parameters γ_i have to be variationally adjusted which provide the variational solutions:

$$\mathbf{J} = \sum_{ij} J_i (P^{-1})_{ij} J_j \mathbf{E} - \sum_{ij} J_i (P^{-1})_{ij} U_j \frac{\mathbf{V}T}{T}, \qquad (4.23a)$$

$$\mathbf{U} = \sum_{ij} U_i (P^{-1})_{ij} J_j \mathbf{E} - \sum_{ij} U_i (P^{-1})_{ij} U_j \frac{\nabla T}{T}, \qquad (4.23b)$$

$$\bar{\bar{\mathbf{\Pi}}} = -\sum_{ij} \tilde{\Pi}_i (\tilde{P}^{-1})_{ij} \tilde{\Pi}_j \bar{\bar{\mathbf{\Lambda}}} .$$
(4.23c)

 P_{ij} and \tilde{P}_{ij} stand for matrix elements $\langle \Phi_i, P \Phi_j \rangle$ and $\langle \tilde{\Phi}_i, P \tilde{\Phi}_j \rangle$ respectively. The tilde refers hereafter to trial functions and other related quantities specialized to viscosity. J_i , U_i and \tilde{H}_i correspond to the rotational invariant part of currents (3.8), computed with trial functions $\Phi_i(\mathbf{k})$ which have to be introduced in the form

$$\boldsymbol{\Phi}_{i}(\mathbf{k}) = \boldsymbol{\varphi}_{i}(k) \, \mathbf{k} \cdot \hat{\mathbf{u}} \,, \quad \tilde{\boldsymbol{\Phi}}_{i}(\mathbf{k}) = \tilde{\boldsymbol{\varphi}}_{i}(k) \, \mathbf{kk} : \hat{\hat{\mathbf{u}}} \,, \tag{4.24}$$

in order to produce a nonzero output. Unit vector $\hat{\mathbf{u}}$ and tensor $\hat{\mathbf{u}}$, which have arbitrary directions in the elastic case, are removed from the variational currents (4.23) through an *ad hoc* projection. For anisotropic systems, or when addressing the calculation of more sophisticated transport quantities such as the Hall coefficient, a tensorial extension of the variational method (D. Léger and C. Deutsch, to be published) can be worked out, which allows us to completely circumvent the dependence of the trial functions on unphysical $\hat{\mathbf{u}}$ or $\hat{\mathbf{u}}$ quantities.

4.3.2 Variational reduced expressions. — As was done for the elastic case, the required variational transport coefficients may be given a more convenient form involving reduced quadratures. In so doing, we first note that through reduced variables t and η (Definitions (4.6)), one can derive the dimensionless currents :

$$J_{i} = \int_{-\beta\mu_{e}}^{+\infty} \mathrm{d}\eta \left(-\frac{\partial f_{e}^{0}}{\partial \eta}\right) t^{3} \varphi_{i}(\hat{\eta}), \qquad (4.25a)$$

$$U_{i} = \int_{-\beta\mu_{e}}^{+\infty} \mathrm{d}\eta \left(-\frac{\partial f_{e}^{0}}{\partial \bar{\eta}}\right) t^{3} \hat{\eta} \varphi_{i}(\hat{\eta}) , \qquad (4.25b)$$

$$\tilde{\Pi}_{i} = \int_{-\beta\mu_{e}}^{+\infty} \mathrm{d}\eta \left(-\frac{\partial f_{e}^{0}}{\partial \eta}\right) t^{5} \tilde{\varphi}_{i}(\hat{\eta}) . \qquad (4.25c)$$

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Functions $\varphi_i(\hat{\eta})$ and $\tilde{\varphi}_i(\hat{\eta})$ correspond respectively to $\varphi_i(k)$ and $\tilde{\varphi}_i(k)$, the latter being implicit functions of $(E_k - \mu_e)$ or also $\beta (E_k - \mu_e)/\pi \equiv \hat{\eta}$. From a general point of view, $\varphi_i(\hat{\eta})$ and $\tilde{\varphi}_i(\hat{\eta})$ may be taken as monomials $\hat{\eta}^n$, or chosen in any set of linearly independent functions.

Let us now set $t_0 = |p - k|/2 k_F$ and $t_1 = (p + k)/2 k_F$ and introduce dimensionless matrix elements P_{ij} and \tilde{P}_{ij} as

$$P_{ij} = \int_{-\infty}^{+\infty} d\omega \int_{-\beta\mu_{e}}^{+\infty} d\eta f_{e}^{0}(\eta) [1 - f_{e}^{0}(\eta - \tilde{\omega})] \int_{t_{0}}^{t_{1}} x \, dx \, \Psi_{ij}(x, \, \hat{\eta}', \, \hat{\omega}) \, V^{2}(x) \, S(x, \, \omega) ,$$
(4.26a)

$$P_{ij} = \int_{-\infty}^{+\infty} d\omega \int_{-\beta\mu_e}^{+\infty} d\eta f_e^0(\eta) [1 - f_e^0(\eta - \tilde{\omega})] \int_{t_0}^{t_1} x \, dx \, \tilde{\Psi}_{ij}(x, \, \hat{\eta}', \, \hat{\omega}) \, V^2(x) \, S(x, \, \omega) \,,$$
(4.26b)

where $S(x, \omega)$ stands for $S(q = 2k_F x, \omega)$. We also define dimensionless integrands Ψ_{ij} and $\tilde{\Psi}_{ij}$ in terms of x and the new variables $\hat{\omega}$ and $\hat{\eta}'$ previously defined in (2.2) so that

$$\varphi_i(k) \to \varphi_i(\hat{\eta}) \equiv \varphi_i(\hat{\eta}' + \hat{\omega}), \quad \varphi_i(p) \to \varphi_i(\hat{\eta} - 2 \ \hat{\omega}) \equiv \varphi_i(\hat{\eta}' - \hat{\omega}), \quad (4.27)$$

and similarly for $\tilde{\varphi}_i$. Upon introducing :

$$A_1 = \varphi_i(\hat{\eta}' + \hat{\omega}) \varphi_j(\hat{\eta}' - \hat{\omega}) + \varphi_i(\hat{\eta}' - \hat{\omega}) \varphi_j(\hat{\eta}' + \hat{\omega}), \qquad (4.28a)$$

$$A_{2} = \varphi_{i}(\hat{\eta}' - \hat{\omega}) \varphi_{j}(\hat{\eta}' - \hat{\omega}) + \varphi_{i}(\hat{\eta}' + \hat{\omega}) \varphi_{j}(\hat{\eta}' + \hat{\omega}) - \varphi_{i}(\hat{\eta}' + \hat{\omega}) \varphi_{j}(\hat{\eta}' - \hat{\omega}) - \varphi_{i}(\hat{\eta}' - \hat{\omega}) \varphi_{j}(\hat{\eta}' + \hat{\omega}), \quad (4.28b)$$

$$A_{3} = \varphi_{i}(\hat{\eta}' - \hat{\omega}) \varphi_{j}(\hat{\eta}' - \hat{\omega}) - \varphi_{i}(\hat{\eta}' + \hat{\omega}) \varphi_{j}(\hat{\eta}' + \hat{\omega}), \qquad (4.28c)$$

and using similar definitions for \tilde{A}_1 , \tilde{A}_2 and \tilde{A}_3 with $\varphi_i \to \tilde{\varphi}_i$, one arrives after a number of lengthy algebraic manipulations at

$$\Psi_{ij}(x, \,\hat{\eta}', \,\hat{\omega}\,) = A_1 \frac{x^2}{2} + \frac{A_2}{4} \left(2 \,\,\hat{\eta}'\,\,\hat{\alpha} + \gamma\,\right) - \frac{A_3}{2} \,\hat{\omega}\,\hat{\alpha}\,\,, \tag{4.29a}$$

$$\tilde{\Psi}_{ij}(x, \ \hat{\eta}', \ \hat{\omega}) = \frac{\tilde{A}_1}{2} x^2 (t^2 - x^2 - 2 \ \hat{\omega} \ \hat{\alpha}) + \frac{\tilde{A}_2}{12} (2 \ \hat{\eta}' \ \hat{\alpha} + \gamma)^2 - \frac{\tilde{A}_3}{3} (2 \ \hat{\eta}' \ \hat{\alpha} + \gamma) \ \hat{\omega} \ \hat{\alpha} + \frac{1}{6} \ \hat{\alpha}^2 \ \hat{\omega}^2 (\tilde{A}_1 + 2 \ \tilde{A}_2) .$$
(4.29b)

Variable $\hat{\eta}'$ is useful in computing transport coefficients at a low temperature, i.e., $\alpha \ll 1$. When addressing the computation of P_{ij} and \tilde{P}_{ij} , we should in fact consider quadratures similar to

$$\langle \hat{\eta}'^{n} \rangle_{1} = \int_{-\infty}^{+\infty} d\eta f_{e}^{0}(\eta) [1 - f_{e}^{0}(\eta - \tilde{\omega})] \hat{\eta}'^{n},$$
 (4.30)

extending to the inelastic case integrals $\langle \hat{\eta}^n \rangle_0$ already considered in (4.15). The analytic properties of these quadratures, both for monomials and other arbitrary functions, will be

detailed in the following paper II. For our purpose, let us just note here that quadratures $(\hat{\eta}'^n)_1$ are identically zero for odd n, while in other cases they express as

$$\langle \hat{\eta}'^{2p} \rangle_{1} = \tilde{\omega} n(\tilde{\omega}) P_{p}(\hat{\omega}^{2}),$$
 (4.31)

where $n(\tilde{\omega}) = (e^{\tilde{\omega}} - 1)^{-1}$ refers to the Planck function, while $P_p(\tilde{\omega}^2)$ is a polynomial of degree p. Expressions (4.31) are thus especially useful in computing inelastic corrections obtained as expansions in $\hat{\omega}^2$ which again explains the basic methodology described above. Finally, one gets the required transport coefficients in the reduced form

$$\sigma^{\text{var}} = L_{\text{EE}}^{\text{var}} = \left(\frac{16}{9}r_{s}^{3}\bar{Z}\rho_{0}\right)^{-1}\sum_{ij}J_{i}(P^{-1})_{ij}J_{j}, \qquad (4.32a)$$

$$-L_{\rm TT}^{\rm var} = \left(\frac{16}{9}r_{\rm s}^3 \,\bar{Z}\rho_0\right)^{-1} 3\,{\rm L}^0 T \sum_{ij} U_i (P^{-1})_{ij} \,U_j\,,\qquad(4.32b)$$

$$-L_{\rm ET}^{\rm var} = \left(\frac{16}{9}r_{\rm s}^{3}\bar{Z}\rho_{0}\right)^{-1}\pi\frac{k_{\rm B}}{e}\sum_{ij}J_{i}(P^{-1})_{ij}U_{j},\qquad(4.32c)$$

$$\eta_{s}^{\text{var}} = \left(\frac{80}{3} \frac{r_{s}^{5} \bar{Z}}{\lambda^{2}}\right)^{-1} \eta_{0} \sum_{ij} \tilde{\Pi}_{i} (\tilde{P}^{-1})_{ij} \tilde{\Pi}_{j}.$$
(4.32d)

Once $\varphi_i(\hat{\eta})$ and $\tilde{\varphi}_i(\hat{\eta})$ are selected, these expressions allow for a variational calculation of transport coefficients at any temperature. As is readily demonstrated from the basic content of the variational principle itself, variational quantities σ^{var} , K^{var} and η_s^{var} have to be *smaller* than their exact counterpart.

4.3.3 Variational transport coefficients in the elastic limit. — Before proceeding further with the estimation of inelastic contributions (Paper II), it proves useful to briefly examine the connection between variational techniques and the elastic transport calculations detailed in previous sections. For that purpose, it is sufficient to derive variational results from the simplest monomial trial functions $\hat{\eta}^n$ which produce a non-zero output for σ^{var} , K^{var} and η_s^{var} . The elastic limit is characterized by $\lim t_0 = 0$, $\lim t_1 = t$ and also $\tilde{\omega} \rightarrow 0$

$$\lim_{\tilde{\omega}\to 0} f_e^0(\eta) [1 - f_e^0(\eta - \tilde{\omega})] = -\frac{\partial f_e^0}{\partial \eta}, \quad \lim_{\tilde{\omega}\to 0} \{A_2, A_3, \tilde{A}_2, \tilde{A}_3\} = 0.$$

Estimating $\rho^{\text{var}} \sim P_{11}/J_1^2$ with $\varphi_1(\hat{\eta}) = 1$ provides straightforwardly

$$\rho^{\text{var}} = (\sigma^{\text{var}})^{-1} = \frac{16}{9} r_s^3 \bar{Z} \rho_0 \int_{-\beta\mu_e}^{+\infty} \mathrm{d}\eta \left(-\frac{\partial f_e^0}{\partial \eta}\right) t^4 L_1(t) , \qquad (4.33)$$

since $J_1 \equiv 1$ in this case; expression (4.33) can be shown to be identical to the well-known Edwards formula for resistivity.

Similarly, the calculation of K^{var} with $\varphi_2(\hat{\eta}) = \hat{\eta}$, is performed through

$$K^{\text{var}} \approx L_{\text{TT}}^{\text{var}} \approx \frac{3 \mathfrak{L}^0 T}{\frac{16}{9} r_s^3 \bar{Z} \rho_0} \frac{\left(\int_{-\beta\mu_e}^{+\infty} d\eta \left(-\frac{\partial f_e^0}{\partial \eta} \right) \hat{\eta}^2 t^3 \right)^2}{\int_{-\beta\mu_e}^{+\infty} d\eta \left(-\frac{\partial f_e^0}{\partial \eta} \right) \hat{\eta}^2 t^4 L_1(t)}, \qquad (4.34)$$

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in agreement with an expression recently derived within a different theoretical framework by Ichimaru and Tanaka [22] for thermal conductivity in dense plasmas. However, it should be appreciated that these authors have replaced the chemical potential μ_e in variable $\hat{\eta} = \beta (E_k - \mu_e)/\pi$ by h_e , enthalpy per electron. This is a simple consequence of the definition retained for the effective electric field, as explained previously. Let us also notice that a complete calculation of K^{var} with the correction term $-TL_{\text{ET}}^2/L_{\text{EE}}$ requires at least two trial functions in order to produce a non-vanishing output for the latter. The complete expression is then much more involved that equation (4.34), even at a level of a two functions approximation.

Finally we compute η_s^{var} with $\tilde{\varphi}_1(\hat{\eta}) = 1$, and obtain

$$\eta_{s}^{\text{var}} = \frac{3}{80} \frac{\lambda^{2}}{r_{s}^{5} \bar{Z}} \eta_{0} \frac{\left(\int_{-\beta\mu_{e}}^{+\infty} d\eta \left(-\frac{\partial f_{e}^{0}}{\partial \eta} \right) t^{5} \right)^{2}}{\int_{-\beta\mu_{e}}^{+\infty} d\eta \left(-\frac{\partial f_{e}^{0}}{\partial \eta} \right) t^{6} L_{2}(t)} .$$
(4.35)

Equations (4.33)-(4.35) derive from the variational principle with one single trial function in each case. In the $\alpha \to 0$ limit, they reduce to exact results (4.20a) and (4.20c-d) respectively. Another interesting problem would consist in demonstrating that a *complete basis* of monomials $\hat{\eta}^n$, or more involved functions, yield back the exact solutions at any *T* provided in equations (4.13). A more immediate program would consist in selecting out trial functions within a limit $\alpha \ll 1$, giving back exact expansions of transport coefficients up to a finite order α^{2p} . By restricting to thermoelectronic coefficients, we have been able to check out that the function pairs $(1, \hat{\eta})$ and $(\hat{\eta}, \hat{\eta}^2)$ yield back respectively σ and *K* up to order α^2 . So, one may conjecture that the thermopower *Q* should be retrieved at order α^2 with $(1, \hat{\eta}, \hat{\eta}^2)$.

Once we have chosen the given trial functions, we can thus apply the above formalism to include inelastic effects. In this fashion, we shall be able to compute σ at order α^2 , the inelastic contributions being included both into the zero-order term and in the α^2 correction. This will be done in the next paper II.

5. Conclusion.

The theoretical framework for computing all the time-independent electronic transport coefficients in strongly coupled and multicomponent ionic mixtures is laid down through the Boltzmann-Ziman approach and the Lorentzian approximation. The latter rests on a few number conditions on the basic parameters Γ and r_s , which have been examined carefully. The present analysis results in a crucial simplification arising from the decoupling depicted in figure 1 of inelastic effects from temperature-dependent corrections. This remark paves the way for a separate analysis given in the following paper II in this series, in terms of exact α^2 and $\tilde{\omega}^2$ expansions. Specific features of Boltzmann-Ziman transport formalism within the context of Lorentz gases have been reviewed with specific attention to the Chapman-Enskog-like treatment of the transport equation. Finally, thermoelectronic and mechanical transport coefficients have been rexpressed under a suitable reduced form, both in elastic and inelastic cases, ready for further algebraic and numerical developments.

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