

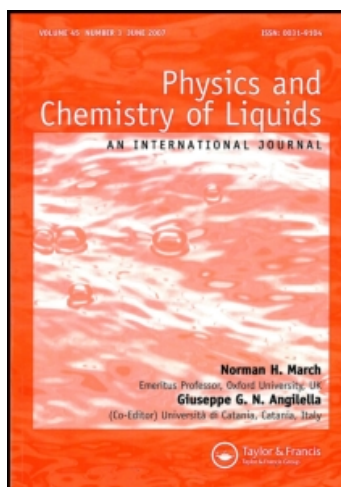
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The calculation of Cs and Rb conductivities in the region of liquid–plasma transition

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The conductivity and thermal conductivity of Cs and Rb are calculated in the liquid phase and in the region between the plasma (gas) and the liquid states. The last area is located at the temperatures higher than the critical one, near the critical point. The Ziman formalism originated from the liquid metal theory was used for the calculations. The results of present calculations were compared with available experiments and calculations of other researchers. It was found that the liquid state formalism can be applied to expanded liquid Cs and Rb at densities higher than the critical one, but another type of models is necessary at lower densities.

Keywords: liquid metals; Ziman theory; liquid–plasma transition

1. Introduction

At the present time the main problem in describing the electronic transport coefficients of metals (conductivity and thermal conductivity) is the region between the rarefied gaseous (plasma) phase and the dense liquid or fluid state. The critical point is also located in this region. Near the critical point, at temperatures higher than the critical one, the values of the transport coefficients increase from gaseous to metallic values. This phenomenon is frequently referred to as the pressure ionisation or the metal–non-metal transition [1–4]. The increase in the transport coefficients will also be referred to as the plasma–liquid transition (note that it is not the thermodynamic phase transition).

There are several theoretical approaches to the description of the coefficients in this region. These are the phenomenological models [1,2], the generalised chemical models (GCMs) [3,4] and the so-called *ab initio* simulations [5,6]. In the frame of GCM a substance is considered as a mixture of positive ions, atoms and electrons. But the validity of GCMs is limited from above by some density because of the degeneracy of the electrons and enhanced inter-particle interaction as a consequence of the ionisation. The *ab initio* simulations are based on the density functional theory. The models with *ab initio* simulations usually consider a substance as a two-component mixture of positive ions and free electrons. The ions consist of the nucleus and core electrons. The ions and free electrons interact by means of some pseudo-potential. Sometimes a substance can consist of the electrons and bare nuclei

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within these models. *Ab initio* approaches successfully describe the region of solid state, liquids and dense fluids, but they fail to reproduce correct ionisation degree at gaseous phase. Phenomenological models are specially constructed to describe the increase in electrical conductivity (and other coefficients) in the vicinity of the critical point.

Various properties of the alkali metals near the critical point are studied more frequently than for non-alkali ones because they have relatively low critical temperatures (the critical parameters are denoted by the index 'c'). There are many wide-ranged measurements of the thermophysical properties of alkali metals under high temperatures (see [1–4] for references). In gaseous phase the alkali metals, i.e. Na, Cs, Rb, Li, are weakly ionised plasma consisting of the neutrals (atoms), the positive single-charged ions and the electrons. The atoms can form dimers and clusters, which also are probably ionised. The presence of clusters makes the number of effective scattering centres smaller for electrons. So GCMs that take into account this effect, can explain the increase in conductivity in alkali metals up to the densities $\sim 0.5\rho_c$ [3,4]. (for Cs $T_c = 1938$ K or $T_c = 1924$ K, $\rho_c = 0.38$ g cm⁻³; for Rb $T_c = 2017$ K, $\rho_c = 0.29$ g cm⁻³ [4,7]). But at higher densities, as we mentioned above, these models cannot describe the interaction between particles correctly.

At the liquid densities near the melting line there are many models calculating the properties of metals. The most advanced of them are the *ab initio* models mentioned above. They give very accurate description of physical properties at the solid state and near the melting line. At the density lowering they are not so accurate because of the problems with choice of pseudo-potentials and exchange-correlation functional [5,6]. There are also more simple models constructed on the basis of the Ziman (or Ziman–Faber) formalism [8], which was generalised for non-zero temperatures. To date these models have been successfully applied to the various thermophysical properties of alkali and non-alkali metals [9–11]. They are even used to describe possible structure transition in liquid Cs [12]. But their application is limited from below by relatively high densities [13] (approximately $\rho \geq 2\rho_c$). The limitation originated from several reasons. Ziman theory considers the electrons as a nearly free degenerated gas, which is weakly scattered by the ion component. That is, the mean free path of the electrons must be much greater than the average distance between the ions [4,8]. So the scattering process can be considered in the first Born approximation (see following section). When a metal expands, this condition is violated because of the recombination of charges and because of the increase in the average distance between the heavy particles. In an expanded medium the electrons are scattered by neutral particles as well as ions. Therefore, some ionic composition models are necessary together with the models of the transport coefficients themselves.

In the case of alkali metals there is an indication [4,14] that near the critical point the substance is fully ionised just like in the liquid phase. It was shown that one of the local pseudo-potentials, [15], can be successfully used in the liquid phase of alkali metals [16] as well as non-alkali ones [17]. If the alkali metal is fully ionised then the ratio of the temperature to the Fermi energy of free electron gas at the critical parameters in alkali metals is ≤ 0.2 . Therefore, the electron gas is still degenerated. So, it is interesting to apply the Ziman-type model to the description of the behaviour of transport coefficients of alkali metals near the critical point and compare the results with available wide-range measurements for Cs and Rb [14,18,19].

The article is organised as follows. The relations for transport coefficients calculation are presented the following section. Section 3 is devoted to the description of results and comparison with calculations and measurements of others researches.

2. Theoretical relations

To calculate the electronic transport coefficients it is possible to introduce so-called the relaxation time. This time coincides with a mean free time for the gases. The Ziman formalism derives the relaxation time for the liquid and the solid state of metals [8]. A metal is considered as the mixture of two components: the positive ions with fixed charge Z_i and the free electrons. The positive ion number density is n_i , the electron number density is n_e ($n_e = Z_i n_i$) and the mass density is ρ . The temperature is denoted as T . The interaction between two components is described by some pseudo-potential. The last object defines the relaxation time too. The relaxation time τ is expressed as (SI units are used in the formulae):

$$\frac{1}{\tau} = \frac{m_e^2}{12\pi^3 \hbar^3 Z_i} \int_0^{2k} S_{ii}(x) \left| \frac{\tilde{w}_{ei}(x)}{D(x)} \right|^2 x^3 dx. \quad (1)$$

In (1) k is the wave vector, $\tilde{w}_{ei}(k)$ is the Fourier-transform of the pseudo-potential $w_{ei}(r)$ mentioned above, $D(k)$ is the static dielectric function (permittivity), $S_{ii}(k)$ is the ion-ion structure factor. The energy of a free electron is $\varepsilon = \hbar^2 k^2 / (2m_e)$. Formula (1) is obtained using the first Born approximation. It is known that the relaxation time in Born approximation is correct if $\lambda_e(n_i)^{1/3} \gg 1$ (or at least $\lambda_e(n_i)^{1/3} \geq 10$), where λ_e is the mean free path of conduction electrons [4]. The mean free path can be estimated when the conductivity is known. (If the electrons are degenerated then the conductivity $\sigma \sim n_e e^2 \tau / m_e \sim n_e e^2 \lambda_e / (m_e \langle u \rangle)$, where $\langle u \rangle$ is the average electron velocity. At $T=0$ $\langle u \rangle = u_F$, u_F is the velocity at Fermi surface.) We will check whether the condition $\lambda_e(n_i)^{1/3} \gg 1$ is true when the results are considered.

In the general case it is necessary to use the Kubo-Greenwood formula, free of any approximation. Therefore, this approach is formally exact. That is why it is used in *ab initio* simulations [5,6]. But the application of any approaches mentioned above to the definition of the relaxation time or conductivity requires the knowledge of some parameters. In the case of *ab initio* approaches to obtain the model parameters one needs to make averaging with exact density matrix. The averaging, in turn, requires the great computational efforts. In the case of (1) these parameters are more simple – $S_{ii}(k)$, $D(k)$, $\tilde{w}_{ei}(k)$, Z_i .

If the relaxation time is known then one can calculate the transport coefficients (σ is the electrical conductivity, S_t is the thermopower, κ is the thermal conductivity) from the following relations [4]:

$$\begin{aligned} \sigma &= -\frac{2|e|^2 \sqrt{2m_e}}{3\pi^2 \hbar^3} I_{3/2}, & S_t &= \frac{1}{|e|T} \left(\mu - \frac{I_{5/2}}{I_{3/2}} \right), \\ \kappa &= \frac{2\sqrt{2m_e}}{3\pi^2 \hbar^3 T} \left(-I_{7/2} + \frac{(I_{5/2})^2}{I_{3/2}} \right), & I_n &= \int_0^\infty \varepsilon \tau(\varepsilon) \frac{\partial f_0}{\partial \varepsilon} d\varepsilon. \end{aligned} \quad (2)$$

Here f_0 is the Fermi-Dirac distribution function, μ is the chemical potential for an ideal electron gas.

As far as the relaxation time is given by (1) then it is possible to calculate the transport coefficients according to formulae (2) for given temperatures and densities. The time τ is defined by means of the electron-ion pseudo-potential $w_{ei}(r)$ and the ion-ion structure factor $S_{ii}(k)$. The structure factor is unambiguously connected with the pair correlation function $g_{ii}(r)$ by the Fourier-transform: $S_{ii}(k) = 1 + 4\pi n_i \int_0^\infty (g(r) - 1)r^2 dr$. There are many techniques to calculate $g_{ii}(r)$ and $S_{ii}(k)$ if the effective ion-ion potential is known. Thus, first we should calculate the effective ion-ion potential. Local ion-ion pseudo-potential $U_{ii}(r)$ can be expressed by means of $\tilde{w}_{ei}(k)$ and the electron linear-response function $\chi(k)$ in the second order of the perturbation theory [4,8,17]. Its Fourier-transform is as follows:

$$\tilde{U}_{ii}(k) = \frac{Z_i |e|^2}{\varepsilon_0 k^2} + \chi(k) |w_{ei}(k)|^2. \quad (3)$$

Here ε_0 is SI constant. The inverse Fourier-transform of $\tilde{U}_{ii}(k)$ gives the effective ion-ion potential $U_{ii}(r)$.

We should note that the ion component in metals under conditions in hand is non-degenerated. It obeys the classical statistics. If the interaction potential for classical system is known then it is possible to calculate its $g(r)$ and $S(k)$ by several ways. The Ornstein-Zernike equation and integral equation theory of liquids were used in [16,17] for this purpose. In this work the NVT Metropolis Monte-Carlo simulations [20,21] with 1000 particles was applied to calculate $g_{ii}(r)$ and $S_{ii}(k)$ for every thermodynamic state. At liquid state, $S_{ii}(k)$ can be measured. The comparison of measured and calculated structure factors are given below.

One can see that all the parameters mentioned above (excluding response functions) are defined by $w_{ei}(r)$. We used the electron-ion pseudo-potential of Fiolhais *et al.* [15].

$$w_{ei}(r) = -\frac{Z_i |e|^2}{4\pi\varepsilon_0 r_0} \left(\frac{1}{x} [1 - (1 + \beta x)e^{-\alpha x}] - A e^{-x} \right), \quad x = \frac{r}{r_0} \quad (4)$$

$$\beta = \frac{\alpha^3 - 2\alpha}{4(\alpha^2 - 1)}, \quad A = \alpha^2/2 - \alpha\beta.$$

Expression (4) is dependent on two parameters – r_0 and α . In [15] there are two possible choices of parameters – ‘universal’ and ‘individual’. ‘Universal’ parameters: for Cs $r_0 = 0.919a_B$, $\alpha = 2.692$ (a_B is the Bohr radius); for Rb $r_0 = 0.823a_B$, $\alpha = 2.749$. Individual parameters: for Cs $r_0 = 0.848a_B$, $\alpha = 3.138$; for Rb $r_0 = 0.76a_B$, $\alpha = 3.197$. In [16] the universal parameters were chosen to obtain the best agreement between calculated and measured structure factors of alkali metals. In [17] both kinds of parameters were used for $S_{ii}(q)$ of Fe, Co, Ni. We also considered both variants of r_0 and α . We indicate below what variant is better on the basis of the comparison with the measurements.

Potential (4) is constructed in accordance with the general theory of pseudo-potentials, developed since 1960s [22]. It belongs to the class of evanescent core potentials [15], i.e. when $r \rightarrow \infty$ it tends to Coulomb potential; but when $r \rightarrow 0$ the interaction is described by some function which is finite at $r=0$ (in contrast to Coulomb potential). This function arises from the contribution of ion core electrons

into the potential, so it should quickly tends to zero when $r \rightarrow \infty$. For reliable calculation of different properties of a metal the whole potential should be a smooth function. The first pseudo-potential of this kind was proposed by Hellmann [23] for potassium. One more analogous potential was derived by Krasko and Gurskii [24]. (The last one can be obtained from (4) if $\beta = 0$, $\alpha = 1$. The main improvements of the evanescent core potential (4) are that it satisfies some general constraints of the pseudo-potential theory (see [15] for details).) These improvements give rise to more exact calculation of different properties of a metal.

As mentioned above, the ionic composition changes when the density decreases. If a metal has multiple-charged positive ions in liquid phase, then this effect can be important even when this metal still consists of only charged components. For example Al has ions with charge +3 in liquid phase (at densities $\sim 2.7 \text{ g cm}^{-3}$). At gaseous state ($\rho \sim 0.1 \text{ g cm}^{-3}$) the neutrals dominate. So there are intermediate densities, where Al is still fully ionised but consists of several kinds of ions. In this case one needs to use a composition model [25,26]. The alkali metals have only single charged positive ions. Near critical point they are possibly still fully ionised [4,14]. So we can set the ion charge as $Z_i = 1$.

Let us consider the last, but not least parameters – $D(k)$ and $\chi(k)$. The static dielectric function entering (1) can be written as [4,8]:

$$D(k) = 1 + (1 - G(k))\chi_0(k)|e|^2/(\epsilon_0 k^2),$$

$$\chi_0(k) = \frac{k_F m_e}{2\pi^2 \hbar^2} \left[1 + \frac{1-x}{2x} \ln \left| \frac{1+x}{1-x} \right| \right], \quad x = k/(2k_F), \quad k_F = (3\pi^2 n_e)^{1/3}. \quad (5)$$

In (5) n_e is the electron particle concentration, $\chi_0(k)$ is the Lindhard response function for non-interacting degenerated electron gas [4,8], $G(k)$ is the local field correction, which accounts for the interaction between the electrons. There are many different forms of $G(q)$, which are usually referred to the names of authors of corresponding model, i.e. Hubbard–Sham, Vashista–Singwi, Taylor, Ichimaru–Utsumi, etc. (see [4,9,10] for references). Here we tested various forms of $G(q)$ and found that the local field corrections offered by Ichimaru and Utsumi [27] and Hellal *et al.* [28] together with the potential [15] can give the best agreement between the calculation and available measurements of conductivity as well as of structure factors of Rb and Cs. So now, we use these $G(q)$.

The response function $\chi(k)$ entering the effective ion–ion potential in (3) is also dependent on $G(q)$:

$$\chi(k) = \frac{\chi_0(k)v(k)}{1 - (1 - G(k))\chi_0(k)v(k)}, \quad v(k) = \frac{|e|^2}{\epsilon_0 k^2}. \quad (6)$$

Now we have all necessary parameters to calculate the transport coefficients.

3. Results

Let us start with the structure factors data. There are many measurements of structure factors of liquid metals near melting (by means of elastic X-ray or neutron scattering). Almost 30 years ago many of these data were accumulated in the well-known monograph written by Waseda [29]. Now they can be downloaded via

internet – <http://www.tagen.tohoku.ac.jp/general/building/iamp/database/scm/>. Up to now these structural data have been described by variety of models and theories. But the maximum temperatures achieved in experiments presented in [29] are near the melting line and far from the critical region. To study the thermophysical properties of a substance in a wider range, the measurements under higher temperatures are necessary. The critical points of alkali metals are located at lower temperatures with respect to the other metals. So, currently we have several sets of structure factor measurements, which are spread up to the critical temperatures. For example there are measurements [30,31] for Cs and [32] for Rb. The initial states (i.e. the densities and temperatures) of both these experiments are located near the melting line, just like in [29], and the results are in agreement with Waseda data.

We have carried out the corresponding calculations of structure factors with potential (3) and have compared the results with the measurements for Cs in Figure 1 and for Rb in Figure 2. In Figure 1 empty circles presents the structure factors for 5 thermodynamics states of Cs measured in [30]. In Figure 2 empty circles presents the structure factors for 5 thermodynamics states of Rb measured in [32]. Our calculations have shown that individual parameters of Fiolhais *et al.* potential [15] can give better agreement with the measurements than universal ones. Consequently, we present our results with individual parameters (i.e. $r_0 = 0.848a_B$, $\alpha = 3.138$ for Cs and $r_0 = 0.760a_B$, $\alpha = 3.197$ for Rb). We have also found that at relatively low temperatures near melting line both $G(q)$ obtained by Ichimaru and Utsumi [27] and by Hellal *et al.* [28] can describe the experimental data. But at higher temperatures (especially near the critical point) $G(q)$ obtained by Ichimaru–Utsumi is better. As one can see in Figures 1 and 2 the calculated data are in agreement with the measured

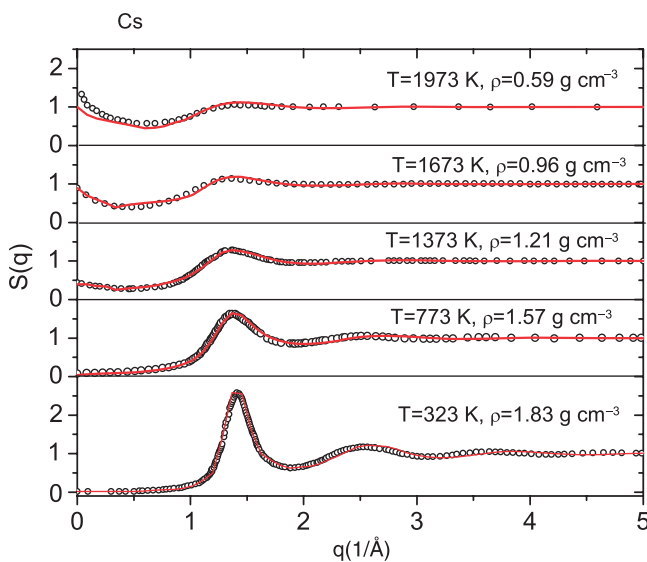


Figure 1. The structure factors of Cs at various temperatures. Empty circles – the measurements of Winter, Hensel *et al.* [30]. Lines – our calculations with Fiolhais *et al.* potential [15] (individual parameters), local field correction of Ichimaru and Utsumi [27].

structure factors. The disagreement is at small wave vectors for the states near the critical points. But all measurements of structure factors is always limited by some k_{\min} , i.e. $k > k_{\min}$ [30–32]. Consequently the values of $S(k)$ at $k=0$ in measurements are always obtained by extrapolation of experimental data. So it is difficult to find real error of our simulations relative to the measurements at small k . Now we move on to the transport coefficients.

The conductivity of expanded liquid Cs has been earlier studied by means of the Ziman formalism [4,33]. The results were compared with the measurements of electrical conductivity, which were also obtained in [30]. In [33] others pseudo-potentials (Ashcroft-empty-core potential, Heine–Abarenkov potential, Hasegawa potential) were used. These potentials have at least one free parameter. For Ashcroft empty-core potential this parameter is the characteristic radius. The free parameters can be fitted to describe some property of a metal. This fitting was used in [33] to obtain the conductivity corresponding to the experimental value near melting line. But the conductivity calculated in [33] was in disagreement with the measured data when the density approaches the critical value. The main reason for this disagreement, as mentioned above, is possible inapplicability of Ziman formalism and nearly free electron approach at the density lowering. A minor reason may be concluded in pseudo-potentials, which was specially fitted in [33] to describe the conductivity at melting. Here we used the pseudo-potential [15] without fitting.

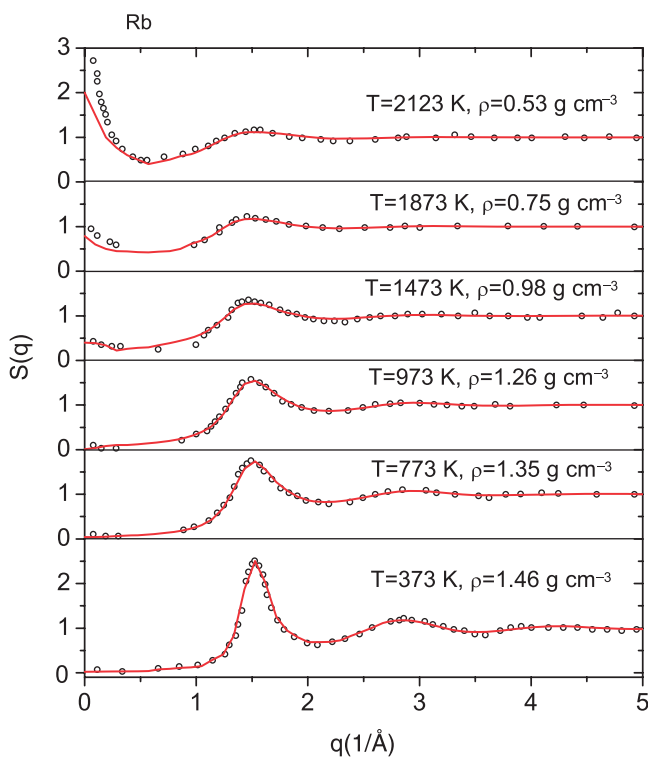


Figure 2. The same as in Figure 1 but for Rb. Empty circles – the measurements of Matsuda *et al.* [32].

The results of our calculations of Cs conductivity are presented in Table 1. The data of Table 1 show that our calculations are in better agreement with the experiment than the results of [33]. But the difference also increases while the density approaches the critical point. The maximum error in measurements [30] was estimated as 20%. The maximum difference in our conductivity relative to the experimental data is 26% at $T=1923$ K. The electron gas is still degenerated, although at $T=1923$ K the ratio of Fermi energy to the temperature is 4.24. The condition $\lambda_e(n_i)^{1/3} > 1$ is fulfilled for every state, but at $T=1923$ K this ratio is only 2.5.

Analogous results for Rb are presented in Table 2. We have made comparison with the experimental data [19]. Their maximum relative error was estimated as 20%. We have also considered the results of *ab initio* simulations [6], which are in agreement with the measurements for all range. Qualitatively we have the same situation as for Cs.

Table 1. The conductivity of Cs in liquid phase. Experiment: the data of [30,33]. Calculation1: the data of [33]. Our data correspond to the individual parameters of Fiolhais *et al.* potential [15].

T (K)	ρ (g cm ⁻³)	Experiment σ (Ω cm) ⁻¹	Calculation1 σ (Ω cm) ⁻¹	Our data σ (Ω cm) ⁻¹	E_F ($k_B T$)
373	1.800	22,196	22,200	2.01×10^4	46.0
773	1.567	10,200	10,100	1.02×10^4	20.2
973	1.452	7800	8060	8.01×10^3	15.3
1173	1.332	5070	5940	6.21×10^3	12.0
1373	1.209	3550	4940	4.32×10^3	9.6
1673	0.956	1170	2760	1.33×10^3	6.7
1923	0.590	500	1370	6.26×10^3	4.24

Table 2. The conductivity of Rb in liquid phase. Experiment: [19], Calculation2: *ab initio* simulation [6]. Our data correspond to the individual parameters of Fiolhais *et al.* potential [15].

T (K)	ρ (g cm ⁻³)	Experiment σ (Ω cm) ⁻¹	Calculation2 σ (Ω cm) ⁻¹	Our data σ (Ω cm) ⁻¹	E_F ($k_B T$)
312.46	1.4785	4.440×10^4	–	4.41×10^4	64.4
373	1.46	–	3.597×10^4	3.68×10^4	53.5
400	1.4495	3.335×10^4	–	3.52×10^4	49.6
573	1.43	–	2.681×10^4	2.8×10^4	34.3
600	1.3603	2.018×10^4	–	2.16×10^4	31.7
900	1.2261	1.135×10^4	–	1.17×10^4	19.7
973	1.26	–	1.107×10^4	1.13×10^4	18.6
1000	1.1826	9.58×10^3	–	1.11×10^4	17.3
1173	1.15	–	7.52×10^3	8.01×10^3	14.5
1200	1.0908	6.91×10^3	–	7.35×10^3	13.7
1500	0.9308	4.21×10^3	–	4.62×10^3	9.7
1673	0.88	–	6.2×10^2	3.61×10^3	8.5
1700	0.8041	2.92×10^3	–	3.25×10^3	7.9
1900	0.6385	1.90×10^3	–	2.21×10^3	6.0

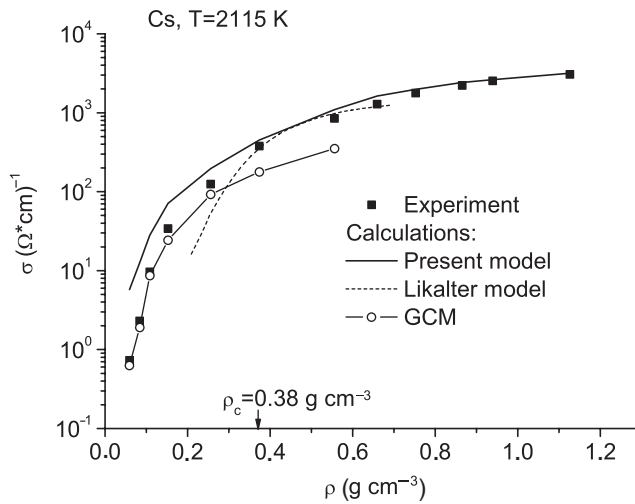


Figure 3. Cs conductivity near the critical point at isotherm $T=2115$ K. Experiment – [14,18], Likalter – [2], GCM – [3].

Now we will try to apply our calculations to the region of plasma–liquid transition. In Figure 3 there are the results of electrical conductivity measurements [14,18] for Cs at $T=2115$ K. There are also the results of calculations according to different approaches. The phenomenological model [2] qualitatively reproduces the conductivity increase but it fails below the critical density. In contrast, the GCM [3] is in agreement with the experiment below the critical densities, but it fails at the densities $\rho > 0.3 \text{ g cm}^{-3}$. Our calculations are in good agreement with the measurements starting from the critical density and higher. Below the critical density our model gives rise to overestimated conductivity. The condition $\lambda_e(n_i)^{1/3} > 1$ is violated at $\rho \sim \rho_c$. At the critical point $\lambda_e(n_i)^{1/3} = 1.2$. Therefore, our model is inapplicable at lower densities. One can also see that none of the models in hand can describe the behaviour of the conductivity in the transition region.

The situation is analogous for Rb. Corresponding results are presented in Figure 4. One can see that there is also no model, which could describe the conductivity at wide-range variation of the density. For Rb the ratio is $\lambda_e(n_i)^{1/3} = 1.1$ at the critical density. Therefore, the conclusion about inapplicability of the present model at lower densities is valid for Rb too.

With regard to the other two transport coefficients (i.e. the thermal conductivity and the thermopower), we can state that high-temperature measurements for them are absent in the vicinity of the critical point. (It is true almost for any pure metals, excluding Hg.) Consequently, the calculations are also rarely presented for these coefficients. So, we have no other results for comparison. But we know that according to the general theory these coefficients also have analogous transition from gaseous to metallic value. So, it is interesting to check the Wiedemann–Franz ratio L : $\kappa = \sigma^* T^* L^* (k_B/e)^2$. The thermal conductivity for Cs was calculated at the same temperature $T=2115$ K to obtain L . At high densities it was just similar to the liquid state i.e. $L \approx 3.29$. But near the critical point it was diminishing. It may be

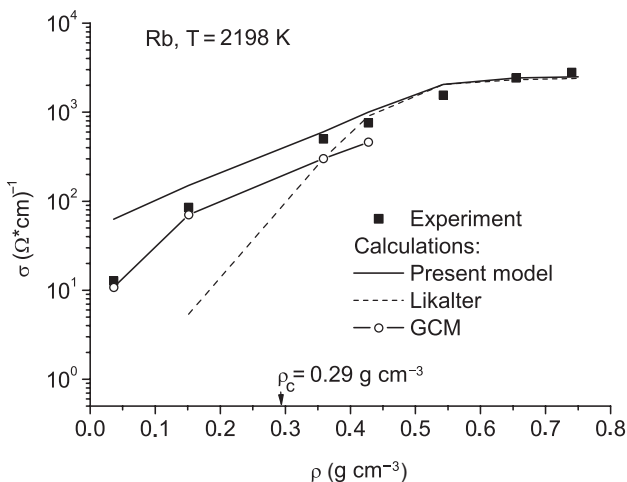


Figure 4. The same as in Figure 3, but for Rb at $T=2198$ K.

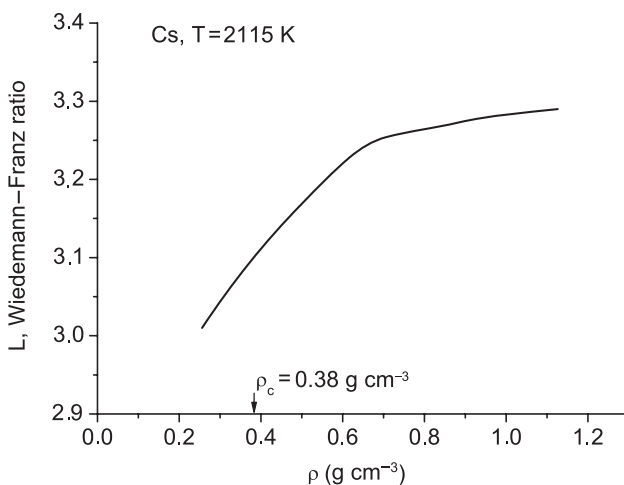


Figure 5. The Wiedemann-Franz ratio for Cs at $T=2115$ K.

the sign of transition from metallic to gaseous state. Corresponding results are presented in Figure 5.

We should note that the GCM approach offered in [3] is not the only one possible. Now there are many variants of GCMs. Some of them describe various properties of metallic plasma correctly from gaseous densities up to critical ones [34]. More advanced variant of GCM was described in [35] to calculate thermodynamical, transport and optical properties of plasma of alkali metals. But these calculations are also limited from above by relatively low densities. Consequently, there is no model describing the transport properties in all density range. But it is possible to use one model (for example, some GCM) for the densities below the critical point and another one (of Ziman type) for the higher densities.

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