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**INVESTIGATIONS OF THE ELECTRICAL RESISTIVITY
AND THERMOELECTRICAL POWER OF LIQUID
LESS SIMPLE METALS**

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Abstract

Electronic transport properties namely the electrical resistivity and thermoelectric power of liquid less simple metals, Zn, Cd, Hg, In, Tl, Sn, Pb, Sb, and Bi are calculated by using the widely used Ziman theory. The effective electron-ion and ion-ion interactions are described by the Bretonnet-Silbert model. The liquid state theory, to evaluate the static structure factors, is described by the thermodynamically self-consistent variational modified hypernetted chain (VMHNC) integral equation of liquids. The results of calculations for the electrical resistivity are found to be fairly good when compared to the experimental data, but the agreement improves significantly when the blurring of the Fermi surface due to finite mean free path of electron is accounted for. The values of the calculated thermoelectric power, for most of the systems, are found to be of the same sign and of the same order of magnitude as predicted by the experiment. The results of the thermopower also exhibit that the contribution of the k dependent term of the electron-ion potential is significant for the systems concerned.

1 Introduction

In a previous work [1] we investigated the structural, thermodynamic, and atomic transport properties of liquid less simple metals namely, for Zn, Cd, Hg, In, Tl, Sn, Pb, and Bi near their melting temperatures. In that work the Bretonnet-Silbert (BS) model [2] for interionic interactions were used in conjunction with the variational modified hypernetted chain (VMHNC) integral equation theory of liquids. Results of those calculations were found to be in good agreement with the corresponding experimental data. In particular, the results of atomic transport properties were found to be excellent.

In the present work we intend to investigate the electronic transport properties, namely, the electrical resistivity and the thermoelectric power for the aforementioned liquid less simple metallic systems. It is well known that the electronic transport property, like the thermodynamic ones, is not an average property and the details of the electron-ion pair potential remains in the heart of the theory [3]. So the investigation of electronic transport properties badly needs a potential which exhibits correct behaviour for the concerned metallic systems.

Though the d-bands in the less simple metals are completely filled by electrons, still the effect of the sd-hybridization exists and it is significant [4,5]. Therefore these systems demand a model which can correctly incorporate this effect self-consistently. In this case the BS model is one of the promising candidates. It is quite relevant to say that the BS model has not been applied to study the electronic transport properties before. Here we describe the BS model very briefly just for completeness.

Bretonnet-Silbert have proposed a local model [6] to describe electron-ion and interionic interactions, primarily, for liquid transition metals. This model treats sp and d-bands separately within the well established pseudopotential formalism. The sp-band is described via the empty core; the d-band contribution is derived from the d-band scattering phase shift by using the inverse scattering approach. The resulting model pseudopotential thus reduces to a simple local form which permits one to extend it to other liquid metals for which the effects of sd-hybridization are significant. It may be noted, here, that the norm conserving non local pseudopotentials are, in principle, to be preferred for accurate predictions. But there are evidences that the local pseudopotentials describe physical properties in some cases, even better [4] than the former ones.

One of the essential ingredients for the evaluation of the electrical resistivity [3] (see eq. (1) below) is the static structure factor, $S(q)$, that involves the interionic interaction through the statistical mechanics. In any way, the theoretical values of the electrical resistivity is very sensitive to the accuracy of the structure factor [7,8]. Therefore, the relevant transport theory thus requires, essentially, a correct profile of $S(q)$ for the realistic description. The variational modified hypernetted chain (VMHNC) is one of the most modern integral equation theories of liquids ever known. It is thermodynamically self consistent for both virial and compressibility

routes [9]. Its accuracy for the liquid transition, noble and the less simple metallic calculations has been tested elsewhere [10,11], and found that the order of accuracy is as good as the computer simulations. In this paper we have used the VMHNC theory to calculate the $S(q)$.

One of the widely used theories for the electrical resistivity is the Ziman theory (ZT) [12]. The starting point of this theory rests on the first order time dependent perturbation theory [13]. This theory successfully takes into account all multiphonon processes, Debye-Waller factors, Umklapp processes, couplings to transverse phonons and anharmonic phonon effects without ever going through an intermediate description of the lattice oscillations in terms of phonons. It proves to be successful for simple metals and their liquids [14]. The Ziman theory was further extended to the noble and transition metals [15,16]. The extended theory involves the t-matrix that depends on the relevant phase shift. The phase shift is derived by solving the Schrödinger equation involving the muffin-tin potentials. Consequently it is much more expensive, computationally, than the Ziman's original theory [12]. In a recent work [8] it is reported that when the t-matrix is expanded for multiple scattering the 2nd and the 3rd term increases the resistivity by 7% and 1%, respectively. It is worth noting that the first term of the expansion alone corresponds to the original Ziman formula for resistivity. In addition, the results of calculations obtained from the extended theory shows a limited success [8] when compared with the experimental data. On the other hand, the original theory has a very simple form, and is easy to handle numerically. Since we intend to investigate electronic transport of the liquid less simple metals we assume that the original Ziman theory [12] is adequate for the present calculations.

The theory of the thermoelectric power [17] used in this work (see eq. (2) below) depends explicitly on the value of the screened potential at $2k_f$ (k_F is the Fermi radius), and the slope of the potential in k -space, and also on the value of the resistivity. Therefore, in our view, the fine features of the electron-ion pseudopotential could be examined correctly by calculating the thermoelectric power of the concerning systems. Because the values of the electrical resistivity sometimes become closer to the experimental data and thus indicates that the potential is of high quality and has right behaviour. But when the thermopower is calculated with the same potential it is seen that the results are of opposite sign than as predicted by the experiment [18].

The Ziman theory of any form is based on the long mean free path (MFP) approximation [19]. But in practice, the MFP of the conduction electrons in liquid metals have finite range. This finiteness of the MFP, following the Heisenberg uncertainty principle, results a blurring of Fermi surface instead of a sharp one which is assumed to be in the Ziman theory [19]. Thus the finite MFP, l , and the width of the blurring, Δq say, are related in the following way $l \Delta q \sim 1$ [20]. Hence it is of great interest to examine the effect of Δq on the resistivity if l is roughly known or assumed to have a value that is permitted by other theoretical or experimental work. It is, here, worth mentioning that a truly self-consistent theory incorporating the blurring effect of the Fermi surface is yet to be developed.

The above aspects and prospects of electronic transport properties aroused our motivation

to do this work. However, this work is important for the following reasons. First, here the BS model has been extended for the first time - which, to the best of our knowledge, nobody did before - to investigate the electronic transport properties of liquid less simple metals. Second, this work along with other previous ones would allow us to draw a decisive conclusion about the quality and transferability of the BS model to describe the static, thermodynamic and transport properties of liquid metals, in particular, for the liquid less simple metals. Third, this work would also permit us to have a feeling about the effect of Fermi surface blurring on the electrical resistivity without exploring any complicated theory.

This paper is organized in the following way. Section 2 describes briefly all theories, relevant to the calculation of electrical resistivity and the thermoelectric power. Results and discussions are presented in section 3. The paper is concluded in section 4 with some remarks.

2 Theories

2.1 Electronic transport theory

Starting from Byam's theory [13] for elastic scattering of neutrons one can arrive to the equation of the electrical resistivity of the form (the well-known Ziman formula)

$$\rho = \frac{\Omega_0^2 m^2}{12 \pi^3 \hbar^3 Z^2 e^2} \int_0^{2k_F} S(q) |w(q)|^2 q^3 dq \quad (1)$$

where S , w , Z , e , m and Ω_0 denote the static structure factor, screened electron-ion pair interaction in q space, effective s -electron occupancy number, electron charge, mass and atomic volume, respectively. k_F is the radius of the Fermi sphere.

The thermoelectric power at a particular temperature may be written as

$$Q = - \frac{\pi^2 k^2 T}{3 |e| E_F} \xi \quad (2)$$

where the dimensionless parameter is

$$\xi = - \frac{k_F}{2} \frac{1}{\rho} \frac{\partial \rho}{\partial k} \Big|_{k=k_F} \quad (3)$$

If one defines

$$\Gamma(q) = |w(q)|^2 S(q) \quad (4)$$

then one can write [14]

$$\xi = \xi_1 + \xi_2 + \xi_3 \quad (5)$$

where $\xi_1 = 3$, $\xi_2 = -2q$ and $\xi_3 = -\frac{r}{2}$, with

$$q = \frac{4 k_F^4 C \Gamma(2k_F)}{\rho} \quad (6)$$

$$(7)$$

$$C = \frac{\Omega_0^2 m^2}{12 \pi^3 \hbar^3 Z^2 e^2} \quad (8)$$

(9)

$$r = \frac{k_F C \int_0^{2k_F} dq q^3 \frac{\partial \Gamma}{\partial k}}{\rho} \quad (10)$$

2.2 The effective electron-ion and ion-ion pair potentials

The electron-ion interaction in a metal experiencing the effect of s-d mixing may be written as [6]

$$w_0 = \begin{cases} \sum_{j=1}^2 B_j \exp\left(-\frac{r}{ja}\right) & \text{for } r < R_c \\ -\frac{Ze^2}{r} & \text{for } r > R_c \end{cases} \quad (11)$$

where a , R_c and Z stand for softness parameter, core radius and the effective s -electron occupancy number, respectively. B_1 and B_2 are expressed in terms of a , R_c and Z [2]

$$B_1 = \frac{Ze^2}{R_c} \left(1 - \frac{2a}{R_c}\right) \exp\left(\frac{R_c}{a}\right) \quad (12)$$

$$B_2 = \frac{2Ze^2}{R_c} \left(\frac{a}{R_c} - 1\right) \quad (13)$$

The unscreened form factor reads

$$w_0(q) = 4\pi n a^3 \left[\frac{B_1 J_1}{(1+a^2 q^2)^2} + \frac{8 B_2 J_2}{(1+4a^2 q^2)^2} \right] - \frac{4\pi n Z e^2}{q^2} \cos(q R_c) \quad (14)$$

where n is the atomic number density and

$$J_j = 2 - \exp\left(-\frac{R_c}{ja}\right) \left(\left[\frac{R_c}{ja} (1 + j^2 a^2 q^2) + (1 - j^2 a^2 q^2) \right] \frac{\sin(q R_c)}{jaq} + \left[2 + \frac{R_c}{ja} (1 + j^2 a^2 q^2) \right] \cos(q R_c) \right) \quad (15)$$

The pseudopotential theory finally gives the interionic interaction of the form (in atomic units)

$$v(r) = \frac{Z^2}{r} \left[1 - \frac{2}{\pi} \int F_N(q) \sin(qr) dq \right] \quad (16)$$

where $F_N(q)$ is the normalized energy wavenumber characteristic

$$F_N(q) = \left(\frac{q^2}{4\pi n Z e^2} \right)^2 w_0^2(q) \left[1 - \frac{1}{\varepsilon(q)} \right] [1 - G(q)]^{-1} \quad (17)$$

Here $\varepsilon(q)$ is the dielectric screening function and $G(q)$ is the local field correction developed by Ichimaru and Utsumi [21].

2.3 The VMHNC Theory

The variational modified hypernetted chain (VMHNC) theory, originally proposed by Rosenfeld [9], belongs to a new generation of fairly accurate integral equation theories of liquids. Like

Table-I: Input values used in this work, and calculated coordination numbers are presented. Here, T , n , R_c , a , Z , and N_R denote temperature, atomic number density, core radius, softness parameter, effective s -electron occupancy number, and coordination number, respectively

<i>System</i>	$T(K)$	$n(\text{\AA}^{-1})$	$R_c(\text{a.u.})$	$a(\text{a.u.})$	Z	N_R	
						Theo.	Expt.
Zn	723	0.0637	1.27	0.285	1.8	11.40	10.5
Cd	623	0.0428	1.23	0.253	1.4	11.48	10.3
Hg	523	0.0386	0.92	0.170	1.3	09.88	10.0
In	433	0.0369	1.32	0.278	1.6	11.03	11.6
Tl	588	0.0332	1.13	0.218	1.5	10.49	11.6
Sn	523	0.0353	1.30	0.273	1.7	10.28	10.9
Pb	613	0.0310	1.47	0.307	1.6	11.92	10.9
Sb	933	0.0320	1.06	0.193	1.5	11.18	08.7
Bi	573	0.0289	1.49	0.317	1.7	10.56	08.8

most other integral equation theories the VMHNC solves the Ornstein-Zernike (OZ) equation with a closure relation

$$g(r) = \exp[h(r) - c(r) - \beta v(r) - B(r)] \quad (18)$$

where β is the inverse of temperature times the Boltzmann constant. The bridge function $B(r)$ is approximated by using the analytic solution of the Percus-Yevick equation for HS namely $B(r) = B_{PY}^{HS}(r, \eta)$. The packing fraction η is the variation parameter which is determined by minimizing the VMHNC configurational Helmholtz free energy. Once η is fixed for a specific thermodynamic state, $S(q)$ or pair correlation function $g(r)$ can be evaluated.

3 Results and Discussions

The pseudopotential model used in this work has three parameters; a , R_c and Z . These are chosen in the following way. Since this work is an extension of our previous work on atomic transport [1], we take the values of a and R_c from that paper where the procedure of choosing is discussed.

Values of the electronic transport properties are very sensitive to the profile of the potential involved [18] and to the static structure factor [7,18] because the value of $2k_F$ generally lies at the principal peak (or near it) of $S(q)$ which in turn depends on potential. In addition, the square of the screened form factor of the electron-ion pseudopotential is also involved directly. Therefore, to fit the theoretical $S(q)$, specifically the position and height of the first peak, to the experimental one as close as possible we have adjusted the value of Z for each individual system. Here, we follow the concept that the effect of hybridization between s and d electrons can be approximately accounted for by changing the relative occupancy of the s and d -bands [22]. This is supported by the self consistent calculations by Moriarty [23] and is also in conformity with the effective charge transfer noted in the augmented spherical waves (ASW) calculations [24].

Here we may also mention that, in principle, there is no restriction as such to use different but suitable values of Z for different systems provided self-consistent calculations of charge transfer support these values. The values of R_c , a and Z are listed in Table-I. It is relevant to note here that in the previous paper [1] we used a constant value of $Z(=1.3)$ for all systems.

The effect of alteration of Z on the effective ion-ion pair potential and as a consequence on the $S(q)$ are shown in figures 1 and 2, respectively.

Having chosen the model parameters the liquid structures for Zn, Cd, Hg, In, Tl, Sn, Pb, Sb, and Bi are calculated by using the VMHNC theory of liquids. Values of the input temperatures and densities are taken from [25]. We have used the Gillan algorithm [26] for a numerical solution of the OZ equation in conjunction with the closure relation (18). In all cases we have found that a 1024 points grid with step size $\Delta r = 0.06\text{\AA}$ is sufficient for the present calculations. We note here that as far as the static structure factors, $S(q)$, are concerned, the difference between the present and the previous work [1] is not found to be significant although the values of Z are different in the two works. So we have not presented the calculated $S(q)$ in this paper.

The average number of atoms near a specific ion is related to the pair correlation function $g(r)$, the Fourier transform of $S(q)$, by the equation

$$N_R = \int 4\pi r^2 n g(r) dr. \quad (19)$$

To verify the accuracy of calculated $S(q)$ we have evaluated the coordination number N_R which is listed in Table-I. It is seen that the coordination number of the concerned metallic systems varies from 9.88 to 11.92. The experimental values lie in the range 8.8 to 11.6 [25]. Other experiments [27] also suggest that the coordination number of liquid metals varies between 10 and 12, this is exactly what our theoretical values predict. The agreement with the experimental data, we would say, has been found to be excellent. This result thus qualifies that the accuracy of the calculated structure factors is undoubtedly good. In (19) the upper limit of integration has been chosen at the first minimum of $g(r)$.

We now turn to the results of the calculations of the electrical resistivity of liquid Zn, Cd, Hg, In, Tl, Sn, Pb, Sb, and Bi near their melting temperatures. Here the original Ziman theory has been employed. The results of the calculations are illustrated in Table-II. The smallest value of resistivity has been found to be 11.23 in Zn and the largest value 43.2 in Bi. The largest discrepancy between the theory and experiment [28] has been found for Bi ($\Delta\rho = 87$) and the smallest for In ($\Delta\rho = 8.1$). But if we compare our results with other calculated values we find that our results are as good as some of others (see Table-II).

It is well known that the Ziman formula for the electrical resistivity is, by construction, useful for the long mean free path situations [19], in this case the Fermi surface from which scattering happens is assumed to be sharp. In practice, the electronic mean free path (MFP) is finite for the metallic systems and could be even smaller than the interatomic distance for metallic fullerenes [29]. The range of MFP for metallic systems could be, roughly speaking, from a few Angstrom

Table-II : Results of electrical resistivity. Electrical resistivity ρ . In the 2nd column values within the parenthesis are theoretical results, taken from different works. Superscripts a, b, c, d and e correspond to [31], [32], [33], [34] and [35], respectively.

System	$\rho (\mu \Omega cm)$		Expt.
	$\Delta q=0$	$\Delta q=0.2 \text{ \AA}^{-1}$	
Zn	11.23(16 ^a)	20.06	37.4
Cd	16.54(17 ^{b,e})	37.13	33.7
Hg	26.34 (30 ^d)	61.96	91.0
In	24.99(24 ^d)	51.94	33.1
Tl	41.16(37 ^e)	97.18	73.1
Sn	28.48	55.35	48.0
Pb	42.70(51 ^b)	108.40	95.0
Sb	33.50	97.58	113.5
Bi	43.20	100.9	130.2

Table-III : Results of thermoelectric power. The dimensionless parameter ξ of thermopower.

System	ξ_1	ξ_2	ξ_3	ξ	
				<i>Theo.</i>	<i>Expt.</i>
Zn	3	-2.942	-0.348	-0.29	-0.1
Cd	3	-3.038	-0.618	-0.66	-0.2
Hg	3	-0.240	1.286	4.05	4.5
In	3	-2.248	0.097	0.85	0.9
Tl	3	-3.286	-0.300	-0.59	0.5
Sn	3	-2.416	-0.098	0.68	0.6
Pb	3	-5.320	-1.624	-3.90	2.1
Sb	3	-5.379	-1.800	-4.18	-0.3
Bi	3	-3.073	-0.350	-0.42	0.9

to more or less a hundred Angstrom [30]. This finiteness of the MFP corresponds to a blurring of the Fermi surface due to the Heisenberg uncertainty principle. The uncertainty, Δq , of blurring may be approximated by the relation $l \Delta q \approx 1$ [20]. In [30] the MFP for different liquid metals is reported, the minimum value of which is $\approx 4 \text{ \AA}$. However, if the value of l is taken, without any rigorous justification, to be $\sim 5 \text{ \AA}$, then Δq appears to be equal to 0.2 \AA^{-1} . We add this value with the $2 k_F$ for all the concerning systems, to obtain an effective diameter of the blurred Fermi surface. With this effective value of $(2 k_F)^{Eff}$ we have again calculated the resistivity. These results are presented in Table-II. We found an excellent improvement in the results when comparing with the experimental data [25]. In this case the discrepancy between theory and experiment is found to be minimum for Hg ($\Delta\rho = 30$) and minimum for Cd ($\Delta\rho = 4.06$).

Results of calculations for thermoelectric power for the concerning systems are presented in Table-III. Here we have demonstrated only the dimensionless parameter ξ because the total thermoelectric power is just a multiplication of it by one third of the free electron contribution of

thermopower. From Table-III it appears that for all systems except for Tl, Pb and Bi, ξ exhibits an appropriate sign as predicted by the experiments [25,28] and has magnitudes which are also comparable. For Tl, Pb and Bi the sign is found to be the opposite to that of experimental data. Since ξ depends on the electron-ion pseudopotential form factor at the level of $2k_F$ and its derivatives with respect to k , we can conclude that electron-ion potentials used for Zn, Cd, Hg, In, Sn, and Sb have correct fine features. For Tl, Pb and Bi the potentials should be improved; this may be achieved by more careful parameterization.

From (3) it is seen that the dimensionless parameter in the formula of the thermopower consists of three essential terms. The first one is due to the free electron contribution, the second term explicitly depends on the screened electron-ion potential at $2k_F$, and the third term is due to k or energy dependence of the potential. The breakdown details of ξ are also illustrated in Table-III. The smallest value of ξ_2 has been found to be -0.24 in Hg, and the largest one to be -5.379 in Sb. The magnitudes of ξ_2 are found to be larger than ξ_1 for liquid Cd, Tl, Pb, Sb and Bi. For the rest of the systems values of ξ_2 are smaller than ξ_1 . Values of ξ_2 are larger in magnitude than those of ξ_1 except for Hg. It is also noticed that the values of ξ_1 and ξ_2 are almost of same magnitudes for Zn, Cd, Tl and Bi. Since their signs are opposite they roughly cancel each other and the decisive contribution to ξ comes from ξ_3 . When the values of ξ_3 are compared with total ξ it is clearly observed that the former values are significant for all systems except for In and Sn. So the 3rd term of ξ cannot be neglected, in general, in the case of liquid less simple metals. It is relevant to mention here that some authors, in their works, have considered the 3rd term as insignificant and have neglected its contribution to the thermopower [18,28]. From Table-III it is noticed that the sign of ξ_3 is negative for all systems except for Hg and In. This finally implies that the slope of $\Gamma(q)$ ($= S(q) | w(q) |^2$) w.r.t. k is positive for all systems except for the latter two elements. During the progress of the calculations we observed that the position $q = 2k_F$ lies just on the right side of the principal peak of $S(q)$ for all systems except for Hg, for which it is right on the peak. Therefore, the slope of $S(q)$ as a function of k would be similar for all systems because of the similar shapes of $S(q)$. So we believe that the different sign of ξ_3 for different metallic systems is solely related to the slope of the potential($w(q)$) profiles.

4 Conclusions

In this work we have investigated the electronic transport properties of liquid less simple metals namely for Zn, Cd, Hg, In, Tl, Sn, Pb, Sb, and Bi. The essential ingredients for the calculations are the Bretonnet-Silbert model potentials, the VMHNC theory of liquids and the Ziman original theory for the electrical resistivity. The results of calculations for electrical resistivity have been found to be in good agreement with corresponding theoretical as well as experimental data. The results of calculations for the thermoelectric power are found to be in very good agreement

for all systems except for liquid Tl, Pb and Bi. In the intermediate step of calculations we have also calculated the coordination numbers for each system, results of which suggest that the accuracy of the static structure factors obtained from the VMHNC theory is adequate for the present calculations. However, the complete analysis of the calculated results of the present and previous ones [1] permits us to draw the following concluding remarks:

(i) The Bretonnet-Silbert model pseudopotential could be a good starting point for the study of structural, thermodynamic, atomic and electronic transport properties of liquid less simple metals.

(ii) Values of the calculated electrical resistivity improves dramatically when the effect of blurring of the Fermi surface due to the finite MFP is accounted for by adding the amount of uncertainty of blurring to the Fermi diameter. These results are supported by the work of March and coworkers [19,20,27].

(iii) Finite MFP of the conduction electrons leads to the relation $l \sim \frac{1}{\Delta q}$ which in turn would allow one to estimate, at least qualitatively, the value of MFP for metallic systems by fitting the experimental values of the electrical resistivity or if Δq can be measured experimentally.

(iv) The contribution of the k dependent term (i.e. $r/2$ of (5)) to the thermoelectric power is significant and cannot be neglected in the case of liquid less simple metals. The fine behaviour of any electron-ion pseudopotential, in our view, may be examined by evaluating the thermoelectric power of liquid metals.

Finally we would like to note that use of the BS model in calculating the various properties of liquid binary alloys is in progress. Preliminary results are found to be very encouraging. Some of these results (viz. on structure) are on the way of publication. The rest on the thermodynamic and transport properties will be reported in due course.

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